# Applied Science Project Logbook

Designing High-Performance PEMFC Electrodes by Optimizing Catalyst Ink Composition



# Antara Krishnamurthy

# **CALENDARS**

This section contains monthly timetables that will help me keep track of my progress. It lists all the tasks to be completed, and the tasks are specific and not open-ended.

AUGUST									
Sunday	Monday	Tuesday	Wednesday	Thursday	Friday	Saturday			
				1	2	3			
4	5	6	7	8	9	10			
11	12	13	14	15	16	17			
18	19	20	21	22	23	24			
25	26	27	28 - <del>No class</del>	29	30 - <del>Intro class</del>	31			

# **SEPTEMBER**

Sunday	Monday	Tuesday	Wednesday	Thursday	Friday	Saturday
1	2	3	4 - <del>Intro class</del>	5	6 - <del>Email mentor</del> - <del>Finish creating</del> <del>logbook calendar</del> - <del>Update notes</del> <del>for the first two</del> <del>classes</del>	7
8 - <del>Go over my calendar and add</del> <del>conflicting</del> <del>events</del>	9	10 - <u>Meeting Dr.</u> <del>Garcia in class</del> - <del>Prep for</del> <del>meeting with Dr.</del> <del>Karan</del> - <del>update logbook</del> - find papers	11 - <del>Meeting Dr.</del> <del>Karan @ 12:50 via Zoom</del>	12 - <del>Update daily</del> <del>notes</del> - <del>Create email</del> <del>communication</del> <del>section</del>	13	14
15	16 - <del>Meeting Dr.</del> <del>Karan @ 4:00 via</del> <del>Zoom</del> - <del>Get acquainted</del> with paperpile	17	18 - <del>Worked on</del> <del>other homework</del>	19	20 - Meeting with Dr. Garcia - Update logbook - Email Dr. Karan meeting reminder	21
22 - <del>Read + annotate</del> <del>Bridging the</del> <del>gap</del>	23 - <del>Meeting Dr.</del> <del>Karan @ 4:00 via</del> <del>Zoom</del>	24 - <del>Update logbook</del> <del>with meeting</del> <del>notes</del> - <del>Read + annotate</del> <del>papers given</del>	25	26 - <del>Read +</del> <del>annotate papers</del> <del>structure,</del> <del>property</del>	27 - <del>Email Dr. Karan</del> <del>meeting</del> <del>reminder</del>	28

29	30			
- <del>Read + annotate</del>	- <del>Create an intro</del>			
<del>papers</del>	outline			
	- Write 3 possible			
	<del>research</del>			
	<del>questions</del>			
	- <del>Meeting Dr.</del>			
	<del>Karan @ 4:00 via</del>			
	<del>Zoom (moved)</del>			

	OCTOBER									
Sunday	Monday	Tuesday	Wednesday	Thursday	Friday	Saturday				
		1 - <del>Email meeting</del> <del>summary (moved)</del>	2 - <del>Biweekly</del> <del>meeting w Dr.</del> Garcin - <del>Finalized RP</del> outline	3 - <del>Meeting Dr. Karan @ 4:00 via Zoom</del>	4 - <del>Read + annotate papers - catalyst ink papers - Email meeting summary</del>	5				
6 - <del>RP intro:</del> <del>background info</del> <del>global shift</del>	7 - <del>Meeting Dr. Karan @ 4:00 via Zoom</del>	8 - Email meeting summary -rewrite background info global shift -RP intro: background info PEMFC	9	10 <del>RP intro - role of CL: function +</del> importance	11	12				
13	14 - Canadian Thanksgiving (no school)	15 - <del>Biweekly meeting w Dr. Carcia</del> <del>RP intro-role of CL: challenges - SH science fair form - Register for the CYSF portal</del>	16 - <del>email meeting</del> <del>reminder</del> - edit RP (edits from dad)	17 <u>Science fair</u> <u>meeting at lunch</u> <u>RP objectives</u> <u>RP intro rationale</u> <u>for the study</u> <u>Meeting with Dr.</u> <u>Karan</u>	18	19 - <del>RP question</del> - <del>RP variables</del> - Edits to the intro from Dr. Garcia - Email meeting summary to Dr. Karan				
20 - RP significance - RP hypothesis	21 -Go over oral presentations -Go through sample oral presentations -Ask about lab permissions -Meeting Dr. Karan @ 4:00 via Zoom	22	23 - Email meeting summary -Read + make edits to the research proposal -Add more about the catalyst ink to intro -Go over ethics	24	25 - <del>Biweekly meeting</del> <del>w Dr. Garcia - RP confounding variable - Go over RP format/Jayout</del>	26				

27	28 I won't be at school	29 I won't be at school	30	31 - <del>RP due (actual)</del> <del>- Meeting Dr. Karan</del>	

# NOVEMBER

Sunday	Monday	Tuesday	Wednesday	Thursday	Friday	Saturday
					1	2
3	4 - <del>RP due</del> <del>(extension)</del> - <u>Meeting with</u> mentor - <u>Make edits to</u> project proposal paper	5	6 - <del>Watch oral</del> <del>presentations</del> <del>- CYSF basic info</del>	7 I won't be at school	8 <del>I won't be at</del> <del>school</del> - Oral presentation slideshow	9
10	11 No school - Remembrance Day (reschedule meeting) - <del>Practice oral</del> <del>presentation</del> <del>speech</del>	12	13 - <del>Oral</del> <del>presentation</del> - Watch oral <del>presentations</del> - meeting with mentor	14	15 - <del>Read papers on the effect of catalyst ink properties</del>	16
17	18 - <del>Meeting with</del> <del>mentor</del>	19 - email meeting summary to mentor - Oral Presentations - CYSF Ethics	20	21 - <del>CYSF portal</del> <del>(variables,</del> <del>hypothesis, and</del> <del>procedure)</del>	22	23

24	25	26	27	28	29	30
	-Meeting with mentor -Biweekly meeting with Dr. Garcia - Make edits to project proposal + oral proposal	- <del>email meeting</del> <del>summary to mentor</del>	- <del>work on the</del> <del>CVSF portal</del> <del>(edits to</del> <del>variables +</del> <del>procedurc, do</del> <del>research section)</del>		- try Paperpile again - email meeting reminder to mentor - work on the CYSF portal - December calendar	

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Sunday	Monday	Tuesday	Wednesday	Thursday	Friday	Saturday
1	2 - <del>Meeting with</del> <del>mentor</del>	3 NO CLASS - PRESIDENT'S BREAKFAST	4 - <del>Email meeting</del> <del>summary to</del> <del>mentor</del>	5 - <del>Biweekly</del> <del>meeting with Dr. Garcia - Reformat documents → <del>Research</del> <del>proposal for the</del> <del>CYSF portal</del></del>	6 - <del>Email meeting</del> <del>reminder to</del> <del>mentor</del>	7
8	9 I will not be at school - <del>Meeting with mentor</del>	10 - <del>Email meeting summary to</del> <del>mentor</del>	11 - og plan: Read <del>papers that Dr.</del> Karan will send -Collect and analyze data -actual: email mentor -areas of improvement of intro	12	13 - <del>Email meeting</del> <del>reminder to</del> <del>mentor</del>	14
15	16 - <del>Meeting with</del> <del>mentor</del>	17 - <del>Email meeting</del> summary to mentor <del>Biweekly</del> meeting with Dr. Garcia - <del>Review</del> background research summary notes	18	19 - <del>Collect and</del> <del>analyze data →</del> <del>Did not end up</del> <del>doing this</del>	20 - <del>Meeting with Vahid at the lab at UofC @ 4:30</del>	21 - Winter <del>break</del> <del>starts at UofC</del> <del>and Webber</del>
22 - Winter break	23 - Winter break	24 - Winter break	25 - Winter break	26 - Winter break	27 - Winter break	28 - Winter break

29 - Winter break	30 - Winter break	31 - Winter break		

		JAN	JUA	RY	-	
Sunday	Monday	Tuesday	Wednesday	Thursday	Friday	Saturday
			1	2 - Winter <del>break</del> <del>ends at UofC</del>	3	4
5	6 - Winter break ends at Webber MIDTERM STUDYING	7	8 MIDTERM STUDYING	9	10 Exam break starts	11 Exam break
12 Exam break	13 Exam break	14 Exam break	15 Exam break	16 Exam break	17 Exam break	18 Exam break
19 Exam break	20 Exam break ends - <del>Meeting with</del> <del>mentor</del>	21	22 <del>Full class</del> <del>meeting</del> <del>Update logbook</del> <del>Send Dr. Karan</del> <del>a meeting</del> <del>summary</del>	23 - s <del>cience fair</del> <del>meeting</del>	24 - <del>biweekly</del> <del>meeting w Dr. Garcia - Update logbook</del>	25
26 <del>– Update logbook</del>	27 - <del>Meeting with</del> <del>mentor</del>	28 - Introduction section of the final paper - logbook calendar Feb	29	30 - Work on introduction section of the final paper - Introduction Section Paper Due (extension next Friday)	31 - Send meeting reminder to mentor - Logbook due December + January	

	FEBRUARY									
Sunday	Monday	Tuesday	Wednesday	Thursday	Friday	Saturday				
						1				
2	3 - Meeting with mentor - Data analysis → take a look at slides sent + ask for raw data points	4 - <del>Send meeting</del> <del>summary to</del> <del>mentor</del>	5 - Biweekly meeting with Dr. Garcia - Data analysis → plot the data I have in a graph on Excel - Email asking for the unaveraged data - Review background research for sci-fair Turnitin - email to set up a time to go over methods in greater detail	6	7 Send meeting reminder to mentor - Background research due on sei-fair Turnitin - Data analysis → understand the patterns in the trends Introduction section due (extended) - Procedures section of the final paper → hypothesis and variables	8				
9	10 - Meeting with mentor - Data analysis → understand the meaning of the data	11 We had an assembly for most of this class Data analysis → analyze what the data means - Begin the procedures section of the final paper → write about the ways that the	12	13 <u>Procedures</u> section of the final paper → Ink preparation, DLS - Watch the video on DLS	14	15 - <del>Procedures</del> section of the final paper → electrical conductivity, BJH average pore width				

		data is collected → wasn't finished because of assembly - <del>U of C @ 4:30 to</del> <del>meet with Vahid</del>				
16 - <del>Procedures</del> section of the final paper → how all the data is graphed	17 - <u>Meeting with</u> mentor (meeting canceled due to family day long weekend)	18	19 - Final edits to procedure - Procedures Section of final paper due (DDDL) - Biweekly meeting with Dr. Garcia - Make the oral presentation for science fair prep -Methods due on sci fair Turnitin - Finish graphing the properties against each other	20 - Make the oral presentation for science fair prep -Finish understanding/a nalysis on data	21 - Final touches on the oral presentation for science fair prep - prepare the oral presentation for science fair prep presentation → practice flow, timing, recitation	22
23	24 - meeting with mentor (canceled) - practice oral presentation and time it	25 - Oral presentations begin (I am presenting here) - Turn in slides from OP (DDDL)	26	27 BE DONE WITH DATA COLLECTION/AN ALYSIS $\rightarrow$ HARD DEADLINE (should be done before for OP) -Oral presentation (watching) -Logbook (DDDL)	28 - Marks close for report cards	

		M	ARC	CH		
Sunday	Monday	Tuesday	Wednesday	Thursday	Friday	Saturday
						1 - Background research, RQ, hypothesis, variables for poster
2	3 - data collection/results + analysis/conclusions due on sei fair Turnitin - meeting with mentor - results, analysis, and conclusion part of the poster	4	5 -Figure out how to add error bars to graphs -Make methods flow diagram for poster -limitations, future direction, acknowledgeme nts, references -Methods for paper -Figure out scaling of poster	6 <del>-meet Dr. Garcia</del> <del>during spare</del>	7 Term 2 report card - redo methods section change poster layout to be trifold ask Dr. Garcia to take another look at the poster	8 - <del>SEND</del> <del>POSTER TO</del> <del>BE PRINTED</del>
9 <del>- PICK UP</del> <del>POSTER</del>	10 - <del>practice poster</del> <del>after school with Dr.</del> <del>Garcia</del>	11 - <del>In-School</del> <del>Science Fair (All Day)</del>	12	13 - hypothesis edits - research edits - Variables edits - procedures edits - add data (graphs) and analysis to the CYSF portal	14	15
16	17 - <del>fill in conclusions</del> <del>for CYSГ portal</del> <del>-fill in the</del> observations section	18	19 - <del>science fair</del> <del>reflections</del> <del>- header image</del> <del>- project image</del> <del>- order a new</del>	20 - download parts of the logbook and combine into one PDF	21 - If you're going to go to the city science fair, the portal is due here	22 SPRING BREAK

	of CYSF portal with photos from the lab and brief descriptions - Biweekly meeting with Dr. Garcia - applications, sources of error,		<del>poster (foam</del> <del>board)</del> - <del>fill in citations,</del> <del>acknowledgment</del> <del>s</del>		- I won't be at school (SPRING BREAK)	
23 SPRING BREAK	24 SPRING BREAK - start writing the results paper $\rightarrow$ wt vs. particle size, wt vs. avg pore width, wt. Vs. conductivity	25 SPRING BREAK - results paper → particle size vs pore width	26 SPRING BREAK	27 SPRING BREAK results paper → particle size vs conductivity	28 SPRING BREAK	29 SPRING BREAK
30 SPRING BREAK	31 SPRING BREAK - results paper → conductivity vs pore width					

APRIL							
Sunday	Monday	Tuesday	Wednesday	Thursday	Friday	Saturday	
		1	2	3	4	5	
6	7	8	9	10 - Biweekly meeting with Dr. Garcia - City science fair	11 - City science fair	12 - City science fair	
13	14 - Results section due	15	16	17	18	19	
20	21	22	23 - Biweekly meeting with Dr. Garcia	24	25	26	
27	28	29	30				

Μ	Δ	$\mathbf{V}$
TAT'		

Sunday	Monday	Tuesday	Wednesday	Thursday	Friday	Saturday
				1 - Discussions and Conclusions section due	2	3
4	5 - Biweekly meeting with Dr. Garcia	6	7	8	9	10
11	12	13	14	15 - Biweekly meeting with Dr. Garcia	16	17
18	19	20	21	22	23	24
25	26	27	28 - Biweekly meeting with Dr. Garcia	29	30 - Final paper due	31

# **DAILY NOTES**

This section contains the details of my daily work, drawings of models I am working on, notes of my meetings with my mentor, notes of topics discussed in the classroom with my instructor, questions I have about procedures learned, and information about what I am reading.

# **August Daily Notes**

# August 30th - Class Time

This was my first ASP class, and we spent the class going over the expectations for the course.

#### **Communication:**

#### With Mentor:

- Check emails 2-3 times per day
- Ask the mentor about the best times to email them
- Ask the mentor about the best communication platforms
- Schedule some meeting times and meeting locations at the initial meeting
- Try and meet at least once a week based on the **mentor's schedule**
- During a meeting with a mentor, go over the work to be done between meetings.

### With Dr. Garcia:

- Keep constant communication either through emails or in-person meetings.
- Email meeting summaries after meetings with mentors to keep her up-to-date as to how your project is going.

#### Email meeting summary to mentor:

- Thank you for taking the time to meet with me.
- Discussed
  - X
  - Y
  - Z
- Tasks with deadlines
  - X
  - Y
  - Z

- Next meeting with date, time, and location
- Ask, "Did I miss anything?"
- Do this after every meeting
- Add a copy of the email to the logbook

#### Preparedness:

- Keep on track of your work
- Mark goals

#### Time management:

- Use a calendar
- Write down tasks/assignments
- Keep track of due dates
- Do what works best for you

Week				-meet mentor (50 min)
ASP				- read intro (20 min)
	ASP			-10glocok entry (10 min) - ernail mentor (10 min)
			ASP	

#### Logbook Content:

- Daily Notes with dates
  - what you did
- Background research/literature
  - Notes on literature
  - Copy of annotated literature
- Methods
- Results/data collection
- Analysis/conclusions

# **September Daily Notes**

# September 03 - Spare

I emailed Dr. Karan asking about setting up a meeting to discuss my project. See <u>Email</u> <u>Communication September 03.</u>

# September 04 - Class Time

During this class, we reviewed more expectations about how the class works.

#### Finding and annotating literature:

- The best place to find literature is Google Scholar
  - Google Scholar is reliable because the literature is cited and accurate.
- Use literature review papers, not literature research papers
  - Literature review papers summarize lots of research done on the topic rather than focusing on new research being done.
  - Include new research if proven and relevant
- Use Paperpile to annotate and store literature
  - Licenses coming soon

### Citation Styles:

- MLA (Modern Language Association)
  - Mainly used in fields such as literature, languages, and philosophy
- APA (American Psychological Association(
  - Mainly used for technical and scientific works
- Chicago
  - Most commonly used when citing sources in history and occasionally social sciences and humanities.
- IEEE
  - Primarily used for electronics, engineering, telecommunications, computer science, and information technology reports.
- IEEE is probably the most beneficial for my project as it is specifically engineering-based.

#### Research proposal:

- The rough deadline for the research proposal will be in mid-October
- The rough date for presentations will be the end of October.

#### First mentor meeting:

- Discuss project ideas
  - Narrow down projects to your research question
- Meeting times
  - Either create a set schedule or decide how meeting times will be decided
  - Provide schedule and availability
- Discuss research proposal
  - Tell the mentor it is the first assignment and go over the guidelines
  - Set up another meeting to talk more about the research proposal

# September 06 - Class Time

☑ Email mentor

- Write an email to the mentor to follow up on the previous email. Mention the research proposal and give possible meeting dates. <u>See Email Communication</u> <u>September 06.</u>
- ☑ Finish creating my logbook calendar
- I marked down when I have ASP classes by highlighting the cells in a specific color, taking into consideration holidays and school breaks.
- ☑ Update notes for the first two classes
- See Daily Notes for <u>August 30th</u> and <u>September 04th</u>

# September 06 - After Class

I got a response back from my mentor about setting up a meeting. <u>See Email</u> <u>Communication September 06.</u>

I wrote back to him confirming a date and time and sending him an invite to a Zoom meeting for September 11th. <u>See Email Communication September 06.</u>

# September 08 - Weekend

I spend a little time going over dates in the next few months when I know I will not be in class.

Dates:

- October 29th I will be in Austin for a prior commitment
- November 08th I will be in Austin for a prior commitment
- December 09th I will not be at school due to a prior commitment -

I also got an email from my mentor with a calendar invite for our meeting on September 11th at 12:50 p.m. See Email Communication September 08.

# September 10 - During Class

Meeting with Dr. Garcia (notes below)

I had my first biweekly meeting with Dr. Garcia (my teacher at school) to go over what I have achieved thus far and things to go over in my upcoming meeting with my mentor (Dr. Kunal Karan).

#### Previous meetings recap:

I have met twice with my mentor thus far. My first meeting with him was on June 04th via Zoom. During this meeting, he told me a lot about fuel cells and their complexity. We talked briefly about this class and the work I will be doing. Before the meeting concluded, we scheduled a meeting in person at the University of Calgary on June 26th. During my second meeting with Dr. Karan at the University of Calgary, he took me to the lab space where he works and showed me all the ongoing projects and equipment in the lab. We did not discuss project ideas during this meeting.

#### Upcoming meeting:

My next meeting with Dr. Karan is tomorrow at 12:50. During this meeting, I need to discuss the following.

- Possible project ideas
- Possible research questions
- My short-term goals for the class and project
- Literature reading I can do to get started

#### **Guidelines for Research Proposal**

Your research proposal should have following elements:

- 1. Working Title (2 marks): The title should be concise, informative descriptive. Can be changed upon completion of the research to reflect more closely the main purpose of the study.
- 2. Abstract (Optional): Summary of the main research question, the rationale for the study, the hypothesis and the methods
- 3. Introduction (30 marks): The introduction will provide the background information. It serves to establish the framework for the research. It will lead to reasons why this study is necessary and its relevance.
- Objectives (10 marks): Short and long terms goals for the investigation have to be stated clearly in the research proposal.
- 5. Variables (20 marks): The proposal has to establish the key variables of the Variables (20 marks): the proposal has to extend to the study a. Independent variable: manipulated or treated in the study b. Dependent variable: responding variable (effect, result, outcome) c. Controlled variable: kept constant during the study d. Confounding variable: May influence the effect of independent variables.
- 6. Questions or Hypothesis (20 marks): If the background information allows Questions of reproducts (commonly, in the background match and/or and/or the researcher to make a prediction, then a hypothesis can be formulated. If that is not possible, a research question (or questions) can be presented. In both cases the variables tested in the study have to be highlighted.
- 7. Methodology (10 marks): Provides an overview of the methods that will be used to test the hypothesis or answer the research questions. The methods do not have to be described in detail. Describes the research design and strategies regarding all aspects of the investigation including: sample size, participants' selection, ethical considerations, instrumentation, data and the selection. collection, and data analysis.
- 8. Significance (5 marks): A brief statement of how this research will impact the field of study and the larger implications of the investigation

- Bring up the research proposal
  - Share guidelines for the proposal with him (see image to the side)
- Set up a rough timeline for the project
- Ask the following questions
  - Is my mentor going to be you or a student?
  - Who will be my direct supervisor/person of contact?
  - What times work best for meetings?
  - Are you available to have weekly meetings?
  - When will our next meeting be (date + time)?
- Never leave a meeting without knowing when your next meeting is. This will reduce the time between meetings, as you will have a clear timeline and won't have to wait for emails.

If time allows, cover the following; otherwise, leave this for the next meeting:

- Outline the project proposal
  - Subheadings
    - Information to cover in subheadings
- Start broad at the beginning of the proposal and narrow it down as you continue
- Talk about how the field works, not just your specific project.



#### Before meeting tomorrow:

- Find 1-2 articles that are reviews on fuel cells
  - <u>https://www.mdpi.com/2077-0375/10/5/99</u>
  - https://www.nature.com/articles/s41467-022-33892-8
- I have added these articles to Paperpile to be annotated soon.

# September 11 - Meeting with my mentor:

Today was my first meeting with my mentor, Dr. Karan, since the start of the school year.

We talked a little about my project and our plan for the future. I have included the main points of our meeting below.

- Due to the length of time fuel cell experiments take, I will be working on a data analysis project using the data collected by a grad student working on the project.
- I shared the research proposal guidelines with my mentor, and he has a project in mind that I could work on. The project already has some results collected and is still generating more results.
- For now, I will be directly supervised by Dr. Karan, but down the line, I could be mentored by the graduate student working on the same project.
- Dr. Karan and I will be meeting every Monday at 4:00 p.m. to discuss my project,
- Following our meeting, I will get my first set of literature to read on Monday.

After the meeting was over, I emailed a summary of the meeting to both Dr. Garcia and Dr. Karan. <u>See Email Communication September 11.</u>

# September 12 - Class Time:

- ☑ Update my logbook with details of my meeting with my mentor yesterday.
  - See <u>Daily Notes for September 11.</u>
- Create a section in my logbook with email communication.
  - ☑ Input all emails between my mentor and me.
    - See the Email Communication section between <u>April 21</u> and <u>September 11</u>.

# September 16 - Class Time:

During this class, we spent a lot of time going over our research proposal and other aspects of the class.

## Science Fair:

- Due to COVID-19, the science fair used to use an online platform that may still be used this year.
- Each person will have to make a poster board for the in-person science fair presentation.
- I joined the Science Fair Google Classroom so I can stay up-to-date on all science fair-related information.

## Paperpile:

- If your mentor sends you a PDF of a paper, find the website it came from and add it to Paperpile.
- You do not have to annotate everything on Paperpile.
  - If you want to print out the PDF and annotate by hand or use an iPad to annotate, then upload images of annotated literature to the logbook.
- If using Paperpile for annotations, then generate a link through Paperpile to the annotated PDF and paste it into the logbook.
- When doing citations, make sure to include a link to the source.
  - Choose the citation style that makes the most sense for your project.
  - <u>Purdue Owl</u> is an excellent source to use to find more information about citations.
- Use <u>IEEE.org</u> to find engineering papers

#### **Research Proposal:**

#### Decide on what kind of project you will be doing:

- Study does not need a variable or hypothesis because it is not your original setup
- Experimental has to have both variables and a hypothesis
- Innovation does not need to have a variable or hypothesis

### Every proposal needs the following:

- Research question(s)
  - It should be as narrow as possible
- Goals
  - Have both long and short-term goals
- Short-term goals
  - It may look more like tasks (things that have to be accomplished)
  - Be ambitious when setting goals (it is okay not to accomplish all of them)
- Long-term goals
  - Things you want to accomplish after finishing short-term goals
  - They can be broader than short-term goals but do not make them too broad
- Introduction section

- Also known as the literature review/background research section
- About 70-80% of the term should be used to study literature
- Since I am probably doing a study-based project, I can dedicate a couple of months to doing literature and background research
- The section should be written with the goal of leading to the research question in mind (write it general to specific about the field that leads to the research question)
- This section should lead the reader to believe that the research question is essential to study
- There is no page limit for the research proposal, but the more you write, the more opportunity you have to make mistakes
- Create an outline of what you want to write in your intro **after** coming up with the research question
  - Think about everything that needs to be talked about to lead you to the research question
  - Add dates to the calendar with dates that you want things done on
    - Mark the day that you want to show Dr. Garcia and your mentor the rough draft of your proposal
    - Then, divide the rest of the work between classes

### After the introduction is figured out

- Start discussing methodology with your mentor
  - Include database, datasets, and setups (how the experiment runner set up their experiment)
  - Talk about what you are looking at and how you are going to look at it
  - Talk about the statistics needed (if needed)
  - You must know the methods in detail by the science fair in April, but for now, just know the methods well enough to connect to the research question.
    - This is how the question is answered.
- Keep Dr. Garcia updated on the research proposal progress and share what you have written for feedback

#### Asking questions to mentor:

- Ask specific questions
- Have work to show them so you can point out exactly what you don't understand

- Don't ask them to re-explain everything they have explained to you
  - Go with specific areas you need further explanation for

### Artificial Intelligence and Plagiarism:

- **Do not** use AI on any papers in this class
- Ask Dr. Garcia if you need help with editing papers
- AI does not help make things specific
  - It makes things very generic and lacks a voice
- AI does not correctly summarize information. It usually leaves information out
- To find the right way to phrase things, ask Dr. Garcia
- Everything will be submitted to Turnitin
- Turnitin will flag copying yourself, but it will be ignored because the sections of the final paper will be submitted in parts prior.
- Do not use AI just to get a good mark.
  - This class is to gain experience with doing research and to help prepare you for university. Using AI does not help with this.

# September 16 - Meeting with mentor:

During our meeting, my mentor walked me through some papers with higher-level content. He will forward the papers to me with specific sections to read. Since I do not have access to the papers we went over, I have typed up the notes I took below.

### Paper Notes:

- Reaction on the surface of the fuel cell.
- The O<sub>2</sub> cathode has to get to the surface of the fuel cell.
- Use proton conductive materials in the polymer to allow the protons to get to the surface of the fuel cell.
- Electrons go through carbon to the surface of the fuel cell.
- $E^{-}$ , P<sup>+</sup>, and O<sub>2</sub> come together on the surface of the fuel cell.
- The performance of a fuel cell depends on many factors, such as how much platinum is used, the size of the fuel cell, and the surface area.
  - How much platinum is used
  - Size of the fuel cell
  - Surface area
    - Increased surface area means increased activity because you are expanding the workforce.

- How much catalyst is used
- How easily protons and  $O_2$  reach the surface.
- A fuel cell is ineffective if oxygen or protons can't reach the polymer.
- Without a polymer, most of the platinum would not be used
- Transport of gas (oxygen) through the structure depends on the size of the pore and how many pores there are
- Electron transport is not limiting
- Carbon is a good conductor as long as the carbon atoms are touching each other.
  - If not utilized, money is being wasted
- To make a fuel cell structure
  - The polymer is attached to a catalyst  $\rightarrow$  catalyst ink
  - The ink is sprayed onto the membrane to get a catalyst layer
- It is crucial to find a ratio that optimizes the utilization of the catalyst.
- The final product depends on more than just the catalyst
  - How is the layer made?
  - How is the ink made?
- Solvent ratios are independent variables.
- Structural parameters are dependent variables.
- The most common solvents used are nPA (normal proponal) and H<sub>2</sub>O (water)
- Ink characteristics should be kept track of
- We don't know how different factors impact performance yet, but we *do* know that different factors influence performance.

### Other important information:

- He mentioned that when citing papers, it is always good to mention the person responsible for the information as well as the place they work (if applicable) in citations. This is because it makes it more specific and easy to find.
- Dr. Karan will be sending Zoom invites for the rest of our meetings as he has the professional version of Zoom with no time constraints. My non-professional account has a time constraint of 40 minutes, which we almost went over during our meeting.

# September 18 - Class Time:

During this class period, I did not have any work to complete for ASP, so I completed homework from other classes.

# September 20 - Class Time:

- Biweekly check-in with Dr. Garcia
  - During this meeting, Dr. Garcia and I discussed everything that happened in my meeting with my mentor the previous Monday.
  - I told her about our plans for our next meeting on Monday, including going over research questions and goals.
  - She looked over a draft of my email, reminding Dr. Karan of our upcoming meeting.
- 🗹 Email Dr. Karan
  - Write an email reminding Dr. Karan of our upcoming meeting as well as ask for papers to read. <u>See Email Communication for September 20th.</u>

# September 22 - Weekend:

- Read and annotate the first three pages of bridging the gap between highly active oxygen reduction reaction catalysts and effective catalyst layers for proton
  exchange membrane fuel cells.
  - <u>See background research for September 22nd.</u>

# September 23 - Meeting with Mentor:

During this meeting with my mentor, we discussed the following items.

- We discussed the one paper that I read prior to the meeting.
- We reviewed some diagrams with zoomed-in images of what a fuel cell works and how the components work together to be effective.
- Dr. Karan sketched a fuel cell structure and will be emailing it to me.
- We discussed the structure of fuel cells and how to optimize performance.
- There are three materials that are used to make the catalyst ink.
  - Catalyst, solvent, and ionomer.



Image from *The Controllable Design of Catalyst Inks to Enhance PEMFC Performance* 

- In the lab at the University of Calgary, they are studying the effect of the solvent on the properties of the catalyst ink and catalyst layer to understand how it affects the connectivity and accessibility of fuel cells.
- We went over some of the variables that the experiment conducted at the lab has.
  - Independent variable
    - The ratio of water to isopropyl alcohol in the solvent used to mix the catalyst ink
  - Responding variables
    - Size of aggregates in the catalyst ink
    - Properties of the catalyst layer
      - Coverage
      - Ionic resistance
      - Electronic resistance
      - Pore size
- Before the next meeting:
  - Have an outline made for the introduction section of the research proposal
  - Have some possible research questions (3 minimum)

# September 24 - Class Time:

- Send an email to Dr. Karan summarizing yesterday's meeting
  - See email communication for September 24th.
- ✓ Finish annotations for the images in Bridging the gap between highly active oxygen reduction reaction catalysts and effective catalyst layers for proton exchange membrane fuel cells.
  - <u>See background research for September 24th.</u>

Upload annotated PNGs to the logbook

## September 25 - After School:

- Dr. Karan sent me the notes from our meeting on September 23rd
  - See email communication for September 25th
  - <u>See mentor written notes for September 23th</u>

# September 26 - Class Time:

- Draft and schedule send an email to Dr. Karan reminding him of the upcoming meeting to be sent tomorrow afternoon
  - Schedule email for tomorrow (September 27th) at lunchtime (around noon)
  - See Email Communication September 27th.
- Add a section for mentor notes and add notes from September 20th and September 23rd.
  - See Mentor Notes for <u>September 20th</u> and <u>September 23rd</u>.
- Update the Email Communication section of the logbook.
  - See Email Communication September 25th.
- Show Dr. Garcia my logbook and get feedback
- Read + annotate more papers
  - Structure, Property, and Performance of Catalyst Layer in Proton Exchange Membrane Fuel Cells

✓ Section 1

- <u>See Background Research for September 26th.</u>

# September 27 - After School:

- Email Dr. Karan meeting reminder
  - See email communication for September 27th

## September 29 - Weekend:

- ✓ Read + annotate more papers
  - Structure, Property, and Performance of Catalyst Layer in Proton Exchange

Membrane Fuel Cells

- ✓ Section 2.1
  - <u>See Background Research for September 29th.</u>
- Section 2.4
  - <u>See Background Research for September 29th.</u>
- Section 4.6
  - See Background Research for September 29th.

# September 30 - Class Time:

- Update the logbook calendar for October
  - Include dates of mentor meetings, biweekly meetings with Dr. Garcia,
  - <u>See Calendars for October</u>
- ☑ Write three possible research questions to be discussed with the mentor.
  - 1. How does the optimization of catalyst layer structures impact the trade-off between cost, performance, and durability in proton exchange membrane fuel cells (PEMFCs), particularly with the reduced platinum content?
    - a. The balance between reducing the cost of PEM fuel cells by decreasing the use of Pt (an expensive material) and maintaining/improving fuel cell performance and durability. Optimizing the structure can influence the efficiency of chemical reactions, water management, and long-term operation.
    - b. The question investigates how changing the CL design can achieve cost savings without compromising on the fuel cell functionality.
  - 2. How do advanced thin-film fabrication techniques (ex., atomic layer deposition and sputtering) affect the long-term performance and mass transport characteristics of ultra-thin catalyst layers in proton exchange membrane fuel cells (PEMFCs)?
    - a. Focuses on the impact of modern thin-film techniques used to create ultra-thin catalyst layers. These methods allow for more efficient use of expensive catalysts such as platinum, but their influence on the longevity of fuel cells and the transport of gases and water is not fully understood yet.
    - b. The question investigates how these techniques affect the overall durability and operational efficiency of PEM fuel cells.
  - 3. How do different catalyst coating methods affect the stability, water

management, and oxygen reduction reaction efficiency in PEMFCs under varying operational conditions?

- a. It looks at how different methods of applying the catalyst impact the overall performance of a fuel cell. The coating methods influence how well the CL facilitates the oxygen reduction reaction, manages water buildup, and remains stable over time.
- b. The question aims to compare methods under different scenarios to determine which one is the best in stability and efficiency.
- 4. How does the composition of non-precious metal catalysts compare to platinum-based catalysts in terms of catalytic activity and stability in PEM fuel cells?
  - a. NPM catalysts are being researched as cost-effective alternatives to platinum; they lack the same level of efficiency and durability.
  - b. The question would investigate the catalytic activity and stability of NPM catalysts compared to Pt, assessing their potential for commercial use in PEMFCs.
- ☑ Research proposal outline
  - I. Background Information
    - A. Global shift toward clean energy and fuel cells (1-1.5 pgs)

<u>Image from UN</u>
<u>Environmental</u>
<u>Programme</u>

#### Targets linked to the environment:

- Target 7.1: By 2030, ensure universal access to affordable, reliable and modern energy services
- Target 7.2: By 2030, increase substantially the share of renewable energy in the global energy mix
- Target 7.3: By 2030, double the global rate of improvement in energy efficiency
- Target 7.a: By 2030, enhance international cooperation to facilitate access to clean energy research and technology, including renewable energy, energy efficiency and advanced and cleaner fossil-fuel technology, and promote investment in energy infrastructure and clean energy technology
- Target 7.b: By 2030, expand infrastructure and upgrade technology for supplying modern and sustainable energy services for all in developing countries, in particular least developed countries, small island developing States, and land-locked developing countries, in accordance with their respective programmes of support
- The problem (causes)  $\rightarrow$  extreme weather conditions (climate change) and human-based carbon emissions.
- International Panel for Climate Change (IPCC)
- Paris Agreement
- Regulations
- Sources of carbon emissions
  - Breakdown of sectors
  - Transportation is a large sector in the US/Canada
- Ways to minimize emissions
- Why the shift is happening
- Increasing demand for clean and sustainable energy sources
- PEMFCs are a promising technology due to their efficiency and environmental benefits
- Applications of PEMFCs in **transportation (mainly)**, stationary power, and portable electronics.
- B. Overview of PEMFCs
  - The basic operation of PEMFCS
    - Splitting hydrogen into protons and electrons at anodes
    - Generating electricity as electrons move through an external circuit
    - Protons react with oxygen at the cathode to form water
  - Challenges in PEMFCs, especially in CLs
    - High cost
    - Performance limitations
    - Durability concerns
- II. Role of Catalyst Layers
  - A. Key functions and importance of CLs
    - CLs facilitate electrochemical reactions (ex., ORR at the cathode)
    - CLs are responsible for transporting reactants, products, electrons, and heat while managing water.
    - CLs make up 42% of the cost of mass-produced PEMFCs due to the use of platinum crystals.
  - B. Challenges in the CL design
    - Cost of PEMFCs due to Pt catalysts
    - Water buildup and flooding in CLs block reactions, therefore reducing performance.
    - Poor CL design can lead to the formation of hydrogen peroxide (H<sub>2</sub>O<sub>2</sub>), which degrades components and reduces the longevity of FC.
- III. Current Efforts to Address CL Challenges
  - A. Reducing platinum content
    - Researchers are exploring platinum alloys and non-precious

metal catalysts to reduce reliance on expensive Pt while maintaining performance.

- NPM catalysts are not as reliable or efficient, leading to cost, durability, and performance trade-offs.
- B. Improving catalyst layer structure
  - CL structure, including thickness, pore size, and arrangement of catalyst particles, impacts short-term and long-term performance.
  - Emerging fabrication techniques like thin-film deposition aim to reduce catalyst loading while maintaining efficiency.
  - Catalyst ink and fabrication of catalyst ink
    - Coating method
    - Building block materials (catalyst, ionomer, carbon supports)
    - Ink composition
- IV. Rationale for Study
  - A. Need for optimization and better understanding of CLs
    - Despite advancements, there is no consensus on the best CL structure for PEM fuel cells.
    - Understanding how Cl structure impacts key factors such as mass transport, catalyst usage, and durability is crucial for improving the overall fuel cell performance.
  - B. Relevance of study
    - Aims to address the gaps in knowledge regarding the trade-offs between cost, performance, and durability in CL design.
    - Optimizing CL structure and reducing platinum usage will allow this research to contribute to making PEMFCs more cost-effective and scalable for widespread industrial use.
- V. Research Aim and Objectives
  - A. Objective
    - Investigate how CL structure and material composition impact the performance, cost, and long-term durability of PEMFCs.
  - B. Relevance
    - The study will help guide future design improvements, accelerating the commercialization of PEMFCs and

#### contributing to global clean energy goals.

- Upload PNGs of annotated papers from September 29th.
  - See Background Research for September 29th.
- ☑ Type up the written summary bullet points on each section of Structure, Property, and Performance of Catalyst Layer in Proton Exchange Membrane Fuel Cells.
  - <u>See Background Research Summary Notes for September 30th.</u>

## September 30 - Meeting with Mentor:

The meeting was moved to Thursday due to Truth and Reconciliation Day

- Dr. Karan sent me an email to reschedule our meeting, and I emailed back to confirm the change.
  - <u>See email communication for September 30th</u>

# **October Daily Notes**

## October 02 - Class Time:

During this class we reviewed a lot of information regarding the class that pertains to everyone.

- September Logbook
  - This logbook is for practice. We are only getting feedback from Dr. Garcia for this one.
  - Common sources of error
    - Having missing information for days in your logbook will result in lost marks for content.
    - Having information written in an unclear fashion will result in lost marks for organization.
  - For papers being annotated, have information that tells Dr. Garcia exactly what paper you were working on
    - Title
    - Author
    - Year
- Do not use sites such as Johns Hopkins, Mayo Clinic, etc., for citing reliable information.
  - These sites are fine to use to gather a basic quick definition or understanding of a concept but not okay to use for citing information.
- Schedules
  - Have schedules planned out to the best of your ability
    - Do not just put class (not specific enough)

### - Research Proposals

- Introduction outline (have done by October 04)
  - Broad
  - То
  - Narrow
- Research Question (have done by October 04)
  - What is it?
- Goals (have done by October 04)
  - Short-term: tasks

- Long-term: future
- Variables and Hypothesis
  - Don't do this if you are not conducting an original experiment
- Methods (by the end of next week)
  - Have a basic understanding
  - There is no need to know super in-depth
- Significance (by the end of next week/beginning of the following week)
  - Contribution to the field
  - Why is it important?
- Have the first draft done by mid-October
- DUE: END OF OCTOBER
- ✓ Meeting with Dr. Garcia
  - By the end of your next meeting with your mentor, have:
    - Goals
    - Methods
      - What are you measuring
      - How is it measured
    - Ask about experimental vs. study
    - Hypothesis and variables
  - Set deadlines for yourself
    - Draft intro
    - Goals
    - RQ
    - Methods
  - Get approval for the intro outline and RQ from Dr. Karan

## October 03 - Meeting with Mentor:

During this meeting with my mentor, we went over the research questions I had written down, as well as my introduction outline.

Pros and cons of each question:

Question 1: How does the optimization of catalyst layer structures impact the trade-off between cost, performance, and durability in proton exchange membrane fuel cells (PEMFCs), particularly with the reduced platinum content?

Pros:

- The current cost for the system
  - Minimize the cost of the most expensive part
  - How much is the fuel cell?
  - How much is the platinum?
  - Measured in \$/kW
    - A car uses about 80-100 kW fuel cell
  - \$3000/kW is the approximate cost of a combustion engine
    - A fuel cell needs to have a similar price

Cons:

- Electric vehicles exist now, so a hydrogen fuel cell car is not as viable.
- Cost is not as big of an issue anymore. Durability and performance are the main issues/concerns.
- Fuel cells are focused on heavy-duty vehicles.

Question 2: How do advanced thin-film fabrication techniques (ex., atomic layer deposition, and sputtering) affect the long-term performance and mass transport characteristics of ultra-thin catalyst layers in proton exchange membrane fuel cells (PEMFCs)?

Pros:

- Scientifically, it is a good question.

Cons:

- The bigger issue is scalability
- Practically looking more towards mass production
- It needs a very clean environment and is a very long process.
- Low material costs but high manufacturing costs.

Question 3: How do different catalyst coating methods affect the stability, water management, and oxygen reduction reaction efficiency in PEMFCs under varying operational conditions?

Pros:

- Links to ink studies (focus of UofC lab)
- How the methods impact the fuel cell
- Tuning the composition of the ink to coating methods

- Can improve performance

Cons:

- Studying the different methods
  - Limited access to the different methods

Question 4: How does the composition of non-precious metal catalysts compare to platinum-based catalysts in terms of catalytic activity and stability in PEM fuel cells?

Pros:

- None

Cons:

- No longer studied for commercial use.
- Platinum is the best now. We are just looking to the performance of them.

After going through all the questions, we decided that the best question would be **question 3** reworded to be more specific to the experiments done at the UofC lab.

Research proposal introduction outline changes:

- What is clean energy for different applications?
- What is the energy used for?
  - Electricity & heat
  - Industries
  - Transportation/vehicles
- What kind of energy specifically?
- Add to intro
  - Factors to urban air quality
    - Emissions
      - Gases
      - Unturned particular matter (PM) approx. 2.5 microns
    - Unburned fuel
  - Why move towards zero-emission vehicles?
  - A fuel cell used in a vehicle would only release H2O, which addresses air quality issues.
  - It can minimize carbon and particulate matter emissions.
- Section IA

- Be more specific about the type of energy.
- Don't use the term global warming; stick to the term climate change instead.
- Why are fuel cells promising?
- What are fuel cells efficient for?  $\rightarrow$  What kind of efficiency?
- Section IIA
  - Cite references
  - Full utilization of the catalyst
  - Looking to get the highest performance
  - Start steering towards research.
- Section IIB
  - Don't bring up the catalyst layer design
  - Talk about the challenges of utilizing the expensive catalyst.
  - I can make the challenges more about what we want to achieve.
  - If doing challenges, talk about what is happening.
  - Flooding does not completely block the reaction from occurring. It just reduces the reaction.
  - Open pores, protons, gases, water removal
  - Current effort
    - Know what we want
      - What can we do to achieve it?
      - What are the problems?
    - Fill in the gaps in the research.
  - Use less catalyst and utilize it all.
- Section IIIA
  - Control the catalyst layer to make sure the pores are large enough
  - What is limiting us?
- Section IVA:
  - Need for optimization
    - Impact of coating parameters
- Section VA:
  - Specific objective  $\rightarrow$  Establish a clear link between the catalyst ink and the structure
  - Catalyst layer structure affecting properties
    - Usual transport properties
      - Water removal
      - Oxygen

- Protons
- The structure is important because of the properties
  - No clear link
  - Trial and error
  - Find optimum
- We discussed the possibility of me coming into the lab to see what everything looks like and to maybe assist with experiments.
- Before our next meeting, I told Dr. Karan that I would have completed the background section of the research proposal introduction.

## October 04 - Class Time:

- Email summary to Dr. Karan about our meeting yesterday.
  - See email communication for October 04
- ☑ Read + Annotate papers about the catalyst ink
  - ✓ Introduction to Dictating Pt Based Electrocatalyst Performance in Polymer Electrolyte Fuel Cells, from Formulation to Application
  - Conclusion to Dictating Pt Based Electrocatalyst Performance in Polymer Electrolyte Fuel Cells, from Formulation to Application
  - ✓ Intro to Tailoring electrode microstructure via ink content to enable improved rated power performance for platinum cobalt/high surface area carbon based polymer electrolyte fuel cells
  - Conclusion to Tailoring electrode microstructure via ink content to enable improved rated power performance for platinum cobalt/high surface area carbon based polymer electrolyte fuel cells
  - ☑ Intro to The Controllable Design of Catalyst Inks to Enhance PEMFC Performance: A Review
  - Conclusion to The Controllable Design of Catalyst Inks to Enhance PEMFC Performance: A Review
  - ☑ Intro to Recent progress in understanding the dispersion stability of catabyst ink for proton exchange membrane fuel cell and water electrolyzer
  - Conclusion to Recent progress in understanding the dispersion stability of catalyst ink for proton exchange membrane fuel cell and water electrolyzer
  - <u>See background research for October 04</u>
- ☑ Write summary notes for each section
  - ☑ Introduction to Dictating Pt-Based Electrocatalyst Performance in Polymer Electrolyte Fuel Cells, from Formulation to Application
    - <u>See background research summary notes for October 04</u>

- Conclusion to Dictating Pt-Based Electrocatalyst Performance in Polymer Electrolyte Fuel Cells, from Formulation to Application
  - See background research summary notes for October 04
- ✓ Intro to Tailoring electrode microstructure via ink content to enable improved rated power performance for platinum cobalt/high surface area carbon based polymer electrolyte fuel cells
  - See background research summary notes for October 04
- Conclusion to Tailoring electrode microstructure via ink content to enable improved rated power performance for platinum cobalt/high surface area carbon based polymer electrolyte fuel cells
  - <u>See background research summary notes for October 04</u>

## October 06 - Weekend:

- ☑ Finish summary notes
  - ✓ Intro to The Controllable Design of Catalyst Inks to Enhance PEMFC Performance: A Review
    - <u>See background research summary notes for October 06</u>
  - Conclusion to *The Controllable Design of Catalyst Inks to Enhance PEMFC Performance: A Review* 
    - <u>See background research summary notes for October 06</u>
  - ✓ Intro to Recent progress in understanding the dispersion stability of catalyst ink for proton exchange membrane fuel cell and water electrolyzer
    - See background research summary notes for October 06
  - Conclusion to Recent progress in understanding the dispersion stability of catalyst ink for proton exchange membrane fuel cell and water electrolyzer
    - See background research summary notes for October 06
- ✓ I wrote the first draft of the background section to the introduction of my research proposal. It was not a very good first draft as I was unfortunately not feeling well all weekend. I also was unable to figure out how to add citations to the sheet using Paperpile.
  - <u>See background research for October 6th.</u>

## **October 07 - Meeting with Mentor:**

Dr. Karan taught me the best way to read a paper without going through every single section, that typically gives too much information for my level.

- 1. Read the abstract of the paper.
- 2. Read the conclusion/summary of the paper to gather the key points
- 3. Go to the images/figures to get a visual representation of what is happening

We went through my outline for the research proposal introduction again and made some changes.

- Updated version below.
  - I. Background Information
    - A. Global shift toward clean energy and fuel cells (1-1.5 pgs)

#### Image from

<u>UN</u>

Targets linked to the environment:

- Target 7.1: By 2030, ensure universal access to affordable, reliable and modern energy services
- Target 7.2: By 2030, increase substantially the share of renewable energy in the global energy mix
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- Target 7.a: By 2030, enhance international cooperation to facilitate access to clean energy research and technology, including renewable energy, energy efficiency and advanced and cleaner fossil-fuel technology, and promote investment in energy infrastructure and clean energy technology
- Target 7.b: By 2030, expand infrastructure and upgrade technology for supplying modern and sustainable energy services for all in developing countries, in particular least developed countries, small island developing States, and land-locked developing countries, in accordance with their respective programmes of support

#### Environmental Programme

- The problem (causes)  $\rightarrow$  extreme weather conditions (climate change) and human-based carbon emissions.
- International Panel for Climate Change (IPCC)
- Paris Agreement
- Regulations
- Sources of carbon emissions
  - Breakdown of sectors
  - Transportation is a large sector in the US/Canada
    - Ways to minimize emissions
- Why the shift is happening
- Increasing demand for clean and sustainable energy sources
- PEMFCs are a promising technology due to their efficiency and environmental benefits
- Applications of PEMFCs in **transportation (mainly)**,

stationary power, and portable electronics.

- B. Overview of PEMFCs
  - The basic operation of PEMFCS
    - Splitting hydrogen into protons and electrons at anodes
    - Generating electricity as electrons move through an external circuit
    - Protons react with oxygen at the cathode to form water
  - Challenges in PEMFCs, especially in CLs
    - High cost
    - Performance limitations
    - Durability concerns
- II. Role of Catalyst Layers
  - A. Key functions and importance of CLs
    - CLs facilitate electrochemical reactions (ex., ORR at the cathode)
    - CLs are responsible for transporting reactants, products, electrons, and heat while managing water.
    - CLs make up 42% of the cost of mass-produced PEMFCs due to the use of platinum crystals.
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    - Cost of PEMFCs due to Pt catalysts
    - Water buildup and flooding in CLs block reactions, therefore reducing performance.
    - Poor CL design can lead to the formation of hydrogen peroxide (H<sub>2</sub>O<sub>2</sub>), which degrades components and reduces the longevity of FC.
- III. Current Efforts to Address CL Challenges
  - A. Reducing platinum content
    - Researchers are exploring platinum alloys and non-precious metal catalysts to reduce reliance on expensive Pt while maintaining performance.
    - NPM catalysts are not as reliable or efficient, leading to cost, durability, and performance trade-offs.
  - B. Improving catalyst layer structure
    - CL structure, including thickness, pore size, and

arrangement of catalyst particles, impacts short-term and long-term performance.

- Emerging fabrication techniques like thin-film deposition aim to reduce catalyst loading while maintaining efficiency.
- Catalyst ink and fabrication of catalyst ink
  - Coating method
  - Building block materials (catalyst, ionomer, carbon supports)
  - Ink composition

## October 08 - Class Time:

- ☑ <del>Fix paperpile</del>
  - I was not able to get Paperpile citations to work, so I spent some time with Dr. Garcia troubleshooting it until I managed to get citations to insert properly and format to the correct citation style.
- 🗹 Email a summary to Dr. Karan.
  - See email communication for October 8th.
- Rewrite the research question to fit better with the research at UofC
  - How do coating parameters impact the structure of the catalyst layer and thereby affect the structure and properties of a proton exchange membrane fuel cell (PEMFC)?
- Rewrite the background information section of the RP with proper citations and follow the flow Dr. Karan suggested at our previous meeting.
  - <u>See background research for October 8th.</u>
- ☑ Work on the role of the background info about PEMFCs section.
  - <u>See background research for October 8th.</u>

## October 10 - Class time:

- ✓ Work on the role of the catalyst layer function and importance section of the RP intro.
  - See background research for October 10th.

## October 15 - Class Time:

- ☑ Fill out the SH Science Fair Form (GC) with the necessary information
  - **Topic:** Effects of the coating parameters of the catalyst ink on the structure and properties of a proton exchange membrane fuel cell (PEMFC)
  - Type of project: Experimental
  - Partner: none
  - Have you done the science fair? No
- Registered for the CYSF Science Fair Portal
- $\square$  RP Intro  $\rightarrow$  role of the CL: Challenges
  - See background research for October 15th.
- ☑ Meeting with Dr. Garcia
  - We went over everything I discussed with my mentor at my last two meetings
    - Research question pros and cons and deciding on a research question
    - Improvements to my outline
    - Went over the first draft of the RP intro and suggested changes/edits for the flow
  - Went over personal deadlines
    - Have the intro done by the end of the week (October 18/October 20)
    - Have the full RP completed by October 25th
    - Send sections to the mentor for suggestions.
      - Don't save it all until the end because then there won't be time to make edits.
    - Work on the oral presentation for the week before presenting on November 6th.

#### **Deadlines**:

- October 31: final draft of written research proposal due
- November 4-8: research proposal oral presentation
  - I am presenting on November 6th

#### **Oral Presentation:**

- Rubrics on Google Classroom
- 10-minute long presentation (almost a hundred percent of your mark comes from this)
  - 1-minute grace period
- 5-minute question period (10% weighting for participation + asking questions)
- The presentation should be about 10-15 slides

- Approximately one minute per slide
- Use the rubric to break down the tasks that need to be done before the presentations

## **October 16 - After School:**

- Schedule send an email to Dr. Karan reminding him of our upcoming meeting tomorrow.
  - <u>See email communication for October 16, 2024.</u>
- Make edits to my research proposal.
  - I sent my dad, a chemical and electrochemical engineer, a copy of my research proposal and asked him to read it and make any edits.
  - I went back through my introduction and made all the edits he proposed.
  - <u>See background research for October 16th.</u>

## **October 17 - Lunchtime Science Fair Meeting:**

We had a quick meeting to go over some general information regarding the senior high science fair.

- The in-school science fair is on March 11th
  - 15 projects will make it to the Calgary Youth Science Fair (CYSF)
- A large tri-fold will be provided to each participant, but we are not required to use it.
  - We are allowed to create a poster board ourselves, but we will have to figure out a way to make it stand up. We will also have to make it ourselves at home + get it printed.

### - Online platform

- Complete **basic project info** as soon as possible
- Complete the **ethics form** as soon as possible
- Be very careful about the ethics form.
  - Everyone must complete the form regardless of whether or not they are working with animals/humans.
  - Provide a brief description of the project and indicate whether or not you are working with data, humans, animals, or animal cells.
  - Be **very clear** if you are not working with human or animal cells.
  - If you are working with living beings
    - "Xyz will be used in xyz way. It will be conducted at the University of Calgary, being mentored by xyz under code 123456."
    - Put the mentor's contact information and name.

- If not directly involved in experiments, be clear that you are using data but not conducting the experiments yourself.
- Only fill out **significant risk** if there is a significant risk associated with your research.

## **October 17 - Class Time:**

- ☑ Reply to Dr. Karan's Email
  - See email communication for October 17th.
- Ask Dr. Garcia if she has had a chance to look over what I have of my research proposal.
  - She has been busy with other stuff, so she has not had a chance to review my research proposal yet, but she will be doing so sometime tomorrow or over the weekend.
- ✓ Write the RP introduction aim + objectives section

Despite all the advancements that have been made in PEMFC technology, there is still no

consensus on how to make the optimal catalyst layer structure [8]. The design of the CL is critical as it has a significant influence on factors such as mass transport, catalyst efficiency, and durability. Understanding how variations to the catalyst layer structure impact these parameters is essential to enhancing the overall performance of PEMFCs. The trade-offs between cost, performance, and durability present significant challenges to the design process of the catalyst layer. Further exploration into how the materials used in the CL react and relate to each other is vital for improving fuel cell technology. The study aims to address the gaps in the understanding of the CL design that is available thus far. Optimizing the CL structure not only makes fuel cells more efficient, but it also reduces the cost of materials and allows for fuel cells to be mass-produced for commercial use. The research will contribute to ongoing studies to create economically practical and durable PEMFCs that will bring countries one step closer to transitioning to renewable energy and addressing climate change [8].

☑ Write the objectives of the research for the RP

This project aims to evaluate the effectiveness of different ratios of isopropyl alcohol in the catalyst ink on the structure and performance of the catalyst layer in proton-exchange membrane fuel cells (PEMFCs). The project aims to understand how varying isopropyl alcohol concentrations affect the properties of the catalyst layer, aggregate size, coverage, and ionic resistance to optimize the fuel cell's durability and efficiency.

#### Short-term:

- Testing and identifying the impact of different concentrations of isopropyl alcohol on the catalyst ink and its properties.
- How each concentration affects the functionality of the fuel cell and its properties, such as aggregate size, coverage, ionic resistance, electronic resistance, and pore size.
- The results will be used to determine which concentration of isopropyl alcohol is most promising for the fuel cell's long-term durability and performance.

#### Long-term:

- Designing a set of manufacturing parameters for applying the ink to the catalyst layer with an optimized concentration of isopropyl alcohol in PEMFCs, especially for applications in heavy-duty vehicles.
- Better the large-scale production of PEMFCs as a sustainable alternative to internal combustion engines in the transportation sector.

## **October 17 - Meeting with Mentor;**

During this meeting with my mentor my mentor and I just discussed some items regarding the research proposal and the science fair portal

- My project will be an experimental based project since the experiment at the University of Calgary is ongoing and all the data has not been collected yet.
- For the science fair portal, there are no ethics that I need to declare in regards to working with human + animals
- There are no significant risks relating to the use of chemicals
  - All chemicals are appropriately handled according to the MSDS (material safety data sheet)
- There are different ways to create a title
  - Provocative
    - Can we...
    - How to...
  - Factual
    - The effect of x on y
  - Snappy
    - Pose a question as the title to make it eye catching
- Methodology
  - We will see if I can get permission to come into the lab regularly
  - I will be asking Dr. Garcia to see if she knows how I can get that permission.
  - If I cannot come in regularly, I can come in as a visitor to learn about the methodology.
  - When I come to the lab, Dr. Karan will be showing me the methods.
- Before our next meeting I will have the introduction the the research proposal fully completed and have started working on other parts of the proposal.

## October 19 - Weekend:

- ☑ I went through the edits that Dr. Garcia suggested and made edits to the parts of the intro I gave her.
  - <u>See background research for October 19th.</u>
- ☑ Write the research question into the proposal

How do the coating parameters impact the structure of the catalyst layer and thereby

affect the structure and properties of a proton-exchange membrane fuel cell (PEMFC)?

- ✓ Write the variables into the proposal
  - <u>See experimental procedure for October 19th.</u>
- Email Dr. Karan meeting summary

See email communication for October 19th.

#### **October 20 - Weekend:**

- ☑ Write the hypothesis for the research proposal
  - See experimental procedure for October 20th.
- ☑ Write the significance of the research for the research proposal
  - I decided to use a paragraph I had written for my intro as the significance as it was the significance of the research.

Despite all the advancements that have been made in PEMFC technology, there is still no consensus on how to make the optimal catalyst layer structure [8]. The design of the CL is critical as it has a significant influence on factors such as mass transport, catalyst efficiency, and durability. Understanding how variations to the catalyst layer structure impact these parameters is essential to enhancing the overall performance of PEMFCs. The trade-offs between cost, performance, and durability present significant challenges to the design process of the catalyst layer. Further exploration into how the materials used in the CL react and relate to each other is vital for improving fuel cell technology. The study aims to address the gaps in the understanding of the CL design that is available thus far. Optimizing the CL structure not only makes fuel cells more efficient, but it also reduces the cost of materials and allows for fuel cells to be mass-produced for commercial use [8]. The research will contribute to ongoing studies to create economically practical and durable PEMFCs that will bring countries one step closer to transitioning to renewable energy and addressing climate change.

### **October 21 - Class Time:**

☑ Whole class discussion about the oral presentation of our research proposal

#### Time:

- 10 minute presentation
  - If you go too long over you may lose mark because you haven't made edits to your presentation and are giving too many details
  - If you go a little bit over, it is fine depending on the complexity of your research as long as you are not giving too much information
  - Everyone is given a one minute grace period
  - Going under the 10 minutes is fine as long as you are clear and have all components
- Spent about 1 minute per slide
- There will be a five minute question period

#### Content:

- Display a deep understanding of your project
- Have the best understanding of your background research
- Convey the research question in the context of your research
- How does the research question relate to the background research

#### **Components:**

- Background research (be about 3 slides)
- Research question (about 1-2 slides, share with objectives)
- Objectives (about 1-2 slides, share with research question)
- Can decide the order of hypothesis, variables, and methodology yourself
  - If you are doing an experimental project, hypothesis (1 slide with variables)
  - If you are doing an experimental project, variables (1 slide with hypothesis)
  - Methodology (2-3 slides depending on how many steps there are)
- Significance (about 1 slide)
  - Need for the research
  - Your contribution to the bigger field
    - My specific study is going to...

#### **Questions**:

- Be able to comfortably answer questions

#### Organization:

- The way things are layed out is important
- Use all the space on the slides
  - Use big font
  - Don't keep things clustered
  - Make graphics easily readable
- Rehearse your presentation so that it flows but do not over-rehearse to the point where you sound like a robot

### Slides:

- First slide title page
- DO NOT GO STRAIGHT TO BACKGROUND RESEARCH IF YOU HAVE NOT EXPLAINED YOUR TITLE
  - Explain title either on the title page or on the next slide
- Background research
  - Few words on the slides
  - Elaborate more
- If you have empty space
  - Make graphics bigger
  - Add more text
- Have just enough information on the slides that audience can summarize it in the time you spend talking
- Methodology
  - Don't just give a list of steps
  - Form some kind of graphic that shows how to get the answer
  - It is okay if you can't explain everything in greate detail but you need to have a basic understanding of the methods
  - Have the methods answer the question
  - The methods to get the audience to understand how you are answering the question.

#### Graphics:

- Prefer graphics over text
- Make sure the graphics are good quality + easy to read
  - If they are not super easy to read/understand but a really good graphic, spend some time explaining the graphic

- Do not put embellishments on your slide for no reason
  - Everything on the slide should correlate to the presentation
- Cite any graphics that you do not make yourself (including graphics from mentor)

#### **BioRendering**:

- A website with graphic templates
- These figures cann help you with your presentation
- You can use whole parts of a template or you can select certain parts of a template that works best with your presentation + topic
- <u>https://app.biorender.com/</u>

#### Presenting:

- You may hve flashcards
- Do not just stand still and read off the flash chards
- Make eye contact with the audience and move around
- Do not cram a presentation longer than 10 minutes into the 10 minutes
  - You do not have to provide every detail
  - Determine what are details and what is critical
  - Edit down your presentation if it is too long
  - Don't just speak faster to cram more information into the 10 minutes
- ☑ Look through previous presentations and go over the pros and cons as a class
  - Do not put too much content on one slide
    - It gets difficult to read for the audience and the audience will be more focused on reading the slides than paying attention to you.
- Ask Dr. Garcia if she knows how to get me lab permissions at UofC
  - There is a young person access to laboratory form that Dr. Garcia will be sending to you.
  - Dr. Garcia thinks that to get me access to the lab, you may have to speak to the health and safety coordinator of the lab.
  - If I am just going to only shadow someone or come in as a visitor, Dr. Garcia does not think that I need permission to be in the lab.
  - I only need permission if I am actively participating in the experiment.

## **October 21 - Meeting with Mentor:**

- Dr. Karan is not sure if I need a confounding variable for this project.
- I shared my research proposal with Dr. Karan and he is going to start making edits to it.
- He is going to be looking to make sure the who proposal flows and tells a story
- The aspects that is important to creating anything
  - Cost, performance, and logevity/durability
- I will be adding more to the introduction about the catalyst ink
- I should add figures to research proposal to connect everything
- While Dr. Karan is editing the document, he will be adding some information about the methodology since I may not be able to go into the lab.
- I will have the rest of the research proposal done by the end of the week.

## October 21 - After School:

Google Docs has recently implemented a new feature where you can create tabs within a document. In order to make my logbook more organized, I went through an gave each section of my logbook a different tab. I transferred all the information from my original page to the different tabs and went through and made sure that all the links to different sections of the logbook corresponded with the new tabs.

## October 23 - Class Time:

- Go over some information as a class
  - CYSF ethics for people who do not have any human or animal-related ethics to declare.
    - Working Title
    - Paragraph that describes project
      - Do this in general terms
    - Second paragraph
      - This study does not require the use of human or animal participants.
    - This project is overseen/supervised by
      - Mentor Name
      - Department
      - Email or phone number
  - CYSF ethics for people who do have animal or human-related ethics to

declare.

- Working title
- Description of the project
  - How are the human and animals going to be used in the project.
- What part of the project will you be working on in regards to the animal and human subjects
- This project is supervised by
  - Mentor Name
  - Department
  - Email and/or phone number
- If the lab already has an ethics document write the lab ethics code
- Significant risks
  - Only have to fill this out if you have significant risks to declare
  - Once you declare ethics, the CYSF will tell you if you nead
- For the methods of the research proposal
  - Don't have to have a full and complete understanding of all the details of every technique used
  - You have to make a link between procedures and how to answer research question
  - Enough details that will show how the methodology will help the question be answered
  - Examples
    - Rats  $\rightarrow$  2 doses anesthetic  $\rightarrow$  brain  $\rightarrow$  morphology of neurons
    - Data will be extracted + parts will be euthanized
  - Always write the methodology in the past usually
    - Since this is a research proposal, methods will be in future tense
    - DO NOT USE PERSONAL PRONOUNS
    - Plan to tell what you will do not what is possible
- Reference
  - Figure out how to title the secion
    - Use owl perdue to find this information
  - Any paper you read should be on Paperpile
  - When you are doing in-text citations
    - Paperpile
    - Insert citation

- Enter citation
- Format citation
- Add citations as you go so you do not miss anything
  - Cite **everything** you did not come up with yourself
- Send an email summary of our last meeting to Dr. Karan
  - See email communication for October 23rd.

## **October 25 - Class Time:**

✓ Full Class meeting

- Oral Presentations
  - We started by going through the schedule for oral presentations and making edits to it.
  - Instead of doing 4, 6, 8 we will be doing presentations 6, 8, and 13.
  - Participation
    - Have to be at a minimum of 4 presentations to get full participation marks
    - Use presentations for ideas for your presentation
  - Dr. Garcia will not be available for individual meetings during this time
    - Stay on top of your own workload
    - Email Dr. Garcia if you need help
  - 15 minute presentation
  - 5 minute buffer period between presentations
    - Feedback from Dr. Garcia and classmates
  - During presentations
    - If you did not attend presentations
      - Have notes of things you read
      - What you worked on
      - Meeting with mentor
      - Etc.
    - If you attended presentations
      - Have notes on each presentation you sat in on
      - Cole's presentation
        - ....
      - Lauren's presentation

• •••

- Go over the research proposal formatting
  - Font
    - Easy to read font (times new roman/arial)
    - 12pt font minimum
    - 1.5-2 spacing
  - Title
    - If you are making a title page
      - "Title"
      - Research proposal
      - Date
      - Applied Science Project
      - Student Name
      - Mentor Name
      - Spread out across the page
    - If you are just putting the title at the top of the first page
      - "Title"
      - Research proposal
      - Date
      - Applied Science Project
      - Student Name
      - Mentor Name
      - Don't spread out across the page
  - It is fine for variables to be in bullet points
  - It is fine for objectives to be in bullet points
  - The methodology **MUST** be written in paragraph form
- Biweekly meeting with Dr. Garcia

I had a biweekly meeting with Dr. Garcia to review my progress.

- My mentor suggested that I add more to the intro about the catalyst ink and I am currently working on that
- Methodology
  - I have still not finished this section
  - I will be emailing my mentor about this today
  - I have another meeting with my mentor on the 31st so hopefully by then I will be able to just review the methodology I have written about
- WRITTEN RESEARCH PROPOSAL EXTENSION UNTIL NOVEMBER 4TH
- I will be comparing the references I have to the template on Perdue Owl to see if

they are accurate

- I have to find the IEEE that gets the citations the closest to the style of Perdue Owl
- ☑ RP confounding variables
  - <u>See experimental procedure for October 25th.</u>

## October 29 - Class Time:

I was not in Calgary attending class today.

## October 31 - Class Time:

I have a meeting with my mentor after school, but I also have a physics test to make up, so I will be writing my test during class.

# **November Daily Notes**

## November 03 - After School:

I sent Dr. Karan an email with the final draft of my written project proposal.

See email communication for November 3rd.

## November 04 - Class Time

- ✓ Class discussions
  - Logbooks
    - Make every task as specific as possible
    - If you don't know what tasks you will be doing
      - Read paper xyz (give specific paper names; don't just say reading papers)
      - CYSF portal xyz (don't just say you will be filling out the portal. Refer to specific sections)
      - Write down meeting dates with mentors
        - Tentative dates should also be written down
      - Biweekly meetings with Dr. Garcia should be written
      - Oral presentations
      - Sending emails to mentors
        - It should never be the only task
  - Oral presentations
    - Which ones are you listening to?
    - Which ones are you skipping?
    - When are you presenting?
  - CYSF
    - Get ethics handed in as soon as possible for approval
  - Long-term planning with mentor
    - What is happening in each month
      - This should be done in general terms
        - Not every meeting but deadlines to make sure the project is done.

- Future classes
  - Literature review sometime in early December
  - Midterms Jan 10-20
  - March  $11 \rightarrow$  School science fair (have poster done)
    - Work backwards
    - What needs to be done for this to happen?
  - May  $\rightarrow$  final paper
- Ask Dr. Garcia about formatting the research proposal
  - How to format and cite figures
  - How to write descriptions of the figures
  - How to introduce the methodology



(water and excess oxygen) Figure 2. Schematic depiction of a PEMFC showing the different layers, compositions, and reactant transport pathways [12]. Black structures are the carbon supports, purple represents the ionomer, red is the PTFE, and green is the catalysts. Note the figure is not drawn to scale, and the

catalyst layer, GDL, and MPL have different porosities and support material sizes.

☑ Go through mentor suggestions again.

Ensure the paper is completed to the best of my ability

## November 04 - Meeting with Mentor

This meeting with my mentor was a very quick one.

- We talked about my final draft of the research proposal before I handed it in.
- He told me to crop out the image of the PEM and electrolyzer to only show the

☑ Find another figure regarding the transport of fuel cells



PEM as the electrolyzer is not relevant to the research.

Figure 1. Schematic depiction of a PEM electrolyzer and fuel cell: (b) The fuel cell combines hydrogen and oxygen to produce electricity and water [11].

- We rescheduled our next meeting to be on Wednesday, November 13th, as Monday, November 11th, is Remembrance Day

## November 06 - Class Time

✓ Watch oral presentations

### Marie-Elise:

Implementation and Evaluation of Alternative User Interfaces for Game Control to Improve Application Accessibility

- Accounts for different people's preferences in modes of control in video games
- 1.3 billion people have difficulty interacting with apps due to disabilities
  - Projected to more than triple by 2050
- Studying the integration of speech, head, and gesture tracking into video games to increase accessibility
- Human-computer interaction (HCI) is the field of study

- User, experience/interactions and computer are all linked
- HCI makes it user-friendly and entertaining  $\rightarrow$  more enjoyable and interactive
- Applications with more modes of control increase accessibility and enjoyability
- Project
  - Preferences in games such as Connect 4 and Checkers
- Short-term goals
  - Program and implement modes of control
  - Complete programming for Connect 4 and Checkers
  - Make sure the program runs smoothly before posting
- Long-term goals
  - Study what modes individuals prefer in different situations
  - How to improve accessibility
  - What alternatives should be integrated
- Variables
  - Manipulated variables
    - Different modes
    - Different disabilities
    - Different ages
  - Responding variables
    - Preferred mode of interaction
  - Controlled variables
    - Types of games (connect 4, checkers)
    - Complexity of game
    - Number of times played total
      - Play a total of 18 times
      - 9 times per game
      - 3 times per mode
  - Confounding variables
    - Personal preference
    - User engagement
    - Experience
    - Enjoyment
    - Biological sex
- Question
  - How do an individual's age and disabilities impact their preference for alternative options to touch when playing video games?
- Null hypothesis

- Older individuals will have the same alternative to touch preference as younger individuals.
- Alternative hypothesis
  - Older individuals will prefer speech, and younger individuals will prefer head-tracking
- Methods
  - Software
    - Website: username, password, surveys
    - Alternatives to touch: speech, gesture, and head tracking programmed with Google Application Program Interfaces
    - Connect 4 Game: same logic, coded to check if they win, if the move is valid, etc.
    - Checkers: same logic, coded to check if they win, if the move is valid, etc.
  - Experience
    - Link, login, survey, games survey
    - Anyone can participate, but they must have a unique username and password
  - Start survey
    - Age
    - Difficulties during stress
    - Conditions
      - Autism
      - Dyslexia
      - ADHD
      - Dyspraxia
    - Video game preferences
  - End survey
    - Preferred mode
    - Ranking of modes
    - Would the play again?
    - difficulties/frustrations
- Significance
  - Accessibility: accessible to all individuals
  - Enhanced experience: advancing application designs for enhanced user experience and user interface

#### **Eleanor:**

A Comparison Study of the Impacts of Extreme El Niño Events on Human Societies in the 1788-1793 and 1982-1983 Episodes

- El Niño is a climate phenomenon caused by a change in the air circulation in the Pacific Ocean
  - Air circulation is normally east-to-west
  - Higher air pressure in the Western Pacific and lower air pressure in the Eastern Pacific
  - A phenomenon that occurs when unusually warm ocean water piles up along the equatorial west coast of South America
  - It happens every 2-7 years and can last for months/years
  - Has effects on global weather patterns
  - Teleconnections: the link between weather patterns in separated areas of the globe
    - India still feels the effects of En Niño even though it is not close to the Pacific Ocean
- El Niño Effects on Human Society
  - Weather anomalies
  - Agriculture
  - Health: known to be associated with floods and droughts that lose access to clean water
  - Infrastructure: the damage to the infrastructure
  - Population: measure to affect the population and economy
  - Economy
- Previous Studies
  - Scientists have established that it impacts global weather and human societies.
  - Few have taken into account how society changes and evolves over time
  - We are more reliant on the digital industry and finance these days
  - El niño has decreased impacts on human society
  - Human society impacts global warming  $\rightarrow$  global weather
- The aim of research is to compare El Niño effects from different periods of different levels of development to study the impact of human society on El Niño societies
- 1788-1793
  - 6 to 7 hundred million people
  - Global temperature rising

- 1 trillion dollars in GDP
- Large-scale manufacturing is the main industry
- 1982-1983
  - 4.4 billion people
  - +1.2 degrees celsius
  - 38 trillion dollars in GDP
  - Digital industry and finance
- Questions
  - What were the agricultural, economic, societal, health, and infrastructural impacts of the 1788-1793 and 1982-1983 episodes?
  - Is modern society more resilient to the socio-economic damages caused by climate variability and extreme weather events?
  - What predictions can we make about how future El Niño may affect human society?
- Short-term Objectives
  - 1788-1793
    - Reconstruct the amplitude of the event
    - Estimate the socioeconomic impacts
  - 1982-1983
    - Gather instrumental records of the event
    - Analyze the statistics
  - Comparison
    - Compare the two events and their socioeconomic effects
- Methodology
  - 1788-1793
    - Create a proxy index
    - Reconstruct the event
    - Look at historical documents
    - Conduct economic reconstructions
  - 1982-1983
    - Analyze instrumental records
    - Look at government statistics on the impact
  - Compare the two events using graphs
- Long-term goals
  - Gain a deeper understanding of how extreme weather events affect human societies.
  - Find mechanisms to reduce the detrimental impacts of future climate

events

- Significance
  - Anthropogenic vs. natural climate variabilities
  - Doubling in the occurrences
  - Predict the socioeconomic influences of climate variabilities in future societies.
- Go over things done well
  - They are very clear about where they are going to go with their project
  - We all know precisely what they will be doing with their projects
  - We do not need to know all the details to understand what is going on
  - The hypothesis and the manipulated variable have to go hand in hand
- CYSF Basic information
  - Name of Project: Coating Parameters of the Catalyst Ink and Their Impact on PEMFC Performance
  - Grade: 11
  - Project Type: Experiment
  - Language: English
  - Project Category: Chemical and Physical Sciences
  - Project Topics: Engineering
  - Brief Description of the Project: The experiment aims to adjust the catalyst ink composition to design the most efficient PEMFC. To improve the ink composition, the ratio of isopropyl alcohol to water will be tested.

## November 08 - Class Time

I wasn't in Calgary to attend this class.

- ☑ Work on oral presentation slideshow
  - I finished putting together all the slides for my oral presentation.



Antara Krishnamurthy Graduate Student Researcher: Vahid Mazinani Academic Supervisor: Dr. Kunal Karan











If the ratio of isopropyl alcohol in the catalyst ink solvent is increased, then the size of the aggregates in the catalyst ink will decrease, leading to improved catalyst layer coverage and reduced ionic resistance.

#### Explanation

This is because a higher concentration of isopropyl alcohol allows particles to spread uniformly across the catalyst surface and promotes better interactions with the membrane.






## November 11 - At Home:

- I worked on my speech for the oral presentation and ran through it a few times to ensure my timing was good.
- I practiced my presentation with my mom so she could give me feedback.
  - She told me that I did a good job explaining everything
  - I should talk a little slower because I am talking fast and taking a lot of pauses because my brain cannot catch up to my mouth.
- I sent Dr. Karan an email with my oral presentation.
  - <u>See email communication for November 11th.</u>

## November 12 - At Home:

- I practiced my oral presentation by myself a couple of times before practicing with my parents again.
- I got my time to be around 10 minutes while speaking slowly and clearly.

# November 13 - Class Time:

During this class, we spent more time presenting oral presentations, and I presented my oral presentation.

✓ Present oral presentation

- My oral presentation went well overall.
- I spent a little over 10 minutes going through my slides and answering questions for a few minutes.
- The questions include some of the following
  - Why is platinum the catalyst used?
  - Can you explain the diagram on PEMFCs in more detail?
  - Why are PEMFCs used in vehicles primarily?
  - Why are PEMFCs only used in heavy-duty vehicles?

✓ Watch Oral Presentations

#### Audrey:

Exploring antiviral defense systems and single-nucleotide polymorphisms in *Escherichia coli* 0157:H7 exposed to bacteriophages T1, T4, T5, rv5

#### *Escherichia coli* 0157:H7:

- Bacteria that produce toxins
- Common outbreaks through food and water
- Types:
  - Shiga-toxin producing
  - Verotixigenic
- Symptoms:
  - Vomiting
  - Stomach cramps
  - Severe/bloody diarrhea
  - Hemolytic uremic syndrome (HUS)
- Treatments
  - Rest
  - Antibiotics don't help and can actually develop HUS
  - Kidney dialysis in extreme cases

#### Bacteriophages:

- Attach to receptors on bacteria to kill it
- Lytic: full takeover (focus of research)
- Lysogenic: replicates passively

#### Antiviral defense systems:

- Mutations that are developed by bacteria as a result of phage attacks
- Absorption inhibition
  - Receptor binding proteins
- Restriction modification
- CRISPR-CAS

#### Single Nucleotide Polymorphism:

- Mutations developed as a result of genetic drift
  - Can potentially affect the reaction of bacteria to phages

#### Significance:

- 97000 registered e-coli cases
- There are antibiotic-resistant bacteria strains
- Can use this research to develop antimicrobial treatments
- Phage therapy can be used as a more generalized treatment

- Evolution of bacteria

Short-term objectives:

- Profile anti-phage defense systems
- Identify single nucleotide polymorphisms from gene sequencing

Long-term objectives:

- Develop a working phage therapy for clinical usage

Methods:

- 1. Bacteria and phages
  - a. Bacteria cultures in TSB
  - b. Phages are propagated using bacteria culture
- 2. Phage exposure
  - a. Mutants are created and purified in TSA
  - b. Microplate assay
  - c. Quantitative resistance assay
  - d. Fitness cost
- 3. 14 phage resistant bacterial isolates
  - a. Nucleospin DNA extraction kit
  - b. Sent to Quebec for WGS
- 4. Bioinformatic analysis
  - a. Galaxy
    - i. FastQC
    - ii. Shovill
  - b. Antiviral defense systems
    - i. defenseFinder
    - ii. PADLOC
  - c. CSV files
  - d. R studio v 1.1
  - e. Snippy

Questions:

- What would be the genetic modifications e.coli develops in response to exposure to phage defenses?
- How quickly do these bacteria develop resistance to bacteriophages?
  - It is relatively fast because bacteria mutate really fast, and mutations happen randomly. Random mutations appear, and it is up to chance which ones become resistant to the bacteriophages.

#### Arth:

Examining the effect of physical activity on muscle mass loss and function loss in peri - and early menopausal females.

#### Simplified:

- How exercise affects muscle mass loss in women 40 - 55

#### Menopause:

- The last menses stage of life, where hormonal change occurs and affects bone mass density
- The average age is 51 in Canada.
- Stages:
  - Reproductive
  - Premenopause
  - Postmenopause
- Menopausal symptoms:
  - Hot flashes
  - Night sweats
  - Mood changes
  - Sleepiness
  - Increased anxiety
- Risk factors for early menopause:
  - Obesity
  - Inactivity
  - Smoking
- Early menopause is influenced by lifestyle factors
- Treatments
  - Hormone replacement therapy (HRT)
    - Gives estrogen to women

#### Muscle:

- One of four soft tissues formed through the body functions through physiological processes
- Slow fibers type 1: endurance, fatigue-resistance
- Fast fibers type 2: power, rapid fatigue

- Muscle loss motor unit absorption compensates
- DXA scan measures muscle and bone density
- Age-related decline  $\rightarrow$  muscle mass loss post 50 years old
- Sarcopenia classes:
  - Class 1: less severe
  - Class 2: inhibits from doing certain things
- Severe sarcopenia: increased disabilities
- Neuromuscular decline impacts muscle mass

#### Physical activity:

- Any movement that requires energy to occur
- Benefits:
  - Physical and psychological health
  - Reduces fat infiltration in tissues
- Resistance training
  - Boosts muscle mass and strength
- Aerobic training
  - Improves insulin production and mitochondria
- Higher-intensity training has more significant benefits
- Measured using an accelerometer and tracks movement intensity
- Regularly physical activity slows muscle mass loss
- Lifelong exercise = younger biological age

#### Objectives:

- Link physical activity to muscle mass loss in peri and early postmenopausal women
  - How muscle loss affects health and balance
- Understudied demographics need more research
- Help others using the data found in the study

#### Research question:

- How does physical activity affect muscle mass loss and function in peri and early menopausal females

#### Hypothesis:

- Participants who perform physical activity at higher-intensity levels show lower levels of muscle mass and function loss in comparison to the control group

because HiRIT training will be an effective way to maintain muscular mass in peri and early menopausal females.

Methodology:

- 40 random people are selected
  - 20 are placed in a control group, and 20 are put in an intervention group
    - The control group does not change anything in their day-to-day life for the experimental period
    - The intervention group is put into HiRIT training
      - Phase 1: taught basic techniques
      - Phase 2: using actual weights
      - Phase 3: increase weights
- 6 tests are conducted before and after the experimental period
  - 6 minute walk test (25m course)
  - Force plate jump test
  - Hand grip test
  - Four square test (balance)
  - Biodex is used to measure muscle power

### Significance:

- Examine exercise effects on menopausal muscle health
- Demonstrate the benefits of exercise
- Fill research gaps on muscle loss
- First exercise program for menopausal muscle maintenance
- Contribution: provide data on HiRIT effectiveness for STOP-EM

Question:

- Was there a survey before the experiments began to see the test subjects' lifestyles?
  - They will be surveyed after the experiment is over to determine how they like the training and how they feel.
  - The project is almost over.

# November 13 - After School:

I sent emails to Dr. Karan confirming our meetings.

- See email communication for November 13th

# November 13 - Meeting with Mentor:

During this meeting with my mentor, we briefly talked about upcoming events.

- I told him that my oral presentation went well and told him about some of the questions I was asked and how I responded to them.
- He told me that a better explanation as to why the solvent ratio is being changed is that.
  - Some studies have looked at different types of solvents, and the ratio is the easiest thing to change.
  - Changing other components is a lot more complicated.
  - Water and alcohol are plentiful, so there is no fear of depleting resources when changing the water-alcohol ratio in the solvent.
- I asked him about how collecting and analyzing data would work for the rest of my project
  - Dr. Karan said that he would need to figure out how to get me permission to work in the lab.
  - He will be talking to a colleague who has already had a high-school student working in the lab to see how she did it.
  - I can come into the lab just to see everything (without doing any work).
- We have set up a time for me to go into the lab
  - November 18th at 4:30 p.m.
  - Meet in Engineering G-block room 330

# November 15 - Class Time:

- Read Intro to Effect of Catalyst Ink Properties on the Performance of Proton Exchange Membrane Fuel Cell and Water Electrolyzer: A Mini Review
  - See background research for November 15
- Read the conclusion to Effect of Catalyst Ink Properties on the Performance of Proton Exchange Membrane Fuel Cell and Water Electrolyzer: A Mini Review.
  - <u>See background research for November 15</u>
- Summary notes Intro to Effect of Catalyst Ink Properties on the Performance of Proton Exchange Membrane Fuel Cell and Water Electrolyzer: A Mini Review.
  - <u>See background research summary notes for November 15</u>
- Summary notes conclusion to *Effect of Catalyst Ink Properties on the Performance*

of Proton Exchange Membrane Fuel Cell and Water Electrolyzer: A Mini Review

See background research summary notes for November 15

# November 18 - Meeting with Mentor:

During this meeting with my mentor, I went to the University of Calgary and looked around the lab for the first time since the summer.

- Dr. Karan introduced me to the graduate student who is working on the project that I am researching.
  - The graduate student's name is Vahid Mazinani.
- Vahid showed me the apparatus used to coat the ink on the substrate.
  - The entire apparatus is cleaned with alcohol.
  - Another tool is placed on top of the apparatus, and the ink is then poured over it.
  - Once the apparatus is turned on, it pushes the tool across the surface of the machine, spreading the catalyst layer into a uniform layer.
  - The ink Vahid was using to show me had been made a year prior and was not a good example of a suitable catalyst ink because all the particles within the ink had dispersed again, creating a non-uniform CI.
- Vahid then showed me examples of catalyst layers that have been made from good ink and dried out to form the CL properly.
- I was then shown how to test the conductivity of the formed catalyst layer.
  - A smaller tool with probes is connected to a machine that can test the layer's electrical conductivity.
  - When the probes touch the CL, it begins to read its ability to conduct electricity.
- Vahid then showed me how he had begun to collect data.
  - He uses many graphs to show the relationship between different properties and the different ratios of alcohol and water in the solvent.
- He has already begun to test different ratios of solvent
  - He changes each test with a 5% difference in water
  - For example
    - Test 1: 5% water, 95% alcohol
    - Test 2: 10% water, 90% alcohol
  - He runs each test with multiple trials to take the average of the data for the most accurate results





















## November 19 - Class Time:

- ☑ Email meeting summary to mentor
  - See email communication for November 19th
- ✓ CYSF Ethics
  - Purpose: This experiment aims to determine the optimum ratio of isopropyl alcohol to water in the solvent used to make the catalyst ink in PEMFCs.
  - Description:

This study explores how changing the ratios of isopropyl alcohol (IPA) and water in the catalyst ink solvent impacts the catalyst ink composition and the performance and durability of proton-exchange membrane fuel cells (PEMFCs). Specifically, it studies how varying ratios of IPA affect catalyst ink properties (viscosity, aggregate size) and catalyst layer properties (pore size, ionic resistance, electronic resistance).

The experiment involves preparing catalyst inks with different solvent compositions and analyzing their physical properties using techniques such as dynamic light scattering. Catalyst layers will be fabricated from these inks and its properties are characterized using BET analysis to measure pore size distribution, four-point probe testing to measure electrical resistance, and cyclic voltammeter for ionomer coverage. This research aims to identify the optimal ink ratio that enhances PEMFC performance for commercial applications.

No human or animal subjects are involved in this study. Proper safety measures are in place for handling chemicals and operating lab equipment. All chemicals are handled appropriately according to the material safety data sheet (MSDS).

- Location: All experiments will be taking place in the lab in the Department of Chemical and Petroleum Engineering at the University of Calgary
- ☑ <del>Watch oral presentations</del>

#### Amber

Changes in the cellular and molecular mechanisms of perturbed genes underlying sevoflurane-induced learning and memory deficits in rats.

Simplified: Does sevoflurane cause changes in genes that affect the learning and memory of rats?

- Paths called synapsis that allow neurons to communicate with each other.

#### Sevoflurane:

- A volatile anesthetic
- Began to be used in the early 1990s
- Gained acceptance as a reliable anesthetic because it is easily administrable and diverse
- Can lead to lifelong changes
- If the sevoflurane blocks synapsis, it can mess with cognitive abilities.
- It is generally safe to use on developed individuals
  - There is very little that is known about the effects of sevoflurane on developing individuals
- The exposure of sevoflurane was shown to have effects on the cognitive abilities of rats

#### Controls:

- Saline
- Dex reduces the neurotoxic effects of sevoflurane

#### Manipulated variable:

- Sevoflurane 3.2%
- Sevoflurane + dex 3.2%

#### Research question:

- Does neonatal sevoflurane exposure alter the cellular and molecular mechanisms of the rats?

#### **Objectives:**

- Use western blotting to decipher between proteins

- Isolate the proteins
- Analyze TBR1, PLP1, and ALDH1A1 proteins

Manipulated variable:

- Exposure to sevoflurane and dex

Responding variable:

- Cognitive effects
- Changes in cellular and mechanical mechanisms

#### Controlled variables:

- State of the rat before (gender, age, overall health, environment raised)

#### Methods:

- The rats are exposed to sevoflurane from a young age
- Their brains are cryopreserved
- Cryosectioning is used to slice the brain into small sections
- The genes are then analyzed to see changes

#### Importance:

- See the effect of sevoflurane on the production of proteins
  - All the proteins are essential in cognitive and motor functions, forming and maintaining myelin sheath, and the development of cells.

#### Significance:

- Understand the molecular altercations underlying cognitive impairments
- Impact the scientific understanding of sevoflurane-induced neurotoxicity
- Develop strategies to prevent molecular changes
- Refine anesthetic protocols and improve the safety of all anesthetics for all demographics.

#### Question:

- Can you explain what the four corners on the grid signify?
  - The red parts are the areas that the rats spent the most time in
  - The dark areas are the least traveled areas
  - The test was to see if sevoflurane affected a rat's desire to move around

- Overtime the sevoflurane made them dormant

#### Maddux and Merrit:

Investigating hemodynamics in postural orthostatic tachycardia syndrome (POTS) patients under stimulated gravitation stress from lower body negative pressure capsule (LBNP)

Simplified: investigating the circulatory system's response in POTS patients under simulated gravity stress caused by LBNP.

#### POTS:

- A chronic condition that causes abnormal heart rate and blood movement
- Only occurs when standing upright
- Within 10 minutes of standing, their heartbeat increases by 30 BPM without changes in blood pressure.

#### Blood pooling:

- In normal humans, blood pools when you stand up, causing your heart rate and blood pressure to change
- The baroreceptors that control this are impaired in POTS patients, so when they stand up, their blood doesn't circulate properly.

#### LBNP:

- A capsule that goes around the lower body creates a vacuum, so there is no pressure on your legs.
- Since there is no pressure on your legs, your blood pressure decreases because it does not have anything to push back against.
- Bernoulli's principle fluids flow from areas of high pressure to areas of low pressure.

#### Head-upright tilt test:

- Strapped down on a table that can tilt up to 90°
- It is tilted about 70° in POTS patients
- When tilted upright, POTS patients' blood pools in their legs, which is what happens when they stand upright.
- Measurements are taken within 10 minutes of standing
  - Heart rate

- Blood pressure

Research question:

- What is the difference in hemodynamic response and controls during the tilt test and LBNP?
- What is the difference in the results of autonomic function testing during LBNP and while recumbent?

#### Hypothesis:

- The difference will be comparable to POTS patients' standing vs. recumbent

Variables:

- MV:
  - LBNP or tilt test
  - LBNP or supine (laying down flat)
- RV:
  - Heart rate
  - Stroke volume
- CV:
  - Severity of pots
  - Degree of tilt
  - Physiology of patients
  - Matching controls within test subjects

#### Measuring:

- Heart rate
- Blood pressure
- Stroke volume
- Cardiac output
- Vascular resistance
- Transcranial doppler entrance of brain from heart
- Oximeter a measure of oxygen in the blood
- Blood cuff measures blood pressure
- SV = EDV ES

Valsalva maneuver:

- Used to test autonomic function and baroreflex response
- Have to blow on closed airways
- 1. Onset of strain
  - BP up
  - Compressed lung vessels
  - HR down
- 2. Continual strain
  - Phase 1
    - BP down
    - HR up
  - Phase 2
    - BP up in non-POTS patients
    - HR up
- 3. Release
  - BP down
  - Release in pressure
- 4. Recovery
  - Bp up
  - SV up

Hyperventilation test:

- BP change of 30 seconds
- HR goes up slightly
  - BP goes down
  - Exaggerated values and lower PT on POTS

Sinus Arrhythmia:

- Deep breathing
  - In HR up
  - Out HR down
- Peak vs. nadir

Short-term objectives:

- Tilt test vs. LBNP
- LBNP vs. recumbent

Long-term objectives:

- Better understanding of POTS
- Cardiac MRIs are not helpful now because symptoms are only present when POTS patients are standing.

Methods:

- 1a:
  - Pots patients from the Calgary Autonomic Lab
  - Matching healthy controls
    - Off medication
- 2a:
  - Hooked up to devices listed above
- 3a:
  - Measure HR, SV, BP, CO, and SVR over the course of 10 minutes
    - LBNP
    - Tilt test
    - Shapiro Wilk
    - t-Test
- 1b:
  - Same as 1a and 2a
- 2b:
  - Asked to perform
    - Valsalva maneuver
    - Hyperventilation
    - Sinus arrhythmia
  - During
    - LBNP
    - Laying down
- 3b:
- Measuring HR, SV, BP, CO, SVR over the course of 10 minutes
  - LBNP
  - Laying down
  - Shapiro Wilk
  - T-test

#### Significance:

- Easy to be misdiagnosed

- 75% misdiagnosis rate  $\rightarrow$  there are many symptoms that overlap with other conditions
- Affects a large population
  - About 1% of the North American population
- Cardiac MRIs
  - Properly simulate

#### Question:

- What is the Shapiro-Wilk test?
  - Taking data and test if the data fits the normal standard of distribution curve
- ✓ Next class
  - Dr. Garcia won't be here
  - Work period
- ✓ Full class discussion
  - References
    - Add a library of used papers to PaperPile
    - When adding citations, find article DOIs
    - Format citations properly
    - AMA vs. APA
      - AMA starts with one and puts superscripts in chronological order. All references are placed chronologically.
      - APA is organized alphabetically and uses brackets, authors, and year of publication
    - Every citation has to have either a DOI or URL
      - Must be turned on PaperPile to include citations with DOIs and URLs
  - Number of sources
    - 5-7: you have to do more reading
    - 30+: this is a lot of sources, so go back through the paper and ensure all citations are in the reference list.
  - Have a long-range plan
  - Have a weekly plan

## November 21 - Class Time:

My CYSF ethics form was approved.

#### ✓ CYSF Portal

- ✓ Hypothesis:
  - <u>See experimental procedure for November 21st.</u>
- ✓ <del>Variables:</del>
  - <u>See experimental procedure for November 21st.</u>
- ✓ Procedure:
  - <u>See experimental procedure for November 21st.</u>

## November 25 - Class Time

- Midterms start on January 10
- We have a study break until Jan 20.
- Meeting with mentors this week and next
- Plan for this week and next
- Create a long-range plan for dec-jan-feb
- Go through the written proposal and oral proposal and make edits
  - <u>See ASP Research Proposal | Antara Krishnamurty</u>
  - <u>See Designing High-Performance PEMFC Electrodes by Optimizing Catalyst</u> <u>Ink Composition</u>
- ☑ Biweekly meeting with Dr. Gacia
  - Review the meetings I had with my mentor previously
  - Plan for when data will be collected
  - Plan for December, January, February
  - Ask mentor what else I should be reading
  - For background
    - What catalysts are being used in different transportation?
    - What are the ratios being used currently?
    - Applications?
    - Best ratio right now?
    - More information on the *now* of transport
    - What stage are we in?
    - Is there field data?
    - More information on why certain alcohols are used

## November 25 - Meeting with Mentor:

- I can maybe assist with some experiments if I get lab clearance.
- I can analyze data.
- Coordinate with Vahid (Graduate student)
- I filled Dr. Karan in on the things I saw at the lab with Vahid.
- He will be coordinating with Vahid on my behalf to figure out dates for when I can come to the lab.
- UofC opens on January 2nd or 3rd from winter break, so I may be able to go there then.
- Figure out how much data I would need.
  - Vahid is writing a thesis, so a lot more data is required.
- Connect with Vahid to figure out specifically what days and times I can go to the lab.
- What is the substrate made of?
  - A Teflon-like sheet

# November 27 - Class Time:

- ☑ Work on the CYSF Portal
  - ✓ Edits to variables
    - See experimental procedure for November 27th.
  - Edits to procedure (I can't switch the citation to APA because my Paperpile is not working at the moment)
    - <u>See experimental procedure for November 27th.</u>
  - Research (Again, I cannot add proper citations because my Paperpile is not working)
    - See background research for November 27th.

## November 28 - After School:

I sent Dr. Karan an email with a list of all the papers I have read and asked if there are any more I should read.

See email communication for November 28th.

## November 29 - Class Time:

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- ☑ Email meeting reminder to mentor
  - See email communication for November 29th
- ☑ Try Paperpile again (change citations to APA for CYSF)
  - I am still unable to get Paperpile to work. It keeps saying that it is analyzing my document without making any progress.
  - I have tried to shut down my computer and try again, but that did not work.
- ☑ Read over CYSF portal sections (specifically the research section)
  - I re-read the sections to the CYSF portal to ensure everything was grammatically correct.
  - I am not able to properly cite the sources using APA on the CYSF portal because Paperpile is not working for me right now, and I have no other way of changing all the IEEE citations to APA.
- ☑ Work on the December calendar
  - See the calendar for December

# **December Daily Notes**

# **December 02 - Spare/After school:**

- My Paperpile is still not working for Google Docs, so I have downloaded Paperpile for Microsoft Word.
- Copy-pasting the research proposal from Google Docs into Microsoft Word does not copy the Paperpile citations, so I will have to go through them again to get the citations working on Word.

# **December 02 - Meeting with Mentor:**

- My mentor has told me that he met with Vahid this afternoon and has discussed what my future with the research is going to look like.
- I will be connecting with Vahid over email to schedule times to come into the lab.
- The things I will be able to see in the lab depend on what is happening on any given day/time.
- For data, only selective pieces of data will be shared with me due to the large amount of data being collected.
- Dr. Karan will be sending additional papers for me to read.

## December 03 - Class Time:

We did not have class today due to President's Breakfast

# **December 04 - Spare:**

- During this spare, I sent a quick email to my mentor asking about papers to read and how to get into contact with Vahid.
  - <u>See email communication for December 04th.</u>

# **December 05 - Class Time:**

☑ Full Class Discussions

- Intro section to the final paper is due on January 31st
  - Spent time reading
  - This section contains most of the same information as the background research section of the research proposal.
    - Improve the section
    - Make sure everything flows well
    - Add more depth to what you have already written
  - It is due 10 days after midterms end, so consider starting now.
- Methods/Procedures section of the final paper is due on February 19th
  - This section needs to be extremely technical and thorough
  - Take notes in your logbook of what is happening in the lab
    - May want to create a methods section in the logbook to make it easier to find information collected.
  - Add more details to the methodology that was written for the research proposal
  - Watch your language when talking about equipment
    - When talking about equipment, describe it (model, manufacturer, place of origin). The same applies to reagents (ex. antibodies)
  - Software formatting:
    - Exel<sup>TM</sup> (Exel 2021)
    - Software (software version)
  - Examples
    - Image J (citation) was utilized to graph....
    - Membranes were incubated at 37°C under continuous shaking using an orbital shaker (model, manufacturer, city/country)
    - Brain slices were visualized under a fluorescent microscope (Nikon TS250, Nikon, Newport, CA)
    - Antibody Rabbit Ig [ ] was mixed with the brain tissue at a 1:5 molar ratio
  - Write in past perfect tense or present perfect tense
  - Do not use personal pronouns
- Biweekly Meeting with Dr. Garcia
  - Don't write the theory in the methods section
    - Only write what is happening and be able to explain the theory behind it

- Read more about why fuel cells are used in certain applications over others.
- Add research question and objectives to the end of the intro
- Variables should be added to the end of the methodology section
  - CORRECTION: Should be added to the start. Depends on how you want to structure the section, but the variables are explained with the design of the experiment usually.
- ✓ Paperpile
  - I finally got Paperpile to format my Google Docs properly.
    - In order to get it working, I deleted every other Google profile I have on my computer, then restarted my computer in order to get Paperpile to restart.
    - After restarting my computer, Paperpile was working again.
  - I reformatted my <u>original research proposal document</u> to include the new citations I added in IEEE style.
  - I reformatted the <u>research proposal for the CYSF portal document</u> to be in APA style so citations can be seen in the portal.
- Update CYSF portal
  - I updated my CYSF portal to have the research and procedure written with APA citations.
  - <u>See background research for December 5th for the research section.</u>
  - <u>See experimental procedure for December 5th for the procedure section</u>

# December 09 - Class Time:

I was not in class today because I was out of town.

# **December 09 - Meeting with Mentor:**

- During this meeting, my mentor and I discussed my coming into the lab in the coming weeks in order to take a look at how the experiments are running.
- He will be reaching out to Vahid and connecting me with him over email in the next few days so I can coordinate with him.
- Dr. Karan will be sending additional papers for me to read soon.
- Dr. Karan has been particularly busy this week because he is finishing making a final.

# **December 11 - Class Time:**

✓ Full class discussion

Have a meeting with your mentor in the next week to check in.

Have a meeting on Jan 3-9 to check in with a summary of results, project status, inform of midterm schedule (don't put too many meetings during this time), and next meeting after midterm.

I sent an email to my mentor to ask about the next steps of my project.

See email communication for December 11th.

I was not able to get much work done for ASP during this class time as my mentor has not sent me any papers to read, and I have no data to collect/analyze.

I looked over Dr. Garcia's previous feedback on my introduction section so I could think about areas of improvement and things to add to the final draft.

- What catalysts are being used in different sectors of transportation?
- What are the current ratios of ionomer : solvent being used currently?
- What is the best ratio of ionomer : solvent at the moment?
- Add more information about the transportation sector *now*
- Is there any field data that can be added?
- Add more information about why certain alcohols are used.

I used what was left of class time to study for upcoming exams at school.

# December 13 - Class Time:

Once again, I did not have much work to get done for ASP because I had no papers or data to collect and analyze. Dr. Karan has not been able to get in contact with Vahid to arrange a meeting.

I sent a quick email to Dr. Karan, reminding him of our upcoming meeting on Monday.

I spent most of this class studying for my upcoming exams in other classes, such as biology and chemistry.

## **December 16 - Morning:**

I sent a quick email to Dr. Karan asking about scheduling a meeting with Vahid.

See email communication for December 16th.

# **December 16 - Meeting with Mentor:**

During this meeting with my mentor, we discussed the next steps of my project.

- We discussed my setting up meetings with Vahid before winter break begins at both the University of Calgary and Webber.
- Dr. Karan and I discussed some dates that are important in the upcoming weeks.
  - Winter break at the university begins on December 21st.
  - Winter break at Webber begins on December 21st.
  - Winter break ends at the university on January 2nd.
  - Winter break ends at Webber on January 6th.
  - Midterm break begins at Webber on January 10th.
  - Midterm break ends at Webber on January 20th.

# **December 16 - After School:**

Dr. Karan, Vahid, and I emailed back and forth about planning an upcoming in-person meeting at the university.

- <u>See email communication for December 16th.</u>

# **December 17 - Class Time:**

During this class, I spent time preparing for my upcoming trip to the lab at the University of Calgary with Vahid, the graduate student Dr. Kraan arranged for me to work with.

- I went through the notes I took on my background research to make sure that I had all the information fresh in my head before going to the lab.
  - <u>See the background research summary notes section of the logbook</u>
- I used my background research to help me figure out areas that I needed to review the most so I could go to the meeting with enough knowledge to

understand everything Vahid told me.

- In doing this, I felt much more prepared for my upcoming meeting.
- ☑ Biweekly meeting with Dr. Garcia
  - During this meeting, I just told Dr. Garcia about how I have a meeting scheduled with the graduate student my mentor has me working with.
  - I told her that I will be trying to get data soon so I can start the analysis portion of my project.

# December 19 - Class Time:

This was our last class before winter break.

Dr. Garcia made us all cookies as a treat for our hard work thus far and before the start of our winter break.

I did not have much work to get done for ASP at the moment because I had no papers to read/annotate or data to collect and analyze. I spent this class studying for my upcoming biology and math tests.

Towards the end of class, I, along with some other people, were tired and not able to focus on our work, so we played some card games for a little break.

# December 20 - Meeting at Lab:

I went to the University of Calgary to meet with the graduate student Dr. Karan set me up with.

- Vahid has been conducting experiments with different ratios of water to IPA (10%, 20%... to 90%)
- The higher the concentration of water, the more clumped together the ionomer is
- The higher the concentration of IPA, the more dispersed together the ionomer is.
- The concentration of water vs IPA forms different structures of all the deposited things.
- An initial dispersion is made of carbon and polymers and is added to the dispersion media (water + IPA)
- You can't see anything in the dispersion
- Once deposited, microscopy can be used to see what's going on.
- In the dispersion, visually all are the same but using instruments, particle size and

other properties can be seen.

- 10% water has smaller particle sizes. Increase size, increase particle size.
  - It is not a direct increase in particle size.
  - It is more complex than just looking at one substance.
  - The mix of substances makes it difficult to have a linear relationship.
- Dynamic light scattering is the instrument used for finding particle size.
  - Reflects light through the dispersion and the instrument gives particle size.
  - For example, at 50% the size is 550nm particle size on average (90% of the whole dispersion) some may be smaller or larger.
- He plots everything to find the information
- Electrical conductivity can be measured using a four-probe tool.
  - Put the probes on the dispersion and find the conductivity
  - Using a formula
    - thickness/RA
    - Thickness measured with calipers
    - Resistance using the device
    - Area is just the area of the sample size
- A certain dispersion (ratio) is deposited then dried for an hour in an over and once dried, electrical conductivity can be measured.
- There is a lot going on in a CL
  - There are carbon, catalysts, ionomers
- All carbon layers = better conductivity
- The structure is slightly different for every layer
- Depending on how the water and IPA evaporate, the structure also is different.
- Dispersion  $\rightarrow$  deposition  $\rightarrow$  evaporation  $\rightarrow$  oven
- Story
  - How is the dispersion made? From what materials (ionomer, carbon, dispersion media)?
  - How do different structures form?
  - What is done with the dispersion?
    - Particle size is the only thing that can be found from instruments in lab using dynamic light scattering (DLS)
    - Explain how DLS works
      - Light goes through
      - Reflected
      - Lots of information online about it
      - Show how the data is collected

- How is sample is prepared?
- How is electrical conductivity found?
- Go through characterisation
- What plot you get and how to extract data?
- Electrical conductivity is a result of the structure formed
- He will be talking to Dr. Karan about sending me data for my project.











# **January Daily Notes**

## January 06 - Morning:

I sent a quick email to Dr. Karan asking if we would still be meeting today as both of us were getting back to school/teaching after a break.

- <u>See email communication for January 6th.</u>

## January 06 - Class Time:

This was our first class back after winter break.

Dr. Garica gave us this period to study for our upcoming midterm exams.

## January 8 - Class Time:

During this class, Dr. Garcia gave us the period to study for our upcoming midterm exams.

## January 10 - Class Time:

No class due to exam break

## January 14 - Class Time:

No class due to exam break

## January 16 - Class Time:

No class due to exam break

### January 19 - At Home:

I sent an email to Dr. Karan asking if he is available to meet tomorrow.

- See email communication for January 19th.

## January 20 - Class Time:

No class due to exam break

## January 20 - Meeting with mentor:

During this meeting, my mentor and I discussed the next stages of my project.

- My mentor will be asking Vahid (a grad student) to share some of his experiment's results with me.
- My mentor will be finding papers that are pertinent to my research and/or related to the results that Vahid has collected.
- We went over all of the important upcoming deadlines for my project.
  - January 30: the introduction section of the final paper is due
  - February 19: the procedures section of the final paper is due
  - March 11: this is the date of the in-school science fair
  - March 21: the results section of the final paper is due
  - April 25: the discussions and conclusions section of the final paper is due
  - May 28: the final paper is due
- I told my mentor that I would be asking Dr. Garcia what section of the final paper should include the hypothesis and variable to send that information to him.

## January 22 - Morning:

I sent an email to my mentor summarizing the information we went over in our last meeting and reminding him to ask Vahid to send me any data possible and papers.

See email communication for January 22nd.

# January 22 - Class Time:

- ✓ Full class discussion (all class)
  - ☑ Make a plan for the remaining time to science fair (six weeks) and be

<del>specific about it</del>

- Reconnect with mentor
  - Set up a meeting/meet with mentor
  - Suggest times + agenda items
- We have the next six weeks to get our projects done for the in-school science fair.
- It is important that we dedicate a lot of free time to ASP (no more time to waste)
- Don't focus on writing the introduction section of the paper, focus on getting data analyzed for (prioritize things to do)
- Submit the literature review to Turnitin and the CYSF portal
- Start entering information into the CYSF portal because it takes a while for all that information to be entered.
  - The CYSF portal is not used for the school science fair on March 11th, but it must be done by **March 21st.**
- Prioritize the poster over the portal for the in-school science fair
  - No one is looking at the portal for the school science fair, but if you are selected for cities, put some extra effort into the portal.
  - The portal may not be used for the city science fair, however, still make sure to do a good job because the judges may use the portal to preview your project and formulate questions before coming to see you.
- The date of the city science fair is right after spring break (April 10-12)
- Make sure you understand the methodology thoroughly
  - Be able to explain this both technically and simply
- Copy-paste all information straight into the portal from writing (don't waste time re-typing or changing stuff)
- For the science fair poster, it is easiest to shorten your background research on the trifold because it can easily be explained orally.
- ☑ Introduction section
  - Finish the introduction section with your research question, hypothesis, and goals at the end.
  - The introduction should flow into the hypothesis and what we are hoping to achieve with the project.
  - Don't need to send this back to your mentor because you already have feedback from the research proposal
    - Make changes based on previous feedback

- ✓ Poster
  - We get to decide what kind of poster we want to use. We will be provided with large tri-folds (60" tall, middle panel 32" wide, side panels 31.5"), but we can choose to create our own.
  - The amount of background information for the poster will depend on how much space you have an how much information you have for other sections.
  - Show Dr. Garcia BEFORE gluing anything down onto the poster.
  - We can plan out our poster on a PowerPoint and show it to Dr. Garcia before printing everything out and sticking it on the poster
- ☑ Poster vs. Powerpoint presentation
  - The physical poster is different from the PowerPoint presentation we will be giving in class prior to the science fair.
  - If you have your poster ready for the presentation, feel free to present with it.
  - Advantages of using the poster in class:
    - It will help prepare you for the science fair
    - It will be exactly like the science fair, and the feedback will be directly applicable to the science fair
  - Disadvantages of using the poster in class:
    - You may be in a rush to get your poster done for class
    - You can't glue stuff down to the poster YET because things might have to be changed after getting feedback from Dr. Garcia.
  - Disadvantages of using a PowerPoint in class:
    - It won't be the same as the actual science fair poster
    - On a PowerPoint, you may be able to fit more information than you can fit on a poster.
    - Images or graphs will not be the same on a poster as they are on screen (size/quality)
    - In a PowerPoint presentation, there won't be any interruptions in the middle, but there can be interruptions during an actual poster-presentation at the science fair.
  - The content will be very similar
- ✓ Presentations
  - Presentations will be between February 21 March 3

- ☑ Misc. information
  - HAVE to be done with data collection/analysis by February 21st.
  - What if you cannot finish your data collection in time for the science fair?
    - Do your best with the data you have
    - Present what you have until February 27th.
    - After February 27th, work on getting a good presentation together for the science fair based on what you have.
    - Present what you have really well, then present the rest of your project as what's going to happen in the future.
- ✓ Science fair
  - The science fair is big on knowing about changes and improvements
  - Changes and improvements are one of the biggest things being judged
    - What are the limitations of your project?
    - What had to be adapted and/or changed?
  - Originality is another big part of your project being judged
    - How do you show that this project is driven by you and your interest, not your mentor?
    - Why are you interested in this topic?
    - Is there a human connection?
    - Exploit your topic in a way that shows you have a connection/interest
  - Don't talk down your achievements, no one else is going to talk about how awesome your project is for you.
  - Show that your work is great and impressive.
  - Show how the background relates to what is being studied
  - Make sure to actually answer your research question
  - All graphs should have error bars
  - Review the rubric before finalizing the presentation (drop a lot of hints throughout your presentation for various categories)
  - End your presentation with the relevance of your project

Science fair rubric
<b>1. SCIENTIFIC METHOD (Choose only one category, 1A, 1E</b> Judge the project in <b>only one</b> of the following categories:	3 or 1C)	Please use the following scale:	
Experimental (1A), Innovation (1B), or Study (1C).	4 Good		
Please contact a member of the CYSF evaluations committee <b>before</b> judging if you have a choosing a category.	lifficulty	<ul> <li>3 Satisfactory</li> <li>2 Weak</li> <li>1 Poor</li> <li>0 Not Present</li> </ul>	
<b>1A. EXPERIMENTAL PROJECT</b> – an investigation undertaken to test a experimentation, usually featuring the identification and control of variables.	scientific hypot	hesis using	
PROBLEM / HYPOTHESIS			
1. Existing knowledge and background research were integrated into the formation of the problet 2. The hypothesis related to the problem, was clearly stated, and provided direction for the project of t	n/hypothesis	012345 012345	
METHOD	SUBTOTAL / 1	0	
<ol> <li>Experimental design was clearly described and appropriate for solving the problem.</li> <li>Controlled, manipulated and responding variables were identified and understood.</li> <li>Repetitions of tests and/or appropriate sample size were used to achieve reliable results.</li> <li>Logbook recorded progress of the project including detailed procedures, results and original detailed procedures.</li> </ol>	ata	0 1 2 3 4 5 0 1 2 3 4 5	
ANALYSIS / CONCLUSIONS	SUBTOTAL / 2		
<ol> <li>Appropriate methods were used to present and analyze data (e.g. graphs, charts and statistics).</li> <li>Sources of error and experimental limitations (e.g. the effect of variables that could not be con</li> <li>Conclusions were related to the problem/hypothesis and were supported by the data presented.</li> </ol>	trolled) were under	012345 rstood012345 012345	
	SUBTOTAL / 1	5	

2. CREATIVITY AND INSIGHT	
1. The problem was approached with originality	
2. Independent motivation, design and thinking were demonstrated.	
3. Resourceful use of equipment and/or materials was shown.	
4. Improvements that can be made to the project were indicated.	
5. Practical applications and future research for the project were identified.	
SECTION	2 TOTAL / 25

3. COMMUNICATION	
1. The oral presentation was clear, logical and concise.       0 1 2 3 4 5         2. Answers to questions were clear and signified depth of understanding.       0 1 2 3 4 5         3. All required written information including credits, citations and applicable ethics/consent forms were presented.       0 1 2 3 4 5	
4. The visual display was effective, with a logical and self-explanatory layout	

#### 4. DEGREE OF DIFFICULTY

1. The project was exceptional (consider the student's grade level).       0 1 2 3 4 5         2. The student gained a deeper understanding of the topic.       0 1 2 3 4 5
SECTION 4 TOTAL / 10

#### 5. TOTAL SCORE

Add the scores from Sections 1 through 4 and record the final mark here.

TOTAL SCORE / 100 \_\_\_\_\_

## January 23 - Science Fair meeting:

- Make sure to excuse yourselves from all classes happening on the day as the science fair will be happening all day on March 11th (with a break during lunch)
- Posters
  - If you want to use the provided trifold, you can pick it up whenever you want.
  - Even if you don't use the trifold, make sure that your poster is able to stand up on its own.
- Portal
  - Be careful about plagiarism
    - Everything must be cited, quoted, in your original words, etc.
    - Use Turnitin first, then put it in the CYSF portal
  - Logbook
    - Find a way to put it into the portal
    - Since I am using a Google Doc, I may be able to copy and paste the document link to the CYSF portal.
- If you are not going to the CYSF, your portal will get deleted
- If you are going to the CYSF, make sure your portal is finished by March 21st.
- Due dates for science fair Turnitin:
  - Background research February 7th
  - Methods February 21st
  - Data collection/results + analysis/conclusion March 3rd
- Spend five weeks to finish data collection/results/analysis and the final week before the science fair on the poster.

## January 24 - Class Time:

☑ Biweekly meeting with Dr. Garcia

- Send another email to Dr. Karan saying
  - as we discussed during our last meeting, I am waiting for data from Vahid.
  - Our teacher has been insisting that we have to get started on analysis and I was wondering whether you had a chance to ask Vahid.
  - See email communication for January 24th.

- Start brainstorming your poster
  - What background research to keep on the poster
  - Howdo you want to lay out the information
  - Do you want to use the trifold or something else?
  - Figure out how much data you have to put on the poster, then decide what you want to use
    - The trifold may be too large for certain projects
      - You don't want to have too much blank spaces
  - You do not have to talk about everything on the posters
    - Just give the judges the main information about the poster
    - Don't overwhelm the poster with TOO MUCH information
  - Don't pack the poster with too much text/graphics
  - More is not necessarily better
- Intro paper
  - Make this your priority
  - Find the information you want to add and add it to the paper
- For the project
  - Don't just take the graphs from the graduate student
  - Go through data analysis with the grad student
  - Understand how it's done + what software is used
  - Understand the details of the process
  - Even if you know all the details of the experiment, you do not have to present everything.
- ✓ Update logbook
  - Prior to winter break, I fell behind on updating my logbook, so I spent the remainder of this class updating my logbook.

## January 26 - At Home:

- Update logbook
  - I finished all the updates to my logbook that I had not had time to finish during class on Friday.

## January 27 - Meeting with Mentor:

- Dr. Karan has met with Vahid

- He has asked Vahid to send me three sets of data, which are all a function of the solvent/dispersion media (five or six different rations)
- X-axis: ratio of water to IPA (isopropyl alcohol)
- Properties:
  - Size of the aggregates and ink found using dynamic light scattering (to find the average size of aggregates and how it varies)
  - Electrical resistance/conductivity
  - Pore size distribution/porosity  $\rightarrow$  important for gas phase transport
- Vahid will be sending the data to Dr. Karan first; then he will send it to me
- I will have to try and make sense of it
  - analyze/write about the trends and patterns I see
- After going through that, we will discuss what else to write about/my thoughts
- Dr. Karan has not yet had a chance to find papers about the data.
  - Will send me some after I get the data.

## January 28 - Class Time

☑ Full class discussion

- Add references to the end of the introduction section being handed in for class.
- There is a specific section in the portal for references
- Pay attention to where things are going in the portal because not all sections are the same for every project type.
- If you are going to the city science fair and you are being considered for a major award, they will scrutinize all the information you give.
  - Make sure you are being honest/ethical about every part of the project
  - There is nothing wrong with taking information from other sources just MAKE SURE TO CITE IT
- March 7th is our next report card
  - Marks lock about a week before (March 1st)
  - Marks added will be:
    - Feb logbook
    - Oral presentation in
  - The biggest portion of marks will come in the last term
    - Logbooks
    - Most of the papers

- Science fair performance
- ☑ February calendar
  - <u>See calendars for February</u>
- ✓ Introduction section
  - I started copying over the introduction section of my logbook into a new document.
    - <u>See background research for January 28th.</u>
- ☑ A quick chat with Dr. Garcia
  - At the end of the introduction section of the logbook, add the research question and objectives of the research.
  - The hypothesis can go into the introduction IF it connects to the RQ and objectives.
  - Variables should go with procedure/methodology.
  - I will be getting data from my mentor in the next couple of days.

## January 30 - Class Time:

🗹 <del>Data</del>

- Vahid sent me the data that I had discussed with Dr. Karan
- I emailed him to see if I could get any raw data points.
  - <u>See email communication for January 30th.</u>
- $\square$  Make sure the logbook is complete  $\rightarrow$  Due tomorrow
  - <u>See daily notes for December</u>
  - <u>See daily notes for January</u>
  - <u>See the calendar for December</u>
  - <u>See the calendar for January</u>
  - <u>See the calendar for February</u>
- ☑ Work on the introduction section of the final paper
  - See background research for January 30th.

# **February Daily Notes**

## February 03 - Class Time:

- ✓ Class Chats
  - February oral presentation schedule
    - I am set to present on February 25th
  - You can use AI to help find sources
    - Enter: find peer-reviewed sources to back up this statement: the statement you made
    - Then, you can just take a look at the main parts of the paper, and you have a peer-reviewed source for your paper to back up the information you are giving.
    - You are not using AI to summarize/do work for you; you are just asking for it to help *find* papers that back up your statements.
  - Put all the data that Vahid gave me into the data collection section of the logbook.

☑ Transcribe data from Vahid into the data collection section of logbook

- See data collection and results for February 3rd.
- ☑ Introduction section of the final paper
  - Figure out a way to incorporate the research question into the introduction section.
    - <u>See background research for February 3rd.</u>
- I did research for finding papers that will fill in any gaps in my background research. I haven't seen any papers that are good enough yet.

## February 03 - Communication with Grad Student

Vahid sent me another file with raw data points.

- <u>See email communication for February 3rd.</u>

## February 05 - Class Time:

Biweekly meeting with Dr. Garcia

- I will be graphing the data I was given
  - Compare the graph made with graduate student's graphs
  - The data I was given is likely average, so I can't do error calculations or standard deviation with what I have at the moment
  - Email Vahid the preliminary graphs and ask for full, unaveraged data in order to get error/standard deviation bars.
- Use Excel to graph data.
  - Excel and Google Sheets are both good. However, Excel has more functions that are helpful for graphing data.
  - Dr. Garcia will help me create the error/standard deviation bars after I get that data.
- Ask graduate student about methods
  - Set up a time to go to the lab and discuss in length
  - How were the different properties measured?
  - How many trials were conducted of each ratio?
  - Was the data averaged out?
  - How was the data graphed?
  - How were the error bars and standard deviations calculated?
- Get data done first before asking about methods.
- ☑ Finish edits to the introduction section + hand into Sci Fair TurnItIn and ASP TurnItIn
  - <u>See background research for February 5th.</u>
- ☑ Take the data that Vahid gave me and make my own graphs.
  - See data collection and results for February 5th.
- Email Vahid asking for un-averaged data so I can add error/standard deviation bars + email asking to schedule a time we can meet to
  - See email communication for February 5th.

## February 07 - Class Time:

- ✓ Full Class Discussion
  - Our logbook quality has significantly declined since our last check.
    - We have to be more specific with our tasks.
    - The experimental procedure section and data collection sections should have some information already.
  - We discussed changing the dates of our oral presentation, and the options were as follows

- 1: move all the oral presentations up to start on Feb 21st.
- 2: move all the oral presentations back so they are marked after report cards
- 3: keep the oral presentations starting on Feb 25th but cram oral presentations in so all eleven are finished in two days.
- We voted and decided on option 3.
  - I am still presenting on Feb 25th.
- Re-plan February to get work done
  - What happens every week? When are you working on your poster?
- Oral presentations
  - For the science fair, the oral presentations should be under fifteen minutes, but around twelve minutes is fine.
- Portal
  - Start plugging in information everywhere you can
  - It does not have to be done, but fill in anything you can
  - PLAN IT OUT
- Science Fair
  - TELL YOUR CLASS TEACHERS THAT YOU WILL BE MISSING ALL DAY FOR THE SCIENCE FAIR
  - Tell teachers before class starts.
  - During breaks in judging, we are allowed to go look at other people's posters.
  - Pack some kind of lunch that you can eat in the PAC  $\rightarrow$  probably won't have time to go get lunch from the cafeteria.
- $\square$  Procedure section of the final paper  $\rightarrow$  hypothesis and variables paragraph
  - See experimental procedure for February 7th.
- $\square$  Data analysis  $\rightarrow$  understand trends in the patterns
  - See data collection and results for February 7th.

### February 09 - Weekend:

- ☑ Vahid and I coordinated a time for me to come to the lab to go over methodology
  - <u>See email communication for February 09th</u>

## February 10 - Spare:

- ☑ <del>Vahid confirmed our meeting time</del>
  - See email communication for February 10th.
- ☑ I finished understanding the trends in the data patterns
  - See data collection and results for February 10th.
- ✓ Speak to Dr. Garcia
  - Ask the mentor if he has unaveraged data today during your meeting.
    - If he can't help, bring it up with the grad student tomorrow when you meet.

## February 10 - Meeting with Mentor:

- I started the meeting by getting Dr. Karan up to date on everything that I have done thus far
  - Got data from Vahid and plotted it
  - Analyzed the trends
  - Finished the introduction section of the final paper
  - Started to write the procedures section of the final paper
- There is no obvious trend in any of the data
  - This tells us that the data is much more complicated than just the ratio of IPA to water
  - He told me not to be perturbed by the fact that there is not a clear pattern in the data
  - One parameter affects multiple structural properties of a PEMFC
    - This can be a conclusion that you don't see an obvious pattern
    - There are no "simple trends"
  - Plot properties as a function of other properties
    - Some trends may be seen
- We will be skipping next Monday's meeting
  - It is family day, and I will be traveling

## February 11 - Class Time:

Most of this class was missed due to an assembly

- ✓ Class discussion
  - Fill out portals

- Submit on Turnitin
- Copy Dr. Garcia on emails
- Send email summaries if you said you would.
- You WILL BE ready for the science fair presentation
  - There is no buffer
- If you want feedback on slides/presentation before presenting
  - Be done a week before a week before the presentation and send it to Dr. Garcia
  - You can arrange a time to present
- The methods section is NON-NEGOTIABLE HARD DEADLINE FEBRUARY 19TH

### I did not get as much done as listed in my calendar because of the assembly.

## February 11 - Meeting with Vahid @ the University of Calgary:

- Dynamic Light Scattering
  - Use a diluted sample of ink
  - If the particle is smaller, it moves faster. The same is true vice versa.
  - Add up all the different values on a bell curve for the particle size
  - Watch this video for more information about how it works.
    - https://www.youtube.com/watch?v=ET6S03GeMKE
- Electrical conductivity
  - The Loresta-gx mcp-t700 is the 4-probe resistance tool
  - A two-probe multimeter is how the data is collected
  - Cut a small sample (2cmx5cm) of the deposited catalyst layer
  - The area and the thickness of this sample are important to measure
  - The multimeter measures the electrical resistance of the sample
  - Place the sample layer face down on copper strips, which conduct electricity, then place the two probes on either strip of copper to measure the electrical resistance.
  - Test the electrical resistance of the sample three times
  - Use Ohm's law to calculate the conductivity of the sample
  - Measure the thickness of the sample
    - The Teflon the ink lays on is 52 microns
    - Measure the thickness of the Teflon plus the catalyst layer using calipers

- Subtract 52 from the measured value to find the thickness of the catalyst layer.
- The electrical conductivity is dependent on the thickness of the sample
  - A thicker layer has lower conductivity
  - According to the data, as thickness increases, conductivity decreases
- \*All the data I have is for a 12-micron sample
- Take the thickness at different points because the sample may not be perfectly even (a good sample should be even)
- Follow the same process for different cut samples of the same deposited catalyst layer (three times)
- The bigger rotator of the calipers is for precise tuning, and the smaller rotator is for rough tuning to get a precise measurement.
- Average pore width
  - Scratch a deposited layer to get 100g of powder, and another lab has the instruments to calculate the width
  - The sample is first degassed.
  - Using BET absorption, the other lab measures how much nitrogen the sample can absorb (porosity)
  - The number that comes from the instrument calculates the pore width and surface area.
- Error bars for dynamic light scattering
  - Vahid took three samples
  - He calculated the averages of each one (area under the curve)
  - After having three samples, he used the error bar formula to calculate this (I have to Google this to figure out more information as Vahid does not remember this formula off the top of his head)
- Have error bars for DLS
- For electrical conductivity, he just found the conductivity of three samples and averaged it out.
  - We did water 60% together.



## February 13 - Class Time:

✓ Class Discussion

- Make sure to fill out the CYSF portal
  - If you have a problem section (only if you're doing a study)
    - Write a super short version of the background
    - Explain the problem
    - It can't just be one tiny paragraph
    - Must explain the problem

- If you are doing an experimental project
  - Your methods cannot be two paragraphs
    - Have a good explanation of your methods
    - Must have citations because you are doing things the way someone else has already done it
      - This test was conducted according to [source]. Briefly.....
    - Use sources that your mentor has used if available
  - Observation is data collection
    - Unmanipulated, unprocessed data
  - Analysis
    - Final graphs, final tables
    - Paragraphs explaining those graphs
  - Conclusions
    - Answer your research question
    - Objectives and conclusion have to go together
      - HAVE YOU PROVEN IT OR NOT
        - The data supports....
        - The data does not support... but this is observable...
        - If it did not come true, explain how you are going to continue the project with a modified hypothesis.
    - Application
      - Significance of your project
        - Why is this important?
        - How did your project help further something?
    - Sources of Error
      - Science fair loves this
      - Find limitations within your project
      - Things you did not think about before
      - Things that may be confounding your results
    - Acknowledgments
      - Not heartfelt messages
      - UofC/Department of....
        - Dr. Karan, Vahid, etc.

- Dr. Garcia from Webber Academy...
- You can acknowledge people for giving feedback

- Person for ....

- Don't be droning on about all the people you love
  - It's not important.
- At the city science fair, they want to see how original your project is.
  - Not even grad students know what they want to study at labs, so there is a bias against ASP students
    - How do you disprove that your project is not mentor-driven without being antagonistic?
    - Use key phrasing in your presentation to show the judges that *you* are the one interested in the project
    - Originality is one of the hardest things to prove.
- Use the rubric from the city-wide science fair to see if you have covered everything.
- When it comes to judging, it is what it is **AFTER** you make sure you have everything
  - Every judge has different opinions
- Between March 1-11
  - Work on the CYSF portal every day
- DEADLINES
  - 27th is the last day of February classes
    - Oral presentations (Slides attached @  $11:30 \rightarrow$  on Feb 25th because that's when I'm presenting)
    - The logbook for February (attached on Google Classroom @ 11:30)
    - Not accepting late work because of marks closing the next day (DROP-DEAD DEADLINE)
  - February 19th
    - Methods deadline
    - DROP-DEAD DEADLINE
- Priority list
  - Data analysis + methods have to be the priority
  - Oral presentation + logbook
  - Poster for the science fair (should be done by the Sunday before

March 11)  $\rightarrow$  March 9th.

- The most important part of the project is TIME MANAGEMENT
  - COMMUNICATE SO THINGS CAN BE SALVAGED
  - No one can help you if you do not communicate.
  - Consider when it's time to say "help"
- METHODOLOGY MUST BE WRITTEN IN THE PAST TENSE
  - By the time the presentation happens, it will already have been done.
- ☑ Watch and take notes on a video about DLS
  - <u>See experimental procedure for February 13th.</u>
- ☑ Write a paragraph on ink preparation for procedures
  - See experimental procedure for February 13th.
- ☑ Write a paragraph on DLS + average particle size for procedures
  - <u>See experimental procedure for February 13th.</u>

## February 15 - Long Weekend:

- ☑ Write a paragraph on electrical conductivity for procedures
  - <u>See experimental procedure for February 15th</u>
- ☑ Write a paragraph on BJH average pore width for procedures
  - <u>See experimental procedure for February 15th</u>

## February 16 - Long Weekend:

- ☑ Write a paragraph on how the data was graphed for procedures
  - See experimental procedure for February 16th

## February 18 - After School:

- Lauren and I read each other's procedure sections and gave each other feedback and edits as people who don't know much about each other's project to ensure that our papers were comprehensive
- I went through her edits and made changes to my paper
  - <u>See experimental procedure for February 18th.</u>

## February 19 - Class Time:

- ✓ Class Discussion
  - To get feedback
    - 7 days is ideal
    - 3-4 days may be possible
  - Results section paper
    - Will be largely based on the science fair
    - Requires
      - Detailed description of the description
      - No raw data
      - Only graphs, tables, diagrams, etc.
    - Paragraph describing the figures, graphs, etc.
      - Reference the figure you are describing
      - You never need to say the figure above/below because you give a number, and the figure should always come below
    - A lot of this will need to be done for the science fair
    - DO NOT INCLUDE WHY IN THE RESULTS
      - This belongs in the discussions and conclusions section
    - Figure legends
      - Goes underneath the the figure
      - Left aligned, not centered with the figure
      - Figure #. <u>Title. Brief description of the figure.</u>
      - The figure has to stand alone
        - Describe the figure in the paragraph above in detail
        - Add a brief description of the figure in the figure legend
    - ANYTHING NOT MADE BY YOU MUST BE CITED BOTH IN THE PARAGRAPH ABOVE AND IN THE FIGURE LEGEND
    - Due on Apr  $14 \rightarrow$  hand in for feedback on the 7th (11th at the latest)
  - Analysis/Discussions & Conclusions
    - Easily the hardest section you will write
      - Complication comes from you trying to describe what your data means
      - You have to go back to the literature
        - Who else said what, and how do my results fit in the

field of study?

- Put your results in the context of the current understanding of the field of study
- explain/provide alternate explanations
- Get back to the research question
  - This happened
  - This didn't happen
  - ...
- Significance and future direction should be in your final paragraph
- By the time this paper roles around, you should have most of the data collected and science fair will be over
- SCHEDULE THIS WELL  $\rightarrow$  AP EXAMS ARE AROUND THIS TIME
- Due May 1st
- Final paper is due on May 30th
  - All edits should be done by here
  - All feedback should be implemented
  - You have a month between the analysis/discussions & conclusions to hand in the final paper
  - SCHEDULE THIS WELL  $\rightarrow$  AP EXAMS ARE AROUND THIS TIME
- Make sure to actually take Dr. Garcia's feedback and implement it
  - She has been giving repeated feedback
  - Make sure each reference has what it has
  - Each reference should have a DOI
  - All references should be peer-reviewed or from a government site
- One more class this week, and then oral presentations start next week
- After the presentations, we will have three classes to prepare for the science fair
- ☑ Biweekly meeting with Dr. Garcia
  - I will try and find a paper to replace the Million Mile paper in the intro because it isn't peer-reviewed
  - I will try to find a government site for the share of greenhouse gas emissions in Canada
    - If I can't find sources for these, we will discuss this closer to the final paper due date
  - I still have a few more graphs to create for the analysis (plotting properties

against each other)

- Add some pictures to the observations section of the CYSF portal with brief descriptions of what is being shown
- I will be starting my presentation for the oral presentation today
  - Find better-quality figures
  - Maybe try to add images to the methodology, so it isn't too wordy
- ✓ CYSF portal
  - I formatted the procedures to fit with the CYSF portal
  - Formatting equations was difficult but I reworked the paper to have it properly formatted.
    - <u>See THIS IS FOR THE CYSF PORTAL document → procedures section</u>
  - Added current list of citations to the CYSF portal
    - See THIS IS FOR THE CYSF PORTAL document → references section
  - Add observations with short descriptions
    - See portal

Check the Procedures paper against the rubric

- I believe that my paper hits all the points that the rubric requires.

Coltonia	Achievement Level				Partial Marks	Mark	
Criteria	Excellent (28-30)	Good (25-27)	Satisfactory (22-24)	Mediocre (19-21)	Not Sufficient (below 18)		
as (20)	Describes experiments with sufficient detail to enable other scientist to repeat the experiment successfully.	Describes experiments with sufficient detail to enable other scientist to repeat the experiment successfully.	Describes how the experiments were performed but some details are missing.	Describes how the experiments were performed with critical details missing.	The description of the experiments is insufficient making it impossible to repeat the experiments.	/5	
Procedur	Presents easy-to-follow steps which are logical and adequately detailed without including standard laboratory procedures.	Most steps are understandable but some lack detail or are confusing.	Most steps are understandable but some lack detail or are confusing.	Some steps are missing in the description of the experiments.	Many steps are missing in the description of the experiments.	/5	
rimental	Specific materials, chemicals and equipment are mentioned in the description of the procedures.	Most specific materials, chemicals and equipment are mentioned in the description of the procedures.	Most specific chemicals and equipment are mentioned in the description of the procedures.	Some specific chemicals and equipment are missing in the description of the procedures.	Chemicals and equipment are in a list format or are not described.	/5	
Expe	Displays a deep understanding of the methods and equipment employed.	Displays a good understanding of the methods and equipment employed.	Displays a basic understanding of the methods and equipment employed.	Displays a basic understanding of the methods and equipment employed.	Displays a poor understanding of the methods and equipment employed.	/5	/20
ie (4)	Methods written in paragraph form.	Most methods written in paragraph form.	Most methods written in paragraph form.	Some methods written in paragraph form.	Some methods written in paragraph form.	/2	
	Materials mentioned in the narrative text, not as a list.	Most materials mentioned in the narrative text, not as a list.	Most materials mentioned in the narrative text, not as a list.	Some materials mentioned in the narrative text, not as a list.	Materials mentioned as a list and not described in the narrative text.	/1	
ŝ	All figures and tables have appropriate legends and/or titles.	Most figures and tables have appropriate legends and/or titles.	Most figures and tables have appropriate legends and/or titles.	Some figures and tables have appropriate legends and/or titles.	Most figures and tables are missing the appropriate legends and/or titles.	/1	/4
т ()	All materials used are presented along with their source	Most materials used are presented along with their source	Most materials used are presented along with their source	Some materials used are presented along with their source	Some materials used are presented without their source	/2	
ions and rences (6	Relevant sources are provided for the methods and procedures employed.	Relevant sources are provided for the methods and procedures employed.	Most sources provided for the methods and procedures employed are relevant.	Some sources provided for the methods and procedures employed are relevant.	Most sources provided for the methods and procedures employed are not relevant.	/2	
Cita	All citations are properly linked to the references list in the correct format.	Most citations are properly linked to the references list in the correct format.	Most citations are properly linked to the references list in the correct format.	Some citations are properly linked to the references list in the correct format.	Most citations are not properly linked to the references list in the correct format.	/2	/6

#### Rubrics for Experimental Procedures Section

- Hand in procedures on Turnitin for Science Fair
- □ Finish graphing properties against each other
  - <u>See data collection and results for Feb 19th</u>

Start oral presentation slides (these are from the research proposal)





## February 20 - After School:

- Understanding the data plotted yesterday
  - See data collection and results for February 20th.
- ☑ Oral presentation slides (methods and results)









## February 21 - Class Time:

- ✓ Conclusions of my project
  - See discussions and conclusions for February 21st.
- Finish slides for oral presentation (analysis and conclusion)



- I ran through the presentation in my head a few times to see if I could do it within the time limit.
  - I think I will have to cut some information out in order to meet the time constraint but I will practice this a few more times to judge whether or not I have enough time to leave the presentation as is.

### February 24 - At Home:

☑ I made changes to some of the slides so there would be fewer words on the slides







- ☑ I ran through the presentation twice with my mom to make sure I was within the time constraint.
  - Both times I was within the 12-minute maximum time limit.
- ☑ I made cue cards just as a guide in case I need prompts for speaking

## February 25 - Class Time:

- □ Class discussion
  - You need a punch line
    - Right from the beginning, talk about what your project is about
    - That way, when you start with the details, you still know that what

you tried to set up makes sense

- We are being too rigid with presentations
  - Need to start looking at flow
- The core of the presentation is the results
  - Results should be taking 5-7 minutes of the 12 minutes
  - Looking at graphs, analysis, conclusion, etc.
- Setup and background should only take 4 minutes
- When you are presenting your poster, you are just talking to one person, and you're pointing to parts of your presentation
- Take time to show graphs
- Conclusions should not have that much information
  - This is how it answers the research question
- Slides with conclusions mean nothing unless it connects to results on graphs
- NEED TO START SHOWING DR. GARCIA PAPERS AND PRESENTATIONS AHEAD OF TIME
- If you are done with your data and presented today, reflect on how this can be better for poster presentation
- ✓ Merrit and Maddux OP

Investigating Postural Orthostatic Tachycardia Syndrome (POTS)

#### What is POTS?

- An autonomic disorder
- Patients experience an increase in heart rate
- Occurs in 10 minutes
- There is no other identifiable cause

#### The problem:

- There is no identifiable cause

#### Solution:

- Find out what's wrong
  - Use MRI to do this

#### Lower Body Negative Pressure

- LBNP has a vacuum that sucks the air out

- Uses Bernoulli's principle  $\rightarrow$  principle of fluid dynamics
- Fluids flow from high to low pressure so LBNP pushes blood to the feet
- When fluid is sucked out, it simulates gravity

#### Head Upright Tilt Test

- Person tilted to 80°
- Actual gravity

#### Autonomic function testing

- Valsalva
  - 4 phases
  - Exaggerated phase 4
  - Increased heart rate
  - Pressure meter monitored on iPad
  - 40mmHg constant pressure
- Sinus arrhythmia
  - Deep breathing
  - Patients follow a ball on the screen
- Hyperventilation
  - Rapid breathing
  - Follows metronome

#### Merrit: Aim 1

#### Maddux: Aim 2

#### Goals:

- Merrit: tilt test vs LBNP
  - Cardiovascular response
- Maddux: autonomic function testing with and without LBNP
  - Parasympathetic response

#### Variables:

#### Merrit:

- Manipulated
  - Tilt vs LBNP
- Responding

- Primary: 10 min HR and strobe pulling
- Secondary 10 min BP and cardiac outlet
- Controlled
  - Length of time
  - Overall health of patient
- Confounding
  - Order of testing
  - Time of day

#### Maddux:

- Manipulated
  - LBNP vs. Recumbent baseline
- Responding
  - Primary: heart rate, valsalva ratio (between maximum over minimum heart rate), surface area ratio (average of all maximum and minimum heart rates)
  - Secondary: BP and cardiac outlet, SVR
- Controlled
  - Length of time
  - Overall health of patient
- Confounding
  - Order of testing
  - Time of day

#### RQ:

- Merrit
  - What is the difference in hemodynamic response and controls?
- Maddux
  - What is the difference in autonomic testing during LBNP and BSL

#### Hypothesis:

- Merrit
  - LBNP and tilt have similar outcomes
    - If LBNP simulated gravity, patients respond similar to gravity
- Maddux
  - LBNP and BSL will have different outcomes
    - LBNP simulates gravity so autonomic function should differ

#### Methods:

- Aim 1
  - 10 minutes of each test
- Aim 2
  - Test autonomic function
  - 1-minute baseline and recovery period
- Lab charts were sent to them and analyzed using Matlab and redcap
- Used SPSS in order to get the results of the mean and standard deviation

#### Procedures:

- Patients from the Calgary autonomic lab
- Participate in a 10-minute baseline
- Then, 1-minute recovery
- Then use autonomic tests
  - 1-minute baseline
  - 1-minute recovery
- 10-minute LBNP baseline
  - 1-minute recovery

#### Results aim 1:

- HR differed by a large margin for LBNP and tilt
- Same with blood pressure

#### Result aim 2:

- Heart rates between BSL and LBNP are different
  - LBNP induces orthostatic stress

### Analysis + conclusions:

- LBNP simulates gravity but is not as effective as the tilt test
  - LBNP shows less drastic symptoms
- LBNP induces orthostatic stress

#### Significance:

- Cardiac MRIs may work, but it might not be as exaggerated as with a normal tilt test that needs to be taken into account

- 75% of people are misdiagnosed with POTS
- 34% patient diagnosed
- There is a large population with POTS (1% of North America)

There were 19 POTS patients and six healthy controls

- You can't really know their health ahead of time
- Sometimes, the instruments don't measure cardiac output correctly

#### Arth OP

Examining the effect of physical activity on muscle mass and muscle function loss in peri and early menopausal females

Menopause:

- Marks the end of a female's reproductive years typically at 51
- It happens in 3 stages
  - Reproductive
    - early, peak, and late
  - peri-menopausal
  - post-menopausal
- symptoms: hot flushes, fatigue, and mood changes
  - worsened by obesity and smoking
- begins after 12 months with no menstruation
  - reduced mobility, balance issues, muscle loss
- menopausal hormone therapy is the only treatment

#### Muscle:

- Slow twitch fiber type 1
- Fast twitch fibre type 2
- Muscle contraction efficiency decreases with muscular function

- Estrogen protects from muscle loss
- Muscle loss leads to mobility issues and a risk of muscular diseases
- As menopause progresses, estrogen decreases, increasing muscle loss
- Muscle mass measured using DXA

#### Physical Activity:

- Promotes muscle health and reduces fat infiltration
- Builds muscle strength
- High intensity > low intensity
- Women who are more active are 20-30 years younger in terms of muscle health

#### Variables:

- MV
  - Levels of PA intensity
    - Sedentary, light, moderate, vigorous, and very vigorous
- RV
  - Lean mass
    - Appendicular lean mass (arm + leg)
- CV
  - Muscle function
    - Dominant and non-dominant

#### Hypothesis:

- higher physical activity intensity creates a positive effect on the improvement of mass and muscle function in peri and post-menopausal women

#### Goals:

- short term
  - immediate effects (different PA levels impact)
  - using data to find significance (importance of variables)
- long term
  - encourage lifelong PA (how staying active is important)
  - expand research in menopause (demographic is understudied)

Research question:

- What is the association between increased levels of PA and muscle mass and function in peri and early menopausal females?

Procedures:

- part of strength training for osteoporosis for early menopause by U of C Kinesiology
- participants were randomly assigned to control or intervention group
  - intervention trained three times with three phases
    - teaching how to lift weights with no weight (30 days)
    - Used a light weight (60 days)
    - increasing weights (6 months)
- all participants wore accelerometers before and after for 7 days
- all were found using six tests
  - 6 min walk test (aerobic fitness)
  - jump test (muscle power)
  - hand grip (max force by forearm)
  - Decus scan to measure lean mass
- Box and scatter plots are used to predict variable value and outliers

#### Results:

- sedentary PA has + significance for appendicular lean mass
  - does not make sense
    - error makes sense because of an outlier with extremely high lean mass but is not active
    - skewed the data
  - caused sedentary physical activity to increase in lean mass
- muscle power (perimenopausal shorter period of menopause, so they are better
   —> vigorous PA)
- leg torque (perimenopausal shorter period of menopause, so they are better All PA)

☑ <del>Nina OP</del>

motivations and expectations for participation in a psilocybin-assisted psychotherapy trial for alcohol use disorder

Alcohol Use Disorder:

- One of the most prevalent substance abuse disorders worldwide
- Linked to chronic diseases
- Previous evidence that psilocybin-assisted psychotherapy may reduce the number of drinks in those with AUD

Psychedelics:

- Cause vision distortion and hallucinations

- used to break addictions
- non-classical
  - ketamine, salvinorin A
  - act as n-methyl D-aspartate NMDA antagonist
- classical
  - small changes in perception, mood, and cognition
  - do not have to worry about addiction

NMDA receptor:

- One of the receptors for neurotransmitter glutamate (memory and learning)
- Antagonists are useful for conditions with excessive neuronal activity Serotonin:
  - Helps appetite, sleep, etc

Research question:

- How are motivations and expectations for participation is a psilocybin-assisted psychotherapy trial for AUD related to treatment outcomes?

Hypothesis:

- Individuals with a higher degree of motivation or positive expectation regarding the therapy experience will have a greater reduction in alcohol consumption

Variables:

- MV
  - motivations and expectations going into therapy
- RV
  - change in alcohol consumption
- CV
  - Age of patients (22-65)
  - Other treatments patients are receiving
    - No benefit from lying about other treatments because participation is a choice

Objective:

- Collect individual motivations and expectations
- Monitor the trends in patients' change in alc consumption
- Fill gaps in knowledge regarding motivations and expectations in trials utilizing psychedelics
- Develop a framework for personalizing psilocybin-assisted therapy

Significance:

- Reduce stigma around AUD
- Enhance the overall effectiveness of psilocybin-assisted therapy
- No research was done comparing motivations and treatment outcomes specifically
- Maximize therapeutic effects

#### Methods:

- Alcohol consumption collected using timeline flow back
- Amount of alcohol consumed over the last 30 days
- Motivations and expectation survey
- 12-week follow-up motivations and expectations survey

#### Results:

- There is a negative correlation between total motivation and change in drinks
   This is a good thing --> means they are drinking less
- The null hypothesis is that motivations and change in drinks are not related, which is untrue

#### Analysis:

- Weak negative correlation between the total MRAC score and the change in drinks
- 13% of the variance in the change in drinks is accounted for by motivation
- The sample size is small
  - Increasing the sample size will decrease the variation

#### Future Steps:

- More data
  - Obtain more accurate estimate of the true correlation
- Intervention development
  - Create a more beneficial expectation (high motivation results in higher drinking)

#### Question:

- Why compare motivation specifically to treatment outcomes
  - We have so little understanding of psychedelics
  - We don't know what causes effectiveness, so trying to get into every subjective part of drug use to see which effect it is to better understand it
- The form reduces bias by having free-response questions and a wide breadth of responses for mcq
- They also do it in isolation

#### ✓ Eleanor OP

A comparison study of the regional impacts of extreme El Niño events on India and Peru in the 1788-1793 and 1982-1983 episodes

- civilisations depend on climate for a steady food supply
- in the 21st century, the effect of climate seems to be less significant
- determine which sector of modern society is more susceptible to weather anomalies and what we can do to mitigate the destruction

El Niño:

- Phase of El Niño southern oscillation caused by a circulation in the Pacific called Walker circulation
- Warmer ocean water in the east and central Pacific
- Higher air pressure in the western Pacific, lower air pressure in the Eastern Pacific
- When the circulation is weak, this is when El Nino occurs

El Niño effect on weather patterns:

- Has teleconnections between separated locations on earth
- El Niño causes weather pattern changes all over the world

Effects in India and Peru:

- The effects of El Niño in these areas are significant
- weather anomalies caused by El Niño cause a monsoon failure in India, resulting in a deficiency in agriculture health and infrastructure, which essentially relates to pop and economy
- Peru impacts fishery because it is highly dependent on the rising sea levels by walker circulation, causing damage to commercial fishery

Proxy reconstruction of ENSO:

- proxy records are sensitive to temperature/rainfall patterns that extend to the 18th century  $\rightarrow$  not enough to analyze El Niño effects further back
- proxy records help record the temperature and rainfall pattern to past centuries that could be used to track El Niño
- can reconstruct ENSO from back in the day
- instrumental record: nino 3.4 SST
- documented as an indicator of the ENSO cycle

Why these years?

- society at these times went through changes and helps show how El Niño of the

same amplitude change affected different societies

- first years
  - 600-700 million pop
  - global temp rise
  - 1 trillion GDP
  - Agriculture
- second years
  - 4.4 billion pop
  - +1.2 degrees celsius
  - 38 trillion GDP
  - digital industry and finance

#### RQ:

- What were the agricultural, economic, and demographic impacts of the 1788-1793 and the 1982-1983 El Niño events in India and Peru?
- Is modern society more resilient to the socio-economic damages caused by climate variability and extreme weather events?
- What predictions can we make about how future El Niño may affect human societies?

#### Significance:

- Anthropogenic Vs. Natural climate variabilities —> so many variability, such as global warming, so it is important to examine the effect of anthropogenic and natural climate change
- A doubling in the occurrences
- Extrapolate the socio-economic influence of climate variabilities in future society by looking at how it changes in different societies

#### methods:

- reconstructing ENSO
  - A primary list of proxy records used in previous study
    - selected as a potential proxy to reconstruct ENSO
  - Raw data gathered from the NOAA Physical Sciences Laboratory
  - Correlations between the proxies and instrumental records Niño 3.4
    - Threshold: |r|>0.3
    - only when the coefficient is larger than 0.3, it would be used for further use in ENSO reconstruction
  - Scatterplots and the equation of regression lines
    - $\rightarrow$  Reconstruction of ENSO
- measuring regional impacts in Peru and India
  - Series of economic/agriculture/ fishery statistics

- Percentage change was calculated to minimize the impacts of increasing economic trends on overall data
- Trends of correlations in different time periods were calculated so that we can identify whether the correlations of ENSO and the economy of the countries are decreasing or increasing
- Qualitative or quantitative data collected from local and colonial government record

#### Analysis:

- Encompassing a large area of El Niño and its teleconnections —> provide a good scope of El Niño
- Consistent results show similar connections between studies
- Similar amplitudes of two El Niño events
- Similar severity of teleconnections in Peru and India

### India:

#### The 1789-1793 El Niño

- Food prices spiked, increasing by 800% in the most destructed regions
- The Skull Famine (caused by monsoon failure from El Niño), resulted in an estimated mortality of 11 million people

### The 1982-1983 El Niño

- A halt in the increase of foodgrain production
- No significant population loss
- Little correlation between India's GDP
- Correlation present for agriculture spiked in the 1990s

### Peru:

### The 1789-1793 El Niño

Qualitative descriptions —> This is the only thing that could be found in documents:

- Fishery crisis, a decline in trade and exports
- Crop failure: torrential rain and floods in coastal areas

### The 1982-1983 El Niño

- Fishery growth decreased by 270%
- Agriculture growth decreased by 550%
- Significant but decreasing correlation between Peru's GDP and fishery

Analysis:

- Controlled and remediable loss in food production in modern society
- No significant demographic loss
- Agriculture remains dependent on stable weather patterns
- Overall, more resilience to extreme El Niño events

Future Directions

- 1. Access to more data (both historical and proxies)—> Spain has more documents from Peru, but it is not digitalized, so it isn't accessible.
- 2. Expand the region of study to more developed countries
- 3. Diminish the influence of anthropogenic factors
- 4. Propose methods and policies that minimize the destruction

Questions:

- Are there any challenges that arise from the data from 1789-1793 El Niño in Peru, only having qualitative descriptions?
  - it is hard to compare the specific impacts of the two events if you don't have very good quantitative data; however, using the economic data from 1920-present, you can still find a trend in how El Niño effects decrease or increase over time and the results from 1789-1793 can be extrapolated
- why India and Peru?
  - Peru is impacted the most because of its location, and the impact is incredibly high

## February 27 - Class Time:

☑ <del>Cole OP</del>

The Significance of Cerebrospinal Fluid(CSF) Protein Biomarkers in Predicting Cognitive Decline in Transient Ischemic Attack (TIA) Patients

- Quality of life has improved
- Advanced life expectancy leads to an increase in the prevalence of neurological diseases
- By the time loss of neurological function has been found, permanent damage has been done

Background:

- TIA is an early indicator of cognitive impairment, presents an opportunity for early clinical intervention after their occurrence

- Strokes
- CSF contains protein biomarkers useful for diagnosing dementia, but have not been thoroughly explored in TIA patients

Looking at Alzheimer's biomarkers, which could be relevant in TIA patients

### Objectives:

Determine if CSF protein concentrations vary between TIA patients and healthy controls and impact cognitive function to affirm biomarkers that can be used to ascertain levels of early cognitive decline

### Methods:

- 5-year longitudinal cohort study (half healthy, half TIA)
  - Clinical review: blood pressure, cholesterol (baseline only)
  - Brain imaging
  - Neuropsychological battery (MoCA, ACE-R)
  - Blood Samples
  - Lumbar puncture was optional to collect CSF (43 TIA and 39 Controls)
    - Total tau
    - Phosphorylated tau
    - Amyloid beta 1-42
    - Amyloid beta 1-40
    - Suggests levels of cognitive decline in TIA patients

#### His role:

- Conducting statistical analysis
  - Data cleaning (34 TIA, 36 Controls left)
  - descriptive/frequency analysis, significance level 0.05

#### Results:

#### Conducting descriptive statistics

- Box and whisker plots control the proteins between the control and the TIA
  - TIA patients have higher levels of Total tau and Phosphorylated tau than controls
  - TIA patients have slightly lower levels of Amyloid beta 1-42 and Amyloid
beta 1-40

- Suggest a correlation between Alzheimer's and TIA patients
- Figure out if the data is statistically significant based on significance values less than 0.05
- Conducted analysis with ratios
  - Amyloid beta 1-42 and Amyloid beta 1-40 are not significant on their own, but are significant together
  - All the ratios corroborate the data
- Linear regressions predicting CSF protein concentrations and ratios based on group status accounting for age
  - Only p-tau has a significance value lower than 0.05
    - Only one that is 100% significant
  - Adjusted R square indicates that the strength of the association is not very good
    - Even for the statistically significant regressions, it isn't that strong
    - Group status is not the only thing at play

Analysis and conclusions:

- Descriptives reveal that CSF protein concentration trends in TIA patients present similarities with AD trends at early stages
- Statistical significance for differences in t-tau, p-tau, and Abeta42 concentrations and both MoCA and ACE-R scores between IA and healthy controls established from t-tests
- Regressions concluded that group status weakly predicts p-tau concentrations ATI MoCa, and ACE-R

Limitations:

- Small sample size  $\rightarrow$  type II statistical errors
- Inconsistent timing of lumbar punctures may have influenced protein concentration, cognitive assessment score statistics, and significance.

Extensions:

- Assess correlations between cognitive test scores and CSF proteins
- Assess more specific cognitive tests to determine specific cognitive domains impacted by TIAs
- Still have statistically significant data

#### Amber

#### Anethetics:

- Used to induce unconsciousness reduce pain and relax muscles
- Growing concerns exist about effects on brain

#### Sevoflurane

- Began to be clinically used in early 1990
- Generally considered safe for healthy individals
- Volatile

#### Synapses

- Used to communicate between neurons through neurotransmitter release and receptor binding
- - 86 billion neurons/100 trillion synapses
- Can strengthen or weaken over time
- Crucial for memory and learning

#### Anesthetics block receptors in order to decrease the action of neurons

Synapses and Anesthethic:

- Neurotransmitter
  - Released into synaptic cleft
  - Binds to receptors
  - Electrical signals are generated

If neurotransmitters remain blocked, the synapse can not fire

#### Synapse proteins

- Synaptophysic
- - located in presynaptic terminal of neurons
- Membrane protein
- Regulates cycling

#### Research aims:

- Question: How does repeated sevoflurane exposure affect synapse formation?

- Changes in synapse formation, density, and proteins

#### Methods:

- Dissection of P0 Pups (day they are born)
- Isolate the hippocampus
- Cell dissociation broke down the hippocampal tissue into single cells for culture
- Neuronal plating
  - Cells distributed onto a dish
  - Grow in an incubated environment
- Monitoring from DIV7
  - Beginning of Synaptic activity
  - Monitored growth and synapsis formation
- Sevoflurane expose
  - Exposed to %% sevoflurane daily for 1 hr
- Fixated cells to stop cellular processes and preserve structure
- Immunostaining
  - Using antibodies to detect proteins in fixed cells
- Imaging and analysis
  - Viewed the juxtaposition of red and green for synapsis
  - Analysis of quality of synapses and length

#### Results:

- Blue shows a single neuron
- Top right: indicator of PSD 95
- Bottom left: synaptic marker
- These ensure markers are working
- Exposed sevoflurane
  - Two main synapses formed
  - Presynaptic neuron  $\rightarrow$  mostly red so channels weren't built
- Not exposed
  - Density is much greater

#### Analysis:

- 1.6
  - Decrease in number of juxtapositions

- Neurons exposed to anesthetic were less synaptically dense
- Red markers remained near the presynaptic neuron
- Green remained near the postsynaptic neuron
- Control
  - More synapses formed
  - Green and red spread out

#### Significance:

- Understand the significance of anesthetic in synapse density
- Inform the public of the risk before inhalation
- Develop post-surgery mitigation strategies
- Refine anesthetic protocols
- Develop an anecdote for an anesthetic

Are there any limitations from a small sample size?

- The little amount shows that the results can't be perfectly formulated, especially because the cells are from the same rat.
- To increase accuracy, use more rats and change the amount of sevoflurane.
- □ Audrey OP

Exploring Antiviral Defense Systems and Single-Nucleotide Polymorphisms in Escherichia Coli 0157: H7 exposed to bacteriophages T1, T4, T5, rv5

- Looking at genetic mutations between a parent genome of E-Coli bacteria and the daughter genome after being exposed to bacteriophages (viruses that link to outside of bacteria + insert on DNA)
- Lytic phages inject DNA and immedietly start reproducing phages and destroy bacteria
- Lysogenic phages inject DNA to replicate through generations

#### Significance:

- 97000 E-Coli cases per year
  - HUS develops in Children under five and immunocompromised individuals are more susceptible  $\rightarrow$  can't fend off the bacteria that caused E-coli

- There is no real cure for it
- Antibiotic-resistant bacteria strains  $\rightarrow$  this strain doesn't have an antibiotic that works
- Develop antimicrobial treatments
- Look into Phage therapy as a generalized treatment
- Evolution of bacteria
- The solution is trying to find bacteriophages that work

#### Genetic components:

- Antiviral defense systems
  - Mutations as a result of phage attacks
  - CRISPR CASP
- single nucleotide polymorphisms
  - Mutations in a singular gene
  - Usually because of genetic drift
  - Can also affect the reaction

#### Objectives:

- Short
  - Profile anti-phage defense systems using WGS
    - Extracted and exposed genomes
  - To identify SNPs from bacterial isolates
- Long
  - Development of a working phage therapy for clinical usage

#### Methods:

- Phage exposure
  - Exposure of E. coli to phages T1, T4, T5, and rv%
- DNA extraction
  - 14 phage resistant isolates were extracted
  - DNA spin kit used to extract DNA and sent to Quebec for analysis
- WGS (whole genome sequencing)
  - fastQ
  - fastQC (reaffirmed quality)
  - FastP (cleave off irrelevant ends of genome)
    - Anything not within the overlay cleaved off to only have significant reeds

- Shovill
  - Reassemble genes
- Step 1 is quality checking the reads
  - Have to reaffirm the quality
- Analysis
  - Defense finder
  - Padloc
  - Just two different pathways
  - Used both to confirm the information collected from one
  - Run through the genes and figure out what is inside and separate into readable data
- Visualisation
  - Conducted using R-studio

#### Results:

- Heatmap of defense systems vs isolates
  - All isolates are similar to a couple of the isolates
  - The isolates didn't change much
- Haccard distance map
  - Maps the genetic similarity of isolates
  - Wasn't much mutation between isolates, any mutation was similar
- Bar graph
  - Looking at polymorphisms
  - Shows the absent isolates
  - There are specific groups in genomes that are present or not present in different genomes/isolates
  - The isolates were measured against the R508 genome
  - There are several groups that were absent from the original strain
- Heat map polymorphisms
  - Which groups and genes are absent compared to R508
  - The blue squares are the isolates where they were absent

- Considering that, some groups are very similar in genetic function
- These are the polymorphisms that happened in every isolate

#### □ Marie Elise OP

Implementation and evaluation of alternative user interfaces for game control

- See how we can improve user accessibility and enhance the experience of technology
- See correlation between age disability and preferred mode of interaction

1.3 billion people in the world with disabilities

- Important to take into account about technology

#### Project

- Coded website with connect 4 and checkers

#### Methodology

- website
  - Link activate
  - Ethics form
  - User name + email
  - Survey

#### Alternatives

- Speech
- Gestures

#### MV: modes of control and limitations, age

RV: preferred mode of control

#### CV: type of game, complexity, number of times played

Confounding: personal preference, user engagement, biological sex

how does age and disability impact prefered mode of interaction when playing video games

#### Hypotesis

- Null: older people with coordination difficulty will prefer same mode as younger
- Alternate: Older people will prefer speech, while younger will prefer gesture tracking

#### Results

- 33 participants
  - 19 females
  - 14 males
  - Mostly 11-18 participants
- The graph shows the number of people with each of the conditions
  - Anxiety is the most represented
- 61% preferred speech and 39% gesture
- Correlation between age group and mode of interaction
  - 11-18 preferred gesture
  - As they get older, people prefer speech recognition
- Speech could be preferred because communication happens through speech, and there are many devices that rely on speech already

#### Conclusions

- People who prefer gesture
  - Adhd
  - Anxiety
  - Difficulty with reading

RQ

- Difficulty with writing
- Speech
  - Focus difficulty
  - None of the above
  - Coordination
- Age
  - Younger prefer gesture
  - Older prefer speech
- Hypothesis is proven correct

Future works:

- Making technology easy and accessible for everyone
- Understanding user control preferences makes it universally accessible and engaging
- Adaptive interface with AI
- Having a larger sample size will allow for more data and more understanding
- More modes of control could be interacted

Other modes that could affect the mode?

- Yes, if you considered more conditions, there would be people, data, and since there is such a small sample size, it's hard to represent everyone.

□ Lauren OP

Identification of novel interventions for stage IIIB/C nonsmall cell lung cancer that may positively impact patient treatment outcomes

- Lung cancer one of the most fatal and most common cancers
- Our obligation to increase research in this area
- Mortality of 73%

#### Importance

- One of the most fata cancers
- Many patients are not able to complete full treatment cycle due to toxicity, discomfort, or death

Objectives:

- Improve treatment outcomes through simple solutions
- Evaluate current interventions against others
- Finding additional treatment methods that can be used after chemoradiation therapy to improve patient survival, comfort, or reduce toxicity

#### Stage IIIB/C lung cancer

- Stage III  $\rightarrow$  infected lymph nodes
- $B/C \rightarrow$  not removable through surgery
- Tend to have larger, more aggressive tumors

#### NSCLC:

- The majority of lung cancer diagnoses (85%)
- Infected epithelial cells
- Adenocarcinoma and squamous cell carcinoma

#### Stand of treatment

- If possible: surgery
- One of
  - Chemoradiation
  - Targeted cancer medication
- Followed by intervention and immunotherapy
- Surgery  $\rightarrow$  chemoradiation/targeted medication  $\rightarrow$  intervention  $\rightarrow$  immunotherapy

#### Interventions:

- Aim to reduce treatment toxicity, improve patient survival and comfort
- Changes to diet, activity, medications
- Range in price, efficacy, and feasibility

#### RQ:

- What are potential interventions, that have yet to be applied to regular NSCLC treatment and that may further improve patient survival, increase the ability of patients to complete prescribed treatment, or improve quality of life beyond existing standards of care?

#### Goals:

- Short:

- Identify interventions to implement into NSCLC treatment
- Score interventions for efficacy, cost effectiveness, and feasability
- Hypothesize and identify intervention with most potential
- Long:
  - Further research on identified intervention
  - Application of scoring system on larger scale
  - Establishment of clinical trial to test hypothesis
- Methods
  - Pull paper from databases
  - Sorted papers by paper type, treatment stage, and intervention
  - Application of exclusion criteria
  - Sorted papers into intervention type
  - Used references lists to gain access to clinical trial information
  - Application of scoring system
- Scoring system
  - Efficacy (0-5)
    - 0 = negative effect
    - 1 = no effect
    - 5 = effective
  - Cost effectiveness (1-5):
    - How prices compares to average in Canada
  - Feasibility (1-5):
    - Difficulty of receiving
- Interventions
  - Dietary
    - advice/caloric intake
    - Fatty acid supplements
  - Activity
    - Mind-body exercises
    - Breathing exercises

Results:

- advice/caloric intake
  - Score 9
    - 1 paper that effectively analyzed this
    - Large possibility of bias based on overviews
- Fatty acid supplements
  - Score 13
    - 2 papers
    - Different supplements

- Quality of life vs. toxicity/decreased enzyme expression
- Difficult to analyze because they were so different
- Breathing exercises
  - Score 14
    - 1 paper
    - Effective for some aspects (physical wellness) however not all the intended effects were achieved
- Mind-body exercises
  - Score 14.17
    - 3 papers  $\rightarrow$  most out of everything
    - Effective for both mental and physical aspects of comfort
    - Only scored three so it didn't completely outweight papers from everything else

#### Analysis:

- Mind body exercises are the most effective
- Correlation between physical fitness and quality of life/emotional well-being
- Large issues of bias in the study

#### Concluding hypothesis:

- If applied to regular stage IIIB/C NSCLC treatment, mind body exercises will be most effective in improving quality of life and patient comfort

#### Errors:

- Small database after application of exclusion criteria
- Large possibility of bias in studies/lack of uniformity
- Results reliant on patient completion/honesty

#### Future direction & significance

- Rerun study with larger database
  - Lack of papers contributed to the error
- More focused study
  - Difficult to evaluate the quality of life to toxicity
- Other directions with scoring criteria
  - Application of scoring system with other types of cancer

Question: you mentioned in sources of error that the results are reliant on patient

honesty, so is there any reason as to why patients may be dishonest?

- Could be a difference between people who are doing their exercises all the time vs partially.
- Some people may not want to admit that they haven't been as good as they could.

# **March Daily Notes**

## March 01 - Weekend

☑ Background research and significance parts of the poster for science fair



## March 03 - Class Time:

- ✓ Class Discussion
  - The poster needs to be able to stand on its own
    - Have all the information needed
  - Slides vs. poster
    - Slides
      - Can be succinct
      - Must flow
      - Linear flow
    - Poster

- Has to be comprehensive
- Must flow
- Non-linear flow because you can point to specific sections of the slides
- Much more space on posters
- When you are in front of the poster, you can point to specific parts of the poster
- Poster structure
  - Background + methods together on one side
  - Results in the center
  - analysis, conclusion, limitation, references, and acknowledgements should be together
- The science fair presentation can be much more informal
  - Start with a punch line
- Poster style was not a determining factor in who did well at the science fair
- Have sections well delineated
- The key for the science fair is understanding your poster
  - Your poster is not going to make or break anything (unless it's particularly bad)
- If you are abbreviating things, say and write it out the first time before using the abbreviated version.
- You can have more things in your poster than you choose to focus on
- Don't write out methods  $\rightarrow$  make a flow diagram
- ☑ Results, analysis, conclusions part of the poster for science fair



Brainstorm ways of making methods less wordy

- I could draw it with my iPad
- I could try and find websites that make flow diagrams or use Google Draw
- Cole told me about how PowerPoint has a smart art feature that allows flow diagrams to be made, so I think that will be the best way to make easy to read methods.

## March 05 - Class Time

- ✓ Class Discussion
  - By Friday, have the final version of your poster done to print, or put it together over the weekend.
- Add error bars to graph
  - I could not figure out how to do this since I couldn't find an option to custom input numbers for the error bars.
  - I talked to Dr. Garcia about it and we looked at it together but could not figure it out.
  - I sent the Excel sheet to her and she emailed me later telling me she figured

it out and she showed me how to do it.

- See data collection and results for March 5th.
- ☑ Make methods flow diagram using Microsoft PowerPoint Smart Art feature
  - <u>See experimental procedure for March 5th</u>
- ☑ Write limitations and future direction
  - See discussions and conclusions for March 5th
- ☑ Limitations, future direction, acknowledgements, and references



Add methods flow diagram



- ✓ Figure out scaling for the poster
  - I used ratios to estimate how large each item on the poster would be,

depending on how I would print it out.

## March 06 - Spare:

- Meeting with Dr. Garcia
  - During this spare I met with Dr. Garcia to go over my oral presentation and my poster draft.
  - She told me that overall my oral presentation was good, but I need to get to the results faster.
  - I should make the methods section less wordy by using a graphic
  - I do not need to explain methods in that great detail. If people want to know, they can ask
  - She said that my poster layout looked good, but I just need to make sure to have graphics spread throughout
  - She told me that I should change the layout of the methods to make more sense/flow better
  - I should also add more images of the methods

## March 07 - Class Time:

- Redo methods section to flow better + add images
  - <u>See experimental procedure for March 7th.</u>
- Add new methods to poster



Change format to three parts of the trifold



- Ask Dr. Garcia for more feedback
  - Change the font to make everything black on the graphs
  - Unbold everything except headings
  - Edit the conclusions to be less wordy
    - See discussions and conclusions for March 7th.
- ☑ I made Dr. Garcia's changes



## March 07 - After School:

- ✓ Poster planning
  - I realized that printing each panel of the trifold would not work because Staples does not custom size paper and I don't know how to cut in straight lines.

## March 08 - Weekend:

- ✓ Poster
  - I resized my poster to be 3ft x 4ft and sent it to Staples to be printed. Unfortunately, I missed the same day deadline, so I will only get it tomorrow.

## March 09 - Weekend:

- ✓ Poster
  - I went to Staples and finally picked up my poster (hallelujah!!)
  - My mom and I looked to see if we could pin the poster to the trifold.
    - It looked comically small on the trifold so I decided I would ask Dr. Garcia if I can pin it up instead.

### March 10 - After School:

- Meeting Dr. Garcia
  - I met with Dr. Garcia to practice my science fair presentation for tomorrow.
  - I made it to the results in about 5 minutes and took another 7 minutes for the rest of the presentation
  - Dr. Garcia said my presentation is really good, but I need to start with a punchline about why this project interests *me* to start off the presentation.
    - Everyone needs a source of reliable energy
    - My parents tell me stories about how their parents stayed up with a manual fan fanning them to sleep.
  - Dr. Garcia said that I will be able to hang up my poster using the art stands

and clips

- The science fair mark we will be receiving is dependent on how we place.
  Gold = 100, silver = 95, bronze = 90, nothing = 85.
- ☑ Presenting to Lauren
  - I presented my science fair presentation to Lauren
  - Make sure to point to the diagram of PEMFC
  - Make the transition between graphs very clear with results
  - Make it clear about why it doesn't matter that pore width peaks at 25wt.%
- ✓ Punchline
  - One in ten people in the world do not have access to a reliable source of energy, and this is not okay. Energy is not a luxury it is a basic human right along with food, water, and shelter. My parents have told me stories about how they did not have access to a reliable source of energy growing up and about how their parents used to stay up all night with a manual fan so they would be able to get a good night's sleep for school the next day. I am lucky enough to have never had to experience this. In addition to energy being reliable and affordable to everyone, it also has to be clean. This is what inspired my project on designing high performance pemfc electrodes by optimizing catalyst ink composition.

## March 11 - Science Fair:

The science fair lasted the duration of the day.

- At school @ 8:00
- Set up science fair poster in the performing arts center (PAC) @ 8:30
- Group meeting @ 8:45
- Morning judging session begins @ 9:00
- Morning judging sessions ends @ 11:00
- Public viewing 1 begins @ 11:00
- Public viewing 1 ends @ 11:30
- Lunch begins @ 11:30
- Lunch ends @ 12:20
- Public viewing 2 begins @ 12:30
- Public viewing 2 ends @ 1:00
- Afternoon judging session begins @ 1:00
- Afternoon judging sessions ends @ 3:00

- Public viewing 3 begins @ 3:00
- Public viewing 3 ends @ 3:30

I had three judging sessions in the morning and two in the afternoon. I feel as though they went pretty well.

## March 12 - Lunch Time:

- ✓ Science fair awards ceremony
  - Everyone who participated in the science fair in junior and senior high had to go to the performing arts center (PAC) for the awards ceremony
    - My project got a gold medal
    - I was one of the top 15 projects and will be going to the city-wide science fair (CYSF)

## March 13 - Class Time:

✓ Class discussion

- Everyone who made it to the CYSF has to finish their portal by March 20th.
  Actually due March 21st in the morning
- Everyone did well at the science fair. It came do to decimal points to determine who went to the science fair.
- ☑ Hypothesis edits for CYSF portal.
  - <u>See experimental procedure for March 13th</u>
- ☑ Research edits for CYSF portal
  - See background research for March 13th
- ☑ Procedures edits for CYSF portal
  - <u>See experimental procedure for March 13th</u>
- ✓ Variables edits for CYSF portal
  - <u>See experimental procedure for March 13th</u>
- Add data (graphs) and analysis to the CYSF portal
  - See data collection and results for March 13th

## March 17 - Class Time:

✓ Class discussion

- Send an email to your mentor telling them about spring break, thanking them for their help, making science fair, what you have been doing, etc.
- ☑ Conclusions for the CYSF
  - <u>See conclusions and discussions for March 17th</u>
- ☑ Fill in the observations section of the CYSF portal with photos from the lab and brief descriptions
  - See data collection and results for March 17th
- ☑ Fill in the applications section of the CYSF portal
  - See conclusions and discussions for March 17th
- ☑ Fill in sources of error for the CYSF portal
  - See conclusions and discussions for March 17th

## March 17 - After School:

- ✓ Film science fair video
  - <u>https://youtu.be/phoBCVW1CYc</u>

## March 19 - Class Time:

- ✓ Science fair reflections
  - Judge 1
    - Check about graphs would be better if all the same type (bar vs. line)
      - Check with mentor
    - Raw data would allow for stats in all
    - Larger sample size
  - Judge 2
    - Perhaps you might want to check if the permeance has an effect on correlation
  - Judge 3
    - Picked a very interesting project with good real-world applications
    - Suggest diving into a holistic perspective of the project as a whole.
    - How does it fit into the clean energy sector, and what will be the real world impact?
  - Judge 4
    - Sample size is pretty small; more samples over a larger time as well

as testing the full fuel cell output, would help validate results.

- Judge 5
  - Fantastic presentation
    - Thorough and clean
    - Good background knowledge and understanding of the process
  - Motivation was exceptional in the
  - Scientific considerations related to the project were meaningful and directional
- ☑ Order new poster (foam board)
  - Ordered from Ryno printing
  - Should be ready by Thursday
- ☑ Email mentor
  - See email communication for March 19th.
- ✓ Header image



☑ Project image



☑ Fill in the acknowledgments section of CYSF

Thank you to Dr. Kunal Karan and Vahid Mazinani from the Department of Chemical and Petroleum Engineering at the Schulich School of Engineering, University of Calgary.

Thank you to Dr. Garcia from Webber Academy for their guidance and support throughout this project.

✓ Fill in the citations section of CYSF

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## March 20 - Spare:

Download parts of the logbook and combine them into one PDF

## March 20 - After School:

I went to Ryno Printing and picked up my poster board.

# **MENTOR WRITTEN NOTES**

This section contains all the PDF images of the notes my mentor has written about the topic and sent for my review.

## **September Mentor Written Notes**

## September 20, 2024:



Fuel Cell Performance





B, B, and C performance could correspond to 3 different catabyst layers or electrodes vorying in catabyst loading or activity of catabyst for example, if we use some catabyst Pt on Corbon (38 out / Pt on Corbon) but use different amount of catabyst per CM<sup>2</sup> (area) of electrode.

Soy, 
$$0.85 \text{ Mg}_{PL}/\text{Cm}^2 - \textcircled{A}$$
  
 $0.10 \text{ Mg}_{PL}/\text{Cm}^2 - \textcircled{B}$   
 $0.25 \text{ Mg}_{PL}/\text{Cm}^2 - \textcircled{C}$ 

we would observe trends shown on grouph

\* Catabyst activity or loading effect are cloninant primonly is high V (or low current i) region. \* At high current (i) region, transport effects become more important. Lo Here we imply transport of 02 gas and protone in membrone and cathode. This is why catabyst layer nucrostruche becomes insportant.

Now, you may ask what is <u>catabyst layes</u> microstructure?

If simply is the shuche of <u>calabyst layer</u> at microscopic / nanoscopic scale.

<u>Consider Cake</u> <u>Cake is fluffy.</u> It has <u>pores</u>. The pores are of certain <u>size</u> and <u>shape</u>. The pores are connected in a certain <u>meandening</u> pathway. Thus, we can say the cake is a <u>microporane</u> or <u>porous</u> material with say, <u>407</u>. porosity (fraction of total volume occupied by pores), with <u>0.005 to 0.05 mm</u> pores. <u>U</u> The pores can contal how moistme (water) diffuses or transport. <u>U</u> Highly porous cake with longe pores can become dry is <u>Calgory</u> easies.

Fuel Cell Catabyst Layer a Microstruche conhols  $o_2$  gas - size and connectivity of pores transport - Porosity - Distribution and connectivity of ionic · conpole utilization of polymer or ionomer. + Pt catabyst · conhols ionic transport · controls 02 transport to pt - Connectivity of combon portuctes supporting Catabyst. 6 controls electron transport CL nuicrostructure depende on - Low it is fabricated from "catabyst ink" - composition of catabast ink Camount of catabase, amount of ionic polymer, amount and type of liquid (water or alcohol - propond) used to "disperse" the catalyst and polyner

- type of catabyst and carbon support - type of ionomer - Ratio of Ionomer to Corbon (I: C votio)

In other words, the "catabyst ink" for mulation is an important factor contalling CL microstructure, which in turn affecte Fuel Cell performance. The intestudy popers are focussed on studying ink parameter effects. J. I'll enail those to you soon.

## September 23, 2024:

Diagram of a Proton Exchange Membrane Fuel Cell





# **BACKGROUND RESEARCH**

This section contains all the PDFs of each paper I have annotated for this research project.

## September Background Research

#### September 22, 2024:

Read and annotate the first three pages of bridging the gap between highly active oxygen reduction reaction catalysts and effective catalyst layers for proton exchange membrane fuel cells.



A highly active catalyst and a high-performance MEA with an integration of highly active catalyst with contained with the contained w

NATURE ENERGY | VOL 6 | MAY 2021 | 475-486 | www.nature.com/natureenergy
### **REVIEW ARTICLE**

#### **NATURE ENERGY**



Fig. 1 | Evolution of market size for fuel-cell electrical vehicles (FCEVs), and cost breakdown of FCEVs alongside production rate. a, Predicted market for FCEVs: the market size up to 2019 is shown in the inset. The scenario data are from ref. 4, b, Cost breakdown of fuel-cell stack components as a function of production rate. PEMFC stack components—GDL, MEA frame, balance of stack, membrane, catalyst and application, and bipolar plates—are all included. Panel b reproduced with permission from ref. 5, Hydrogen and Fuel Cell Technologies Office, Office of Energy Efficiency and Renewable Energy, US Department of Energy. TSURFACE AREA TSTODINITY

the ligano

what are

2

common challange

+ scalability + durability Shrain effects? fabricating well-defined structures, such as nanopolyhedrons<sup>10,11</sup> <sup>4</sup>, nanoplates<sup>15</sup>, nanocages<sup>16</sup> nanowires nanoframes1 core-shells<sup>21,22</sup>. Sometimes, various strategies have been combined. Alloying Pt with a transition metal is one of the most promising ways to improve catalytic activity, as the incorporation of transition metal atoms into the Pt face-centred cubic structure forms an alloy phase that increases ORR performance via the ligand and and strain effects<sup>16,23</sup>. In Pt-based alloy catalysts, the {111} facet is more favoured for the ORR than the {100} and {110} facets<sup>24</sup> Hence, octahedrons and icosahedrons dominated by the {111} facet have garnered notable attention. According to previous reports, a shape-controlled Pt-Ni system seems to yield the most active catalysts for the ORR and has continued to generate the highest ORR activity records in the past decade<sup>25,26</sup>. Departing from the octahedral design, jagged Pt nanowires obtained by the electrochemical dealloying of Pt-Ni nanowires in 2016 created the highest ORR mass activity yet, at 13.6 A mg $_{Pt}^{-1}$ , with a specific activity of 11.5 mA cm $_{Pt}^{-1}$ (ref. <sup>12</sup>). So far, despite massive research efforts, the record set by these jagged Pt nanowires under RDE testing has not been broken to our knowledge. Catallysts Stay dwave & efficient In addition to efforts at improving mass activity, there have been urabil significant undertakings to enhance the stability of Pt-M alloy nanoparticles. It has been found that doping octahedra with trace significant undertakings to enhance the stability of Pt-M alloy nanoparticles. It has been found that doping octahedra with trace amounts of a third element, such as Mo, Rh, Co or Au, can stabilize both Ni and Pt atoms against dissolution, or suppress the migration Sd rate of Pt atoms and consequently mitigate against loss of the octa-AStoi hedral shape during the ORR process<sup>11,27,28</sup>. Transformation of traā ditionally disordered Pt-M alloy catalysts into structurally ordered e most ideal h intermetallic alloys can also suppress the dissolution of transition metal atoms, which not only significantly improves catalyst stability but also enhances the ORR catalytic activity2 Yet while the ORR activity and stability of the state-of-the-art novel Pt-based nanocatalysts achieved in labs far exceed commercialized Pt/C at RDE levels (in some cases by 100 times), it is very difficult to draw conclusions on expected MEA-level activities based IND VS. Y on such seemingly impressive RDE performance because RDE and MEA tests are substantially different (Fig. 2)<sup>16,19,21,31-33</sup>. Remaining g

challenges need to be overcome for state-of-the-art highly active ORR catalysts to gain widespread application in commercial PEMFCs, including scaling up production of these catalysts without losing their activity and stability, and successfully translating their superior RDE performance into MEA performance. Make it just as effective in real-life

#### Challenges for achieving ultralow Pt loading in MEA

In this section, we outline the remaining obstacles to achieving high MEA performance with ultralow Pt loading: lack of intermediate testing technologies; achieving a catalyst design that takes mass transport into consideration; and designing effective CLs.

Lack of intermediate testing technologies. To effectively develop assess the performance of novel catalysts and compare results across sile boratories. The RDE testing method (Fig. 3a) is a well-established methodology that has been widely accepted for determining the set of mass activity and the fundament. methodology that has been widely accepted for determining the by mass activity and the fundamentally more meaningful specific activity of catalysts<sup>34</sup>.

Two key features of the RDE method are the low solubility of  $O_2$  in the HClO<sub>4</sub> aqueous electrolyte and the very thin CL (under 1  $\mu$ m). As a result, ORR activity through RDE measurement is typically evaluated at 0.9V in a very-low-current-density region typically evaluated at 0.9 V in a very-low-current-density region  $\searrow$  (normally  $\leq$ 10 mA cm<sup>-2</sup>), in which the electrochemical behaviour is dominated by reaction kinetics. However, in practical fuel-cell operation or MEA-level tests where the operating current densities are mostly  $\geq$ 1 A cm<sup>-2</sup> both kinetics and mass transport significantly Scenarios are mostly >1 A cm<sup>-2</sup>, both kinetics and mass transport significantly affect the performance. That is because of the completely different proton and O<sub>2</sub> transport mechanisms in an MEA compared with in D an RDE.

In an RDE (Fig. 3), the CL is in a thin-film structure with two-phase interfaces (liquid electrolyte and catalyst) as the reaction  $\mathbf{F}_{2}$  supplied through rotation of the electrode. However, in an MEA, the CL is about six to ten times thicker and the reaction zones are the well-known three-phase interfaces (gas, catalyst and ionomer). In particular, oxygen transport over the last few nanometres to the 5 active catalyst surface, possibly across a thin ionomer film, presents a much bigger mass transport resistance than in the RDE condition  $^{5:6}$ . We speculate that the well-known poisoning effect caused by the adsorption of the ionomer's -SO3- groups on the Pt surface might be more pronounced in the CL of an MEA than in an RDE

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Fig. 2 | Performance of state-of-the-art catalysts evaluated in RDE and MEA. The asterisk indicates that the MEA data are not available in the reference but have been extracted from the fuel-cell polarization curves. The question marks indicate that the catalyst was not tested in a fuel cell<sup>12,15,27</sup>. All the RDE data were obtained in O2-saturated 0.1 M HClO4. MEA test conditions, Pt3Ni nanoframes (NFs)<sup>10</sup>: cathode Pt loading is 0.035 mg<sub>Pt</sub> cm<sup>-2</sup>, in 150 kPa H<sub>2</sub>/ O2 (80 °C, 100% RH, gas flow is not mentioned); L10-CoPt (ref. 21): cathode Pt loading is 0.105 mg<sub>Pt</sub> cm<sup>-2</sup>, in 150 kPa H2/O2 (80 °C, 100% RH, 500/1,000 s.c.c.m.); ultralow concentration of Pt alloy supported over precious-group-metal (PGM) free materials (LP@PF-2) (ref. 3): cathode Pt loading is 0.035 mg<sub>Pr</sub> cm<sup>-2</sup>, in 150 kPa H<sub>2</sub>/O<sub>2</sub> (80 °C, 100% RH, 200/200 s.c.c.m.); PtNi bunched nanocages (BNCs) (ref. <sup>16</sup>): cathode Pt loading is 0.15 mg<sub>Pr</sub> cm<sup>-2</sup>, in 200 kPa H<sub>2</sub>/air (80 °C, 100% RH, 150/300 s.c.c.m.); L1<sub>0</sub>-PtZn (ref. <sup>32</sup>): cathode Pt loading is 0.104 mg<sub>p</sub>, cm<sup>-2</sup>, in 150 kPa H<sub>2</sub>/O<sub>2</sub> (80 °C, 100% RH, both 500-1,000 s.c.c.m.); Pt/C (ref. 33): cathode Pt (commercial 46.5 wt% Pt/C catalyst (TANAKA)) loading is 0.09 mg<sub>P1</sub> cm<sup>-2</sup>, in 100 kPa H<sub>2</sub>/O<sub>2</sub> (80 °C, 100% RH, both 500-1,000 s.c.c.m.). The MEA data for Mo-Pt<sub>3</sub>Ni, PtPb nanoplates and jagged Pt nanowires (J-Pt NWs) are not reported. Images reproduced with permission from: Pt<sub>3</sub>Ni NFs, ref. <sup>19</sup>, AAAS; Mo-Pt<sub>3</sub>Ni, ref. <sup>27</sup>, AAAS; PtPb nanoplates, ref. <sup>15</sup>, AAAS; J-Pt NWs, ref. <sup>12</sup>, AAAS; L1<sub>0</sub>-CoPt, ref. <sup>21</sup>, Elsevier; LP@PF-2, ref. <sup>31</sup>, AAAS; PtNi BNCs, ref. <sup>16</sup>, AAAS; L1<sub>0</sub>-PtZn, ref. <sup>32</sup>, Wiley.

nsistent ivironment in consisten because the affinity of -SO3- groups for the Pt surface might be weaker due to the stronger hydrophilicity of aqueous HClO<sub>4</sub> electrolyte in RDE conditions. In addition, the maintenance of a highly active CL structure is more challenging in MEAs because of the harsher reaction conditions, including higher operating currents Nev N and temperatures, as well as more frequent voltage changes during automotive applications.

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Therefore, in spite of the convenient and versatile nature of the RDE method and its importance in early catalyst screening, the results obtained by RDE cannot be used directly to compare the results obtained by RDE cannot be used directly in the second E DCC the same excellent performance in an MEA. Hence, intermediate catalyst-screening technologies are required to bridge the discrepancy, particularly to address the narrow range of accessible current £ξ density in RDE tests, which we discuss later.

Obstacles from catalysts to CLs. The biggest challenge to achieving an ultralow-Pt-loaded MEA is translating highly active, mass-produced catalysts into CLs with superior performance. The CL in the MEA is where the electrochemical reaction takes place, and where the transport of O2, protons, electrons and water occurs, all of which are of particular importance for the ORR. In this sense, how to minimize the mass transport resistances in a CL to maximize the utilization of a given highly active catalyst becomes Critical importance of opposing most france is advance efficiency of oxygen reduction of the second second

fusion layer (GDL) and the proton exchange membrane (PEM), across which O<sub>2</sub> and protons are respectively transported into the cathode CL. The mass transport limitation across their interfaces is an obstacle and need to be minimized. A closer look at this CL reveals ionomer-coated agglomerates and aggregates of Pt/C par-

NATURE ENERGY | VOL 6 | MAY 2021 | 475-486 | www.nature.com/natureenergy

ticles, forming a porous network with macropores) and mesopores respectively. The pressure-dependent molecular diffusion at macro pores and pressure-independent Knudsen diffusion at mesopores of O<sub>2</sub> and water need to be optimized. Oxygen mass transfer resistance also occurs locally across interfaces, including the ionomer/ gas interface ( $R_{I/gas}$ ) and the ionomer/Pt interface ( $R_{I/Pt}$ ,  $-SO_3^-$  poisoning) and resistance in the bulk ionomer thin film  $(R_I)$ . Local  $O_2$ mass transfer resistance contributes the most to the total O2 transport resistance35,37,38

Reducing the ionomer content of the CL can drastically decrease the overall  $O_2$  transport resistance, particularly the local  $O_2$  mass transport resistance caused by -SO3<sup>-</sup> poisoning. As the impact of -SO<sub>3</sub><sup>-</sup> poisoning may be more pronounced in ultralow-Pt-loading MEAs due to higher ionomer/Pt ratio, lower ionomer content may improve local O2 transport more significantly. However, sufficient onomer is needed to coat catalyst agglomerates, form a porous catalyst and solid electrolyte network, and facilitate proton transpor throughout the CL crucial for one of voromer in clumer to the Electron transport is not as much of an issue in the CL, as mos

of the catalyst aggregates and agglomerates in the layer form a continuous electron transport network. However, depending on the ink formulation and ionomer content, some catalyst particles may become totally electronically isolated by the ionomer, forming dead zones. Cracks between catalyst islands in the layer can also result in large dead zones if the contact between catalyst islands and the GDL is lost.

Of particular note is the continuous reduction in mass transport along with catalyst decomposition during fuel-cell operation. As most highly active catalysts are made of a Pt-M alloy, the leached cations may lower water absorption ability and reduce the conductivity of the membrane and the cathode CL ionomer due to cation exchange resulting in poorer proton transport<sup>39,40</sup>. Even

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# September 24, 2024:

✓ Finish annotations for figures 4 and 6c in Bridging the gap between highly active oxygen reduction reaction catalysts and effective catalyst layers for proton exchange membrane fuel cells.



**Fig. 4 | Sources of mass transport resistance inside the MEA of a PEMFC.** The functional layer abbreviations denote microprous substrate (MPS), MPL and CL). The resistance symbols denote Knudsen resistance ( $R_{knr}$ , pressure independent), molecular diffusion resistance ( $R_{Molr}$ , pressure dependent), ORR kinetics resistance ( $R_{kinr}$ , proton transport resistance ( $R_{kinr}$ , pressure independent), molecular diffusion resistance ( $R_{Molr}$ , pressure dependent), ORR kinetics resistance ( $R_{kinr}$ , proton transport resistance ( $R_{kinr}$ , pressure independent), molecular diffusion resistance ( $R_{Molr}$ , pressure dependent), ORR kinetics resistance ( $R_{kinr}$ , proton transport resistance ( $R_{kinr}$ , pressure independent and equal to  $R_{UPR} + R_i + R_{U}$  ( $R_{pinr}$ ) which represents the O<sub>2</sub> transport resistances through the ionomer/gas interface ( $R_{Ugas}$ ) and the ionomer/Pt interface ( $R_{UPR}$ ) and local resistance in the bulk ionomer thin film ( $R_i$ )). Micropores (<2nm) are pores in carbon supports, mesopores (2-20 nm) are pores formed between catalyst particles and macropores (>20 nm) are larger pores formed between catalyst agglomerates. **a**, Equivalent circuit model of mass transport, showing the O<sub>2</sub> transport pathway (orange in **c**) and the proton transport pathway (blue in **c**) through the CL. **b**, Enlarged model of an agglomerate and the interfaces of CL/GDL and CL/PEM. **c**, Spatial deconvolution of the  $R_{LOTR}$  through macropores and partially across macropores before the reactive gases reach the catalyst's surface (black dots).



**Fig. 6 | Mass transport enhancement at interfaces. a**, Evolution from a two-dimensional interface to a three-dimensional engineered interface. DMD technology and a three-dimensional engineered interface between the PEM and CL can be explored to improve contact at the PEM/CL interface, thereby boosting proton transport as well as water back-diffusion at that interface. **b**, Schematic of MPL/CL interfacial contact. Produced water could accumulate in the interfacial gap between the MPL and CL, affecting O<sub>2</sub> flux to the CL. **c**, Polarization curves of three interfacial geometry models of MPL/CL: case 1, perfect contact ( $\delta = 0$ , where  $\delta$  is the height variables that was scaled for numerical convenience); case 2, the measured MPL/CL interface ( $\delta$ ) obtained from ref. <sup>20</sup> was incorporated into the model; case 3, the same MPL/CL interface as in case 2, but with a 1-µm-larger space ( $\delta + 1$ ). *E*, potential. Panels adapted with permission from: **b**, ref. <sup>20</sup>, IOP; **c**, ref. <sup>91</sup>, Elsevier.

# September 26, 2024:

Section 1 Structure, Property, and Performance of Catalyst Layer in Proton Exchange Membrane Fuel Cells

13	Page 2 of 61		Electrochemical Energy Reviews (2023) 6:13		
Gree	ak letters	ve me	Using smaller amounts of noble menals (ex. platinum	n	
a	Transfer coefficient	200	erformance, durability and catalyst loading are usually in		
ß	Non-Darcy coefficient $[m^{-1}]$	P P	a trade-off relation, which requires rigorous optimizations		
δ	Thickness [m]	De + g	with multiple design parameters, including the materials		
E	Porosity		formulation and microstructure of CLs.		
n	Over potential [V]		In a PEM fuel cell, hydrogen fuels and oxidants are sup-	FC.SH	nucture
θ	Contact angle [rad]		plied into the flow channels, gas diffusion layers (GDLs),	``ر	
λ	Mean free path [m]		and CLs. In anodic CLs, hydrogen molecules are firstly	se s	
μ	Dynamic viscosity [Pa s]		adsorbed on the catalyst surface, where the hydrogen-hydro-	βŧ <sub>H</sub>	B
v	Poisson's ratio		gen bond (H-H) is broken and produces adsorbed atomic	ર્ટ ગ	E
ρ	Density [kg $m^{-3}$ ]		hydrogen (H*) [2]. Subsequently, each adsorbed hydrogen	5 3	)e(
$\sigma$	Surface tension $[N m^{-1}]$	0	atom gives up an electron $(e^{-})$ and a proton $(H^{+})$ . The gener-	εğ	2
τ	Tortuosity	1 al	ated electrons and protons will be transported by electron-	5 A	te
$\Phi$	Volume fraction	allock	conducting components (e.g., carbon supports) and iono-	9-0	8
ω	Volume fraction of ionomer in catalyst layer	Yoll	mers, respectively, releasing the occupied catalyst surface,	y '	So o
~ .		×.	which is known as the hydrogen oxidation reaction (HOR).	Xid Xid	e o
Sub	scripts		Protons are transported through membrane to cathodic CLs,		e e
act	Activation		while electrons are blocked by the membrane and have to	ЧÏ	3
an	Anode		move into the external circuit, where electricity is gener-		
D	Bulk properties		ated. In cathodic CLs, the oxygen reduction reaction (ORR)		
с	Capillary		occurs via two major pathways under different conditions:		
ca			dissociative and associative pathways [2, 3]. For the disso-		
еп	Effective		ciative pathway (a.k.a. the four-electron pathway), oxygen		
ele	Electronic		is adsorbed by the catalyst surface, where the oxygen-oxy-		
eq	Equivalent		gen bond (O=O) is broken and generates adsorbed atomic		
g	Gas phase		oxygen (O*). Each adsorbed oxygen atom is protonated by		
geo	Geometric		H <sup>+</sup> and reduced by e <sup>-</sup> to give the surface bonded hydroxyl		
Kn in	Knudsen		(OH*) groups. The OH* can be further reduced and proto-		
in ion	Iniet		nated to form water. When the water is removed from the		
1011	Ionic Liquid water		catalyst surface, the reaction sites are released and will be		
1	Liquid water Mambrong		ready for the next reactions. For the associative pathway		
m	Membrane Membrane water		(a.k.a. the peroxide or two-electron pathway), oxygen is		
niw	Outlot		firstly adsorbed by the catalyst surface while the O=O bond		
n	Bore		may remain unbroken. The adsorbed oxygen reacts with pro-		
p rof	Pole		tons and electrons to finally form hydrogen peroxide (H <sub>2</sub> O <sub>2</sub> ).		
ICI 6	Solid phase		Therefore, the ORR is more complicated, and generally		
s	Solution		more sluggish than the HOR [4]. It should be mentioned that		
sat	Saturation Standard anasimon		water is formed at the triple phase boundary (TPB) in the		
sub	Substrate		cathodic CLs, where catalyst, ionomer, and reactants meet.		
sub	Test specimen		The electrochemical reaction cannot be facilitated effectively		
w	Water		unless most catalyst surface is concurrently accessible to the		
w	water		reactants, protons, and electrons, with excellent capabilities		
			of liquid water release. Otherwise, excessive liquid water		
			products can either occupy the reactive surface or block the		
11	ntroduction		reactant transport, which is known as water flooding in PEM		L.
			fuel cells.	-	
Cost	t, performance, and durability are the major bar	riers to	A poor selection of catalysts or the poor design of the	٦	<u>ŝ</u> S

the high-volume manufacturing of catalyst layers (CLs) for proton exchange membrane (PEM) fuel cells. It is estimated that the cost of CLs and their applications can be around 42% in a PEM fuel cell stack with a high-volume production of 500 000 systems per year [1]. The cost reduction of CLs can be achieved by two pathways: improving performance/

A poor selection of catalysts or the poor design of the CL structure may result in the generation of a large amount of H<sub>2</sub>O<sub>2</sub> during the cell operation, which can attack and decompose ionomer, polytetrafluoroethylene (PTFE), or carbon supports. The most prevalent catalyst employed in PEM fuel cells is Pt based due to its excellent capability to facilitate the dissociative pathway reactions, to enhance

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### Electrochemical Energy Reviews (2023) 6:13 What is Gibbs function

types of Pt-based electrocatalysts has been enhanced sig-

nificantly (e.g., in the range from 0.2 to 14 A  $mg_{Pt}^{-1}$  [8]) by

reducing particle size, controlling particle shapes, alloying

Pt with transition metals, and optimizing CL formulation.

employed in an actual fuel cell is not improved as much

Pt with transition metals, and optimizing CL formulation. C However, the comprehensive performance with catalysts t amployed in an actual fuel cell is not improved as much

 $S_{\rm S}$  as expected due to the limited reactant transport capabil-

Sity and low utilization of catalysts under practical operating + conditions. As a result, carbon-supported Pt (Pt/C) remains S the most commonly used catalyst for commercial PEM fuel

cells. To further reduce the cost, many efforts have also been

devoted to non-precious metal (NPM) catalysts [2, 9-15] for

PEM fuel cells; however, their performance, reliability, and

Therefore, a well-designed CL should be (1) chemically

active to activate the oxygen, (2) easy to release the product

water from the catalyst surface, (3) stable under corrosive

operating conditions, (4) easy to transport reactants and

products, and (5) easy to transport the electrons, protons, and

transfer heat, which requires an optimized structure resulted

durability need to be further verified.

of arctivation?

reaction rates, and to reduce the Gibbs function of activaby its physicochemical and electrochemical properties, tion [5, 6]. Compared with other metal catalysts, pure Pt has which are resulted from its structure at multi-scale levels; the a more suitable oxygen binding energy for ORR. In addimulti-scale structure of the CLs will be deteriorated during tion to pure Pt, substitute catalysts, including binary (e.g., the long-term cell operation, causing gradual and irrevers-PtCo), ternary (e.g., Pt-Cr-Ni), or even quaternary (e.g., ible performance degradation. Therefore, the CL structure Pt-Ru-Ir-Sn) Pt-transition metal alloys, are widely invesis of great significance for the development of electrochemitigated in order to improve the ORR activity of catalysts cal devices. In this review article, the CL structure formaand simultaneously reduce the cost resulted from expensive catalysts [7]. In the past decade, the mass activity of various

tion, visualization, and characterization have been comprehensively reviewed, and the state-of-the-art experimental techniques and results have been scrutinized. The relation between the CL structure and its physicochemical and electrochemical properties has been reviewed along with the corresponding experimental methods for their characterization. Finally, the interconnection among the CL multi-scale structure, physicochemical and electrochemical properties, performance, and durability is examined and discussed.

#### 2 Formation, Visualization and Characterization of Catalyst Layer Structure

The practical structure of CLs, which is conventionally composed of carbon-based platinum (e.g., Pt/C), ionomer (e.g., Nafion polymer), and void regions (i.e., porous space) [3], can be determined by various manufacturing parameters, including material specification (e.g., nature of catalyst and ionomer materials, size and shape of particles, and composition), catalyst ink composition, preparation procedures, ink application techniques, and drying and hot-pressing conditions [23-25]. The development of novel catalyst and ionomer materials and the optimization of CL composition have gained significant attention, while little progress has been made to the understanding of CL structure formation and the effect on the PEM fuel cell performance. The highly random and delicate nature of CL structure typically ranging from a few nanometers to a few micrometers makes it challenging to capture all details of the CLs using the existing visualization and characterization techniques. Recent innovative fabrication methods have modified traditional CL materials and composition, e.g., plasma sputtering [26], ion-beam-assisted deposition [27], and atomic layer deposition [28], making the corresponding structure more complicated. Therefore, the major factors affecting the CL structure formation and the recent progress in advanced experimental techniques for CL structure visualization and characterization are reviewed in this section.

#### 2.1 Structure Formation

The CL cannot stand alone and is formed during the fabrication process, and the CL structure can be affected by many

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from the manufacturing processes [5]. Unfortunately, the CL structure and its impact on the reaction pathways, rates, and component durability have not been fully understood, and there is still no agreement on what the best CL structure should be and how the CL structure affects the short- and laver Structure properties of long-term performance. Therefore, the understanding of the CL structure, properties, performance, and their relationships is urgently needed.

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The CL structure covers a wide range of length scales, involving the CL thickness from a few nanometers to tens of microns, the pore sizes at the levels of nanometers and Varying catalyst microns, the agglomeration of the Pt/C with ionomer of a few microns, Pt particles of several nanometers, and the accompanied local reactant, water, and charged species transport within the multi-scale solid and porous structure. Examples of typical multi-scale structure-related features

in CLs are shown in Fig. 1 based on the characteristic dimensions. Waking them more accessible Many efforts have been devoted to developing low-cost, high-performance, and high-durability CLs for the PEM fuel cells; however, the CL still requires improvements to further enhance the mass transport capability and the utilization of

> how efficiently reactants are delivered to reaction sites & how quickly products one removed. Affects overall performance and efficiency.

catalyst to enhance the performance and reduce the cost of

CLs for mass production. The CL performance is determined

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### September 29, 2024:

Section 2.1 Structure, Property, and Performance of Catalyst Layer in Proton Exchange Membrane Fuel Cells

Electrochemical Energy Reviews (2023) 6:13 What is Gibbs function

reaction rates, and to reduce the Gibbs function of activa-S tion [5, 6]. Compared with other metal catalysts, pure Pt has Opti a more suitable oxygen binding energy for ORR. In addition to pure Pt, substitute catalysts, including binary (e.g., effective PtCo), ternary (e.g., Pt-Cr-Ni), or even quaternary (e.g., pensive Pt-Ru-Ir-Sn) Pt-transition metal alloys, are widely investigated in order to improve the ORR activity of catalysts and simultaneously reduce the cost resulted from expensive most catalysts [7]. In the past decade, the mass activity of various types of Pt-based electrocatalysts has been enhanced significantly (e.g., in the range from 0.2 to 14 A  $mg_{Pt}^{-1}$  [8]) by the E reducing particle size, controlling particle shapes, alloying Pt with transition metals, and optimizing CL formulation.  $\nabla$  Pt with transition metals, and optimizing  $\Sigma$  However, the comprehensive performance with catalysts  $\underline{\circ}$ employed in an actual fuel cell is not improved as much lofinum. S as expected due to the limited reactant transport capabil-Sity and low utilization of catalysts under practical operating conditions. As a result, carbon-supported Pt (Pt/C) remains the most commonly used catalyst for commercial PEM fuel  $\overline{\frown}$ cells. To further reduce the cost, many efforts have also been devoted to non-precious metal (NPM) catalysts [2, 9-15] for PEM fuel cells; however, their performance, reliability, and 9000 Billyer durability need to be further verified.

Therefore, a well-designed CL should be (1) chemically active to activate the oxygen, (2) easy to release the product water from the catalyst surface, (3) stable under corrosive operating conditions, (4) easy to transport reactants and products, and (5) easy to transport the electrons, protons, and transfer heat, which requires an optimized structure resulted from the manufacturing processes [5]. Unfortunately, the CL structure and its impact on the reaction pathways, rates, and component durability have not been fully understood, and there is still no agreement on what the best CL structure should be and how the CL structure affects the short- and long-term performance. Therefore, the understanding of the CL structure, properties, performance, and their relationships is urgently needed.

Varying properties of Catalyst laver Structure

The CL structure covers a wide range of length scales, involving the CL thickness from a few nanometers to tens of microns, the pore sizes at the levels of nanometers and microns, the agglomeration of the Pt/C with ionomer of a few microns, Pt particles of several nanometers, and the accompanied local reactant, water, and charged species transport within the multi-scale solid and porous structure. Examples of typical multi-scale structure-related features in CLs are shown in Fig. 1 based on the characteristic dimensions. WOWiNG there were processible >

dimensions. WOWING them more QCCESSIBLE Many efforts have been devoted to developing low-cost, high-performance, and high-durability CLs for the PEM fuel cells; however, the CL still requires improvements to further enhance the mass transport capability and the utilization of catalyst to enhance the performance and reduce the cost of CLs for mass production. The CL performance is determined

how efficiently reactants are delivered to reaction sites & how quickly products are removed. Affects overall performance and efficiency.

by its physicochemical and electrochemical properties, which are resulted from its structure at multi-scale levels; the multi-scale structure of the CLs will be deteriorated during the long-term cell operation, causing gradual and irreversible performance degradation. Therefore, the CL structure is of great significance for the development of electrochemical devices. In this review article, the CL structure forma-5 tion, visualization, and characterization have been compre-B hensively reviewed, and the state-of-the-art experimental techniques and results have been scrutinized. The relation COVEY between the CL structure and its physicochemical and electrochemical properties has been reviewed along with the corresponding experimental methods for their characteriza-tion. Finally, the interconnection among the CL multi-scale structure, physicochemical and electrochemical properties, performance, and durability is examined and discussed.

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#### 2.1 Structure Formation

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Fig. 1 Multi-scale catalyst layer structure with representative phenomena. Adapted with permission from Ref. [16]. Copyright O 2012, Elsevier. Adapted with permission from Ref. [17]. Copyright O 2004, the Electrochemical Society. Reprinted with permission from Ref. [18]. Copyright O 2015, Elsevier. Adapted with permission

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factors, including the CL ingredients, fabrication methods, procedures, and conditions, as well as the support substrates. The CLs for PEM fuel cells made in the 1960s were composed of Pt black and PTFE with a high Pt loading of  $17-45 \text{ mg cm}^{-2}$  [29]. PTFE in the CLs not only is a binding material to stabilize the catalysts (to avoid being washed away by liquid water and reactant gas) but also improves the hydrophobicity of the CL to decrease the transport resist-▶ ance of water and reactants [30]. However, the PTFE content should be optimized as excess PTFE material may cover the surface of catalyst particles, reducing protonic conductivity and active catalytic surface. To reduce the proton transport resistance, the PTFE-bounded CLs are routinely impregnated with proton-conductive Nafion polymer. However, the utilization of catalyst is still as low as ~20%, leading to a significant material cost, although excellent durability is đ observed [31]. SSS

To decrease the catalyst loading, Ticianelli et al. [32] adopted carbon-supported platinum (Pt/C) instead of the Pt black in the 1980s. The carbon supports are typically carbon

<sup>3</sup> black with high surface areas, such as Vulcan XC-72, Ketjen black, and Black pearls 2000. Recently, carbon supports

with different morphology and sizes are actively investigated to support catalyst nanoparticles (e.g., Pt nanoparticles), including nanofiber [33], nanotube [34, 35], graphene [36], and composite supports [37]. The carbon supports can create an efficient network for electron transport between Pt surface and GDLs. The substitution of Pt/C for Pt black significantly reduces Pt loading to 0.35 mg  $\text{cm}^{-2}$  with fuel cell performance equivalent to that of CLs fabricated with Pt black [38]. Furthermore, Wilson et al. [39] employed hydrophilic Nafion polymer instead of hydrophobic PTFE 5 material, which further enhanced the cell performance. By this means, the catalyst particles can maintain excellent contact with Nafion polymer, not only stabilizing the catalyst particles but also improving the transport of protons lyst particles but also improving the transport of protons to between the electrode and electrolyte. The binding materials with high dissolubility and diffusivity for reactant gases are favorable as the catalyst surface is often covered by a thin layer of binding materials. The gas dissolubility and diffusivity of the binding materials determine the reactant concentration on the catalyst surface, which affects the reaction rate [5, 40]. With Nafion polymer, the power density is doubled in comparison with that of the PTFE-bound CLs,

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and the electrochemical surface area (ECSA) is increased from 22% (PTFE-bounded CLs) to 45.4% (ionomer-bounded CLs). It should be noted that ionomer-bounded CLs are usually thinner than 50  $\mu$ m with reduced overall mass transport resistance through CLs. The ionomer-bonded CL fabrication methods are often referred to as thin-film methods [41], which are widely employed in the industry.

According to the types of coating substrates and experimental procedures, three types of thin-film methods are widely used for CL fabrications, i.e., catalyst coated on GDL substrate (CCS) [42, 43], catalyst coated on membrane (CCM) [42, 44], and decal transfer method (DTM) [41, 45], as shown in Fig. 2. For CCS methods, the catalyst ink (a mixture of Pt/C, ionomer, and solvent) is firstly coated on one side of GDL to form a gas diffusion electrode (GDE), and then, the prepared GDEs are assembled with a membrane in between to form the membrane electrode assembly (MEA) [43]. It should be mentioned that the GDL can have a two-layer structure, including a layer of PTFE-treated carbon fiber and a microporous layer (MPL) composed of a mixture of carbon particles and PTFE. The CCS method is easy for implementation; however, it remains challenging to minimize the penetration of Page 5 of 61 13

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catalyst ink into GDLs, which can cause catalyst isolation and pore blockage. Zhao et al. [42] sprayed the catalyst ink on the surface of MPLs and observed catalyst penetration into MPLs and GDLs, reduced porosity, and increased mass transport resistance. For CCM methods, catalyst ink is directly coated on both sides of the membrane, with two GDLs covering on the outer sides of CLs to form the MEA [44]. The CLs fabricated by the CCM methods demonstrate excellent interfacial properties between the CLs and membrane, resulting in superior cell performance. However, the swelling of membrane caused by the solvent has a detrimental influence on the CL microstructure; therefore, a vacuum table is often used during the fabrication process to hold the membrane in place, which increases the complexity of the manufacturing system [44, 46]. For DTM methods, the catalyst ink is coated onto a decal substrate, followed by a hot-pressing process to transfer the CLs onto the membrane to form the CCM. The DTM method often requires experienced operators or high-precision automa-tion externs to excid the new uniform and incomplete tion systems to avoid the non-uniform and incomplete transference of catalysts from substrate to membrane; thus, this method may be limited when the catalyst loading is further reduced to much less than 0.1 mg  $cm^{-2}$  [47].

Fig. 2 Three major approaches of the thin-film methods for the catalyst layer fabrication. Adapted with permission from Ref. [48]. Copyright © 2019, the author(s)











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As can be seen, the structure of the thin-film CLs is primarily formed during the ink coating process. The coating of catalyst ink can be implemented by various techniques, including blading [49–51], brushing [31], spraying [44, 52, 53], rolling [54], screen printing [55, 56], and inkjet printing [56, 57] as shown in Fig. 3a-f. Many methods have been recently developed and employed to achieve ultra-low-Ptloading thin-film CLs, including ultrasonic spraying [58],

electrospraying [59-62], and electrospinning [63], which are summarized and illustrated in Fig. 3g, h. Currently, the catalyst ink-based thin-film CLs with balanced performance,

durability, and cost are the most commonly used in the industry as the catalyst loading and thickness have been significantly reduced [64].

To further reduce catalyst loading and increase catalyst utilization, direct deposition of Pt on GDLs or membrane without carbon supports and with Nafion polymer partially covered is widely investigated. Typical methods employed for direct deposition of Pt to form an ultra-thin CL (typically thinner than 1 µm with an ultra-low Pt loading of much lower than 0.1 mg cm<sup>-2</sup>) include sputtering deposition [66, 67], ion-beam [68-70], and atomic layer deposition (ALD)



Fig. 3 Schematic of various catalyst ink coating techniques. a Doctor blading. b Brushing. c Spraying. d Rolling. (c, d) Reprinted with permission from Ref. [54]. Copyright © 2009, Springer Nature. e Screen printing. Reprinted with permission from Ref. [25]. Copyright

© 2011, Elsevier. f Inkjet printing. g Ultrasonic spraying. (a, f, g) Reprinted with permission from Ref. [65]. Copyright © 2018, Elsevier. h Electrospinning and electrospraying. Reprinted with permission from Ref. [63]. Copyright © 2014, Elsevier



Fig. 4 Schematic of various fabrication techniques for ultra-low-Ptloading catalyst layers. **a** Plasma sputtering. Reprinted with permission from Ref. [26]. Copyright © 2004, Elsevier. **b** Ion-beam-assisted deposition. Reprinted with permission from Ref. [27]. Copyright

© 1992, American Vacuum Society. c Atomic layer deposition. Reprinted with permission from Ref. [28]. Copyright © 2009, American Chemical Society

[71–74] as shown in Fig. 4. In the past decade, the order structural CLs have been actively investigated in the literature due to their excellent capabilities of minimizing Pt loadings and improving reactant transport. Yao et al. [75] developed porous Pt-Ni nanobelt arrays by following a procedure of hydrothermal processing, magnetron sputtering, decal transferring, and acid treatment. In comparison with traditional CCM methods, the new developed CLs with ultra-thin, ionomer-free, porous and oriented microstructure demonstrated better catalytic activity and mass transport capabilities. Ozkan et al. [76] developed titania nanotubes for cathode CLs. It was found that longer nanotubes (10  $\mu m)$ demonstrated better performance than shorter ones (5  $\mu$ m), and in comparison with photodeposition, ALD methods can create more uniform and better dispersed Pt distribution on nanotube surfaces. Murata et al. [77] developed vertically aligned carbon nanotubes for cathode electrodes, and the

MEA produced superior performance of 2.6 A cm<sup>-2</sup> at 0.6 V with ultra-low cathode Pt loading of  $0.1 \text{ mg cm}^{-2}$  due to enhanced transport capabilities of oxygen, protons, electrons, and water. Recently, the ionomer-free ultra-thin CLs, e.g., 3 M nanostructured thin-film (NSTF) CLs prepared by sputtering, have gained significant attention to reduce the Pt cost for PEM fuel cells with plausible stability [78]. A comparison of the NSTF electrodes and traditional Pt/C electrodes is shown in Fig. 5, demonstrating that the NSTF electrodes are much thinner and have smaller pore volume and no ionomer coverage in comparison with traditional Pt/C electrodes. However, due to the nature of hydrophilic NSTF surface, liquid water tends to accumulate in cathode CLs during the actual fuel cell testing. In addition, as no ionomer is applied in the ultra-thin layer of NSTF catalysts, the proton conductivity is relatively low. To overcome these drawbacks, a thin "interlayer" of dispersed catalysts and



Fig. 5 Cross-sectional scanning electron microscopy (SEM) images of a traditional Pt/C electrode, b NSTF electrode, and c enlarged view of NSTF electrode structure. Reprinted with permission from Ref. [78]. Copyright © 2014, the Electrochemical Society

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ionomers were applied between the NSTF layer and the
MPL by Kongkanand et al. [79]. However, as the Pt loading
is very low, the durability of the ultra-thin CLs may be a
problem although the material cost can be reduced. There fore, efforts have been continuously made to further improve
these techniques for enhanced manufacturing efficiency and
durability for industrial applications [80].

#### 2.2 Structure Visualization

The CL structure is complicated at different length scales from atomic to macroscale levels [81]. It is vital to visualize the multi-scale multi-dimensional structure of CLs to identify any morphology defects, to recognize the catalyst crystallinity, shape, and size, to inspect carbon agglomeration and connectivity, to check the ionomer coverage, and to understand pore structure. The typical CL thickness ranges from several nanometers to tens of microns, which often requires a combination of two or more microscopy techniques to visualize the exterior and interior structure of CLs at different scales. The commonly used microscopy techniques for CLs are reviewed in this section based on different dimensions: 2D, 3D, and 4D techniques. 2D techniques are the most commonly used for CL structure visualization from the exterior sample surface, including optical microscopy, scanning electron microscopy (SEM), transmission electron microscopy (TEM), and atomic force microscopy (AFM). The interior structure of CLs can be visualized by 3D techniques, such as focused ion-beam/scanning electron microscopy (FIB/SEM) and 3D X-ray computer tomography (3D X-ray CT). Recently, 4D techniques have been developed to obtain more detailed information about the CLs, and the fourth dimension can be chemical composition, time, temperature, or other physical parameters in addition to 3D spatial structure.

#### 2.2.1 2D Microscopy Techniques

The exterior structure of the CLs is commonly investigated by a variety of 2D microscopy techniques including optical microscope, SEM, TEM, AFM, and other techniques to obtain information about catalyst dispersion, carbon support connectivity, ionomer coverage, and pore structures from the surface. Table 1 summarizes the commonly used 2D microscopy techniques for CL visualization.

Optical microscopy (a.k.a. light microscopy) utilizes a system of lenses to magnify images of small objects based on visible lights with a typical resolution of ~0.2  $\mu$ m. Optical microscopy is commonly used in characterizing the morphology of the CL surface, e.g., the dispersion of the catalyst, the catalyst agglomerates, pinholes, cracks, and even ice crystals, which are in the size of a few microns [16, 84]. SEM is frequently used to generate magnified images of CLs

with higher resolution (around 10 nm) than optical microscopy by using focused electron beams instead of light waves as probing species [85]. SEM is very helpful and widely used for the characterization of the CL structure at the nano- and microscale levels [86, 87], e.g., micro-cracks and agglomerates of Pt/C particles in the CLs in a few nanometers [82]. Traditional SEM performs imaging in a vacuum environment for better resolution, and environmental SEM (a.k.a. ESEM) allows visualizing the samples in their natural state in wet and gaseous environments, which can be used to visualize the tiny water drops on the surface of CLs [83]. TEM is suitable for imaging specimens at the atomic level with a maximum resolution of 0.5 nm by focusing a beam of high-energy electrons onto the specimen [41]. TEM is broadly used to visualize the nano- and microstructure of the electrocatalysts and ionomer in CLs, e.g., the catalyst particle size, shape, and dispersion of Pt nanoparticles with tiny size of 0.33 nm [37], ionomer coverage [88], three-phase microstructure of the Pt, ionomer, and carbon [22]. AFM utilizes a cantilever with a probing tip to detect the surface of the specimen with a maximum resolution of 0.5 nm [89, 90]. When the probing tip scans over the specimen surface, the cantilever will be deflected in response to the forces between the tip and specimen. This technique is suitable for the detection of the sample surface at atomic levels, e.g., roughness, cracks, holes, although it is limited to recognize the interior structure of a specimen [17].

#### 2.2.2 3D Microscopy Techniques

Due to the complex manufacturing process, the near-surface and interior structure of the CLs may be significantly different. To investigate the interior structure of the CLs, 3D microscopy technologies have been applied to CLs to investigate their morphology and topology. The most commonly used techniques for CLs in PEM fuel cells have been reviewed in this section, such as FIB/SEM and 3D X-Ray CT.

(1) Focused ion-beam/scanning electron microscopy FIB/SEM utilizes a focused ion beam to etch the sample and SEM to visualize the exposed interior surface, as shown in Fig. 6a. During the practical visualization process, a cubic fiducial mark is first milled on the sample. The specimen is then milled in a particular tiny thickness (e.g., 10 nm), after which SEM is used to take an image for the exposed surface. The cycling of the milling and imaging processes is repeated until a sufficient number of SEM pictures are achieved. The milling direction is often perpendicular to the ion beam, and the SEM images are aligned with the fiducial mark, which will be used to reconstruct the 3D images. The FIB window is demonstrated in the dash-line region, Section 2.4 Structure, Property, and Performance of Catalyst Layer in Proton Exchange Membrane Fuel Cells

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Pt and oxidized Pt species [156]. EDX is another technique widely used for material analysis by detecting X-rays emitted from a material surface after interacting with an electron beam. EDX is widely used to identify and quantify the elements [157], to analyze the distributions of elements coupled with SEM or TEM [158], and to characterize nanostructure, e.g., core–shell and alloy nature [159].

### 2.4 Summary

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The microstructure of CLs, formed during the fabrication process, can be affected by many factors, including materials, composition, fabrication methods, conditions and procedures. The PTFE-bonded CLs are durable due to the extremely high Pt loading applied; however, the high cost resulted from the large amount of noble Pt catalyst unfavored this method in industrial application. Vice versa, the ultra-low-Pt-loading CLs prepared by the plasma sputtering method, ion-beamassisted deposition, or atomic layer deposition can considerably decrease the material cost; however, these methods remain impractical for large-volume manufacturing due to technical challenges in complex fabrication apparatus and unconfirmed long-term performance [31]. The ionomer-bounded method (a.k.a. the thin-film method) demonstrates a good balance between durability and cost, which can be further optimized by improving the CL microstructure. The multi-scale structure of CLs can be visualized by different microscopy techniques, including optical microscopy, SEM, TEM, and AFM, which are suitable to identify the morphology and topology of the CL surface with different spatial resolution. The interior structure can be visualized by FIB/SEM and 3D X-ray CT methods. Advanced 4D microscopy techniques have been also adopted for fuel cell studies to investigate the fourth "dimension", e.g., chemical composition, temperature, time, and other information. Quantitative characterization of the multi-scale CL pore structure includes porosity, PSD, surface area, mean pore size, tortuosity, and other parameters. The pore structure can be characterized by the MSP, MMP, BET, and densometer, and other techniques. The solid structure can be studied by XRD, electron diffraction, Raman spectroscopy, TGA, XPS, EDS, and other methods.

#### 3 Physicochemical Properties of Catalyst Layers

The physicochemical properties, which significantly affect the transport of reactants, water, and heat in the CLs, are determined by the compositional ingredients and multi-scale structure. The performance and durability of CLs can also be affected by various transport and mechanical properties, such as the effective diffusion coefficient, permeability, capillary pressure, contact angle, effective thermal conductivity, and Young's modulus [123, 160, 161]. Unfortunately, the experimental data of these effective properties are very limited for the CLs, due to the difficulties in measuring a thin layer of porous media. Therefore, various experimental techniques specifically designed and potentially applied for the CLs have been comprehensively reviewed in this section. The physicochemical properties are strongly structure-dependent, and the relation between these properties and structural parameters is scrutinized in this section.

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### 3.1 Effective Diffusion Coefficient

#### 3.1.1 Fick's Law of Diffusion

Diffusion, one of the key mass transfer mechanisms in fuel cells, is defined as the net movement of molecules as a result of random molecular motion, which can be caused by a gradient of concentration, temperature, pressure, or external force [160, 162, 163]. The rate of diffusion is governed by Fick's law of diffusion [164].

$$J_{\rm m} = -D\frac{\partial c}{\partial r} \tag{12}$$

where  $J_{\rm m}$  represents the mass flux caused by diffusion in [kg m<sup>-2</sup> s<sup>-1</sup>], c denotes the concentration in [kg m<sup>-3</sup>], x is the diffusion distance in [m], and D denotes the diffusion coefficient in [m<sup>2</sup> s<sup>-1</sup>].

In the open spaces, the diffusion is driven by the collisions between molecules without the interference by any object. The diffusion coefficient is known as the bulk diffusion coefficient, which is governed by not only the gradients of temperature, pressure, and concentration but also the nature of the diffusion substances. In porous media, e.g., the CLs of PEM fuel cells, the reactant gas molecules can collide with a solid CL surface, which slows down the diffusion rates. Therefore, the Fick's law needs to be modified for the diffusion in porous media, where an effective diffusion coefficient is used to replace the bulk diffusion coefficient.

$$J_{\mathrm{m},i} = -D_{\mathrm{eff}} \frac{\partial c_i}{\partial x} \tag{13}$$

where the subscripts, *i* and eff, denote species *i* and effective properties, respectively. The diffusion coefficient in porous media is lower than that in the bulk region as the collision with solid surfaces makes the transport of gas species more difficult.

It should be noted that with the current trends to fabricate CLs with ultra-low loadings much less than  $0.1 \text{ mg cm}^{-2}$ , the thickness of the CLs can be only a few nanometers. Therefore, the reactant transport resistance, especially for oxygen at the cathodes, through pores can be reduced, while that through the thin films of ionomer covered on the surface of

### Section 4.6 Structure, Property, and Performance of Catalyst Layer in Proton Exchange Membrane Fuel Cells

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Model	Formula	Remark	Component	Eq.	Ref.
Springer et al.	$k_{\rm m} = (0.005139\lambda - 0.00326) \exp\left[1268\left(\frac{1}{303} - \frac{1}{T}\right)\right]$	$\lambda > 1$	Membrane	(88)	[234]
Sone et al.	$k_{\rm m} = -19.8 \times 10^{-3} + 16.6 \times 10^{-4} x -$ 34.5 \times 10^{-6} x <sup>2</sup> + 28.4 \times 10^{-8} x <sup>3</sup>	293 K	Membrane	(89)	[267]
Sone et al.	$k_{\rm m} = -8.01 \times 10^{-3} + 6.72 \times 10^{-4} x -$ 11.6 × 10^{-6} x <sup>2</sup> + 11.8 × 10^{-8} x <sup>3</sup>	303 K	Membrane	(90)	[267]
Sone et al.	$k_{\rm m} = -1.75 \times 10^{-3} + 1.45 \times 10^{-4} x + 0.0161 \times 10^{-6} x^2 + 3.45 \times 10^{-8} x^3$	318 K	Membrane	(91)	[267]
Sone et al.	$k_{\rm m} = -3.41 \times 10^{-3} + 2.73 \times 10^{-4} x -$ 2.67 \times 10^{-6} x^2 + 5.72 \times 10^{-8} x^3	333 K	Membrane	(92)	[267]
Sone et al.	$k_{\rm m} = -1.56 \times 10^{-3} + 1.21 \times 10^{-4} x + 1.01 \times 10^{-6} x^2 + 3.95 \times 10^{-8} x^3$	343 K	Membrane	(93)	[267]
Boyer et al.	$k_{\rm m}^{\rm eff} = 0.078 \Phi_{\rm m} + 0.004$	Experimental correlation	Catalyst layer	(94)	[266]
Boyer et al.	$rac{k_{\mathrm{m}}^{\mathrm{eff}}}{k_{\mathrm{m}}}=oldsymbol{\varPhi}_{\mathrm{m}}^{n}$	n=1.2-4.5	Catalyst layer	(95)	[266]
Das et al.	$\frac{k_{\rm m}^{\rm eff}}{k_{\rm m}} = 1 - \beta \left\{ \frac{3\left(1 - \boldsymbol{\Phi}_{\rm m}\right)}{3 - \boldsymbol{\Phi}_{\rm m}} + \frac{3\varepsilon \left[1 - \frac{3\left(1 - \boldsymbol{\Phi}_{\rm m}\right)}{3 - \boldsymbol{\Phi}_{\rm m}}\right]}{2 + \varepsilon} \right\}$	Spherical catalyst particles covered by ionomers	Catalyst layer	(96)	[180]
Das et al.	$\frac{k_{\rm m}^{\rm eff}}{k_{\rm m}} = \left[\boldsymbol{\varPhi}_m(1-\varepsilon)\right]^{1.5}$	Bruggeman correlation	Catalyst layer	(97)	[180]

 $\Phi_{\rm m}$  is the volume fraction of the Nafion in CLs;  $\lambda_{\rm m}$  is correction factor;  $k_{\rm m}$  is bulk membrane protonic conductivity in [S cm<sup>-1</sup>];  $k_{\rm m}^{\rm eff}$  is effective protonic conductivity of catalyst layers in [S cm<sup>-1</sup>];  $\lambda$  is water content;  $\beta$  is a correction factor for the geometrical structure of membrane phase in CLs; and x% is the relative humidity which ranges from 40% to 100%

ionomer and water content determines the intrinsic protonic conductivity of ionomer, while the microstructure affects the overall effective conductivity. Many correlation models have been developed to estimate the intrinsic protonic conductivity of ionomers and effective protonic conductivity of CLs, as summarized in Table 15. Springer et al. [234] established an empirical correlation of protonic conductivity based on Nafion 117 membranes as a function of water content and temperature, which is widely used for fuel cell modeling even though different types of membranes are employed. Sone et al. [267] proposed another polynomial empirical equation about the protonic conductivity of Nafion 117 based on experimental studies at a different temperature between 293 and 343 K with relative humidity levels between 40% and 100%. Boyer et al. [266] built an empirical correlation based on experimental data obtained from polarization curves and found that the ohmic resistance of CLs shows a linear relation with the volumetric fraction of ionomers in the CLs. Boyer et al. [266] also suggested that the effective protonic conductivity of the CLs and the bulk protonic conductivity of the membranes are in exponential relation to the power of 1.2-4.5. Das et al. [180] derived a model to calculate the effective protonic conductivity of the CLs based on the volumetric ratio of ionomer and void space based on the assumption that the CL is composed of multiple spherical catalyst particles covered by thin uniform ionomer layers. In this study, the derived model was compared with Bruggeman correlation (also proposed by Das et al. [180]) under different membrane-catalyst ratios, and the comparison demonstrated good agreements. It should be noted that limited experimental data on effective protonic conductivity of CLs are available in literature due to the difficulty in experimental measurements. Therefore, the validity of various empirical and analytical models should be further explored.

### 4.6 Summary of Structure-Dependent Electrochemical Properties

Many experimental methods and empirical models have been employed to investigate the electrochemical properties of CLs, including exchange current density, charge transfer coefficient, electrochemical surface area, electrode roughness factor, effective electronic conductivity, and effective protonic conductivity. These electrochemical

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Fig. 27 A typical polarization curve of a single PEMFC. Reprinted with permission from Ref. [268]. Copyright © 2014, the Electrochemical Society

Ś properties are vital to understanding the electrode kinetics, ohmic loss, transport phenomena, and cell performance. However, in comparison with physicochemical properties, experimental methods and apparatus for the measurement of electrochemical properties are usually complicated, and some particular properties have to be indirectly measured. Therefore, the accuracy and uncertainty analysis of the experimental methods should be carefully performed. Due to the lack of experimental data on these properties, the analytical or empirical models are very scarce for some of these parameters, including the exchange current density, charge transfer coefficient, and electrochemical surface area (or electrode roughness factor). Some correlation models are available for the effective electronic conductivity and protonic conductivity of CLs; however, the validity of most of these models should be further explored when more experimental data are available.

important to study

### 5 Performance of Catalyst Layers

The overall performance of the PEM fuel cells is determined by all components including membrane, CLs, GDLs, and distribution plates, among which the CLs play a dominant role. The performance is often characterized by a polarization curve for PEM fuel cells, i.e., the voltage-current relation, as shown in Fig. 27. There exists a maximum voltage if all energy stored in hydrogen and oxygen can be converted to electric energy without any losses, and this maximum voltage is called thermo-neutral voltage. However, the thermo-neutral voltage is unachievable as heat generation

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is always accompanied by electricity production during cell operation. Theoretically, the maximum achievable voltage under the thermodynamically reversible condition is always lower than the thermo-neural voltage and is called reversible voltage. In a practical PEM fuel cell, the output voltage will be reduced with an increase in the current density owing to four categories of irreversible polarization or energy losses: (1) reactant (fuel or oxidant) crossover and internal current, (2) activation loss, (3) ohmic loss, and (4) concentration loss, among which the latter three are closely related to the microstructure of the CLs.

#### 5.1 Fuel Crossover and Internal Current

Fuel crossover is a waste of hydrogen molecules by penetrating the electrolyte membrane without effective electrochemical reaction, and internal current is caused by unused electrons which are transported from anodic to cathodic electrodes directly through the membrane [5, 81]. Ideally, only protons and water can pass through the polymer electrolyte membrane, while hydrogen fuel and electrons are rejected. However, a small quantity of fuels and electrons are always possible to diffuse into the membrane from the anode, and the diffusion has a considerable influence on the open-circuit voltage (OCV), which is always smaller than reversible voltage. Each hydrogen molecule that directly crosses the membrane and reacts with oxygen at the cathode will result in two fewer electrons passing through the external circuit. In practical fuel cell operation, this type of energy loss is insignificant as the rate of fuel crossover and electron penetration is a few orders of magnitude lower than that of hydrogen consumption and electrical current in external circuits [231]. However, if the current density is very small, the voltage drop resulted from fuel crossover and internal current may not be negligible. Fuel crossover and internal current can be significantly affected by the nature of membrane material, the thickness of the membrane, and the sealing of the fuel cell stack [269].

#### 5.2 Activation Polarization

Activation polarization is caused by the sluggish kinetics of the electrochemical reactions in CLs, and a certain amount of energy has to be consumed to overcome the activation energy of the electrochemical reactions. The activation loss causes a sharp voltage drop when the operating current density is small, as shown in Fig. 27. The nature of catalyst materials and the nano- and microstructure of CLs determine the activation polarization. However, how the multi-scale structure of the CLs affects the activation loss has not been fully understood but a higher ECSA may help lower the activation over-potential. It should be noted that the activation

# **October Background Research**

### October 04, 2024:

✓ Introduction to Dictating Pt-Based Electrocatalyst Performance in Polymer Electrolyte Fuel Cells, from Formulation to Application

> ACS APPLIED MATERIAL & INTERFACES

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Research Article

### Dictating Pt-Based Electrocatalyst Performance in Polymer Electrolyte Fuel Cells, from Formulation to Application

Tim Van Cleve,<sup>†©</sup> Sunilkumar Khandavalli,<sup>†©</sup> Anamika Chowdhury,<sup>‡,§</sup> Samantha Medina,<sup>||</sup> Svitlana Pylypenko,<sup>†,∥</sup><sup>©</sup> Min Wang,<sup>†</sup><sup>©</sup> Karren L. More,<sup>⊥</sup> Nancy Kariuki,<sup>#</sup> Deborah J. Myers,<sup>#</sup> Adam Z. Weber,<sup>‡</sup><sup>©</sup> Scott A. Mauger,<sup>†</sup><sup>©</sup> Michael Ulsh,<sup>†</sup> and K. C. Neyerlin<sup>\*,†</sup><sup>©</sup>

<sup>†</sup>Chemistry and Nanoscience Center, National Renewable Energy Laboratory, Golden, Colorado 80401, United States <sup>‡</sup>Energy Conversion Group, Energy Technologies Area, Lawrence Berkeley National Laboratory, Berkeley, California 94720, United

<sup>§</sup>Department of Chemical and Biomolecular Engineering, University of California, Berkeley, California 94720, United States <sup>||</sup>Colorado School of Mines, Golden, Colorado 80401, United States

 $^{\perp}\textsc{Oak}$  Ridge National Laboratory, Oak Ridge, Tennessee 37830, United States

<sup>#</sup>Argonne National Laboratory, Lemont, Illinois 60439, United States

Supporting Information

ABSTRACT: In situ electrochemical diagnostics designed to probe ionomer ABSTRACT: In situ electrochemical diagnostics designed to probe ionomer interactions with platinum and carbon were applied to relate ionomer coverage and conformation, gleaned from anion adsorption data, with  $O_2$  transport resistance for low-loaded (0.05 mg<sub>pt</sub> cm<sup>-2</sup>) platinum-supported Vulcan carbon (Pt/Vu)-based electrodes in a polymer electrolyst fuel cell. Coupling the in situ diagnostic data with composition is explained by both ink-level interactions that dictate the electrode microstructure during fabrication and the resulting local ionomer distribution near catalyst sites. Electrochemical techniques (CO displacement and ac impedance) show that catalyst inks with higher water content increase ionomer (sulfonate) interactions with br sites without significantly affecting ionomer coverage on the carbon support. Supersingle, the higher anion adsorption is shown to have a minor impact on specific



ionomer coverage on the carbon support. Surprisingly, the higher anion adsorption is shown to have a minor impact on specific activity, while exhibiting a complex relationship with oxygen transport. Ex situ characterization of ionomer suspensions and catalyst/ionomer inks indicates that the lower ionomer coverage can be correlated with the formation of large ionomer aggregates and weaker ionomer/catalyst interactions in low-water content inks. These larger ionomer aggregates resulted in increased local oxygen transport resistance, namely, through the ionomer film, and reduced performance at high current density. In the water-rich inks, the ionomer aggregate size decreases, while stronger ionomer/Pt interactions are observed. The reduced In the water intrins, the follower aggregate size decreases, while storiger forbult T interactions are observed. The reduced ionomer aggregation improves transport resistance through the ionomer film, while the increased adsorption leads to the emergence of resistance at the ionomer/Pt interface. Overall, the high current density performance is shown to be a nonmonotonic function of ink water content, scaling with the local gas ( $H_{22}$  O<sub>2</sub>) transport resistance resulting from pore, thin film, and interfacial phenomena.

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KEYWORDS: Pt/C catalyst inks, ionomer coverage, ink formulation and processing, in situ electrochemical diagnostics, oxygen transport resistance

Polymer elect Polymer electrolyte fuel cells (PEFCs) are an attractive technology for mobile and stationary electric power generation combustion engines, including higher efficiency and lower emissions. PEFCs convert the chemical energy stored in  $H_2$ and  $O_2$  into electrical energy, while producing only  $H_2O$  as the product. Despite their significant promise, commercially-available fuel cell vehicles currently utilize total areal platinum available fuel cell venicles currently utilize total areal plathnum
boadings greater than 0.3 mg<sub>Pr</sub> cm<sup>-2</sup>/<sub>1</sub> exceeding both the US
Department of Energy's (DOE) 2020 target of 0.125 grow
kW<sup>-1</sup> at rated power (kW<sub>rateb</sub> total areal loading of 0.125 mg<sub>Pt</sub> cm<sup>-2</sup>) and an industry-proposed stretch goal of 0.0625 g<sub>PGM</sub>

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 $kW_{rated}^{-1}$ , which would require cathode loadings from 0.1 to 0.05 mg<sub>Pt</sub> cm<sup>-2</sup>, respectively.

To improve the overall PEFC performance and achieve to improve the overal PEPC performance and achieve these targets, research groups have applied various strat-far(gefing) egges,<sup>5-7</sup> from the incorporation of novel materials<sup>8-12</sup> to excessive PE modified electrode fabrication methods<sup>13-18</sup> and conditioning we issue protocols.<sup>19-22</sup> While advancements have been plentiful, both in scientific understanding and in PEFC performance, material improvements tend to be discussed relative to their targeted

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focus (e.g., oxygen reduction reaction mass activity of cathode catalysts), rather than their collective impact on electrode structure and performance.

The performance of PEFCs with low Pt loading has been shown to be impacted by ionomer chemistry,  $^{23-25}$  Pt accessibility,  $^{11,26,27}$  ionomer film thickness,  $^{28-30}$  ionomer loading (I/C),  $^{31-33}$  and other properties related to the local Pt Foctors ionomer distribution and morphology in the catalyst layer. To that extent, recent studies have been able to visualize the ionomer distribution in membrane electrode assembly (MEA) cross sections using electron microscopy [scanning electron microscopy (SEM), transmission electron microscopy (TEM), scanning TEM (STEM), energy dispersive X-ray spectroscopy (EDS)] and X-ray tomography (nano-CT) techniques, with the purpose of examining the influence of process variables such as ionomer loading and the solvent ratio on the electrode microstructure. Orfanidi et al. observed that MEAs with smaller ionomer aggregate structures exhibited superior ORR and O2-transport performance.<sup>34</sup> Lopez-Haro et al. utilized a series of high angle annual dark field (HAADF)/STEM images at different tilt angles and a tomographic reconstruction algorithm to produce 3D images of Nafion/carbon black layers, reporting an increase in ionomer coverage from 50 to 80% as the ionomer to carbon ratio was increased from 0.2 to 0.5 (by mass).<sup>35,36</sup> Cetinbas and co-workers utilized a combination of nano-CT and hybrid reconstruction techniques to refine the 3-D agglomerate microstructure and calculate ionomer film thickness distributions.<sup>37,38</sup> However, given the urea of current resolution limitations, these techniques do not provide Microsoft information on nanoscale phenomena such as ionomer adsorption or configuration, which has been hypothesized to impact ORR kinetica<sup>39,40</sup> sites.41

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Along these lines, ex situ characterization of catalyst inks has provided insight into the molecular interactions between the ionomer, solvent, and catalyst particles that govern the electrode structure. For example, Khandavalli et al. described how ionomer content impacts the stabilization of different catalyst/support aggregates, which is relevant for electrode fabrication,<sup>11</sup> and Berlinger et al. showed how the solvent ratio (and more specifically pH) affects ionomer's conformation in solution<sup>26,45</sup> While these studies are very insightful, a knowledge gap

exists that would relate ionomer/catalyst, and/or ionomer/ support, interactions with performance for as fabricated electrodes and validate any proposed structure-property relationships. This work aims to provide better resolution of the ionomer/catalyst interface by measuring Pt-sulfonate coverage and ionomer coverages on Pt and C surfaces utilizing in situ electrochemical diagnostics obtained on fully conditioned MEAs. Specifically, 50 wt % Pt/Vulcan (Pt/Vu) cathodes containing the Nafion 1000 EW ionomer prepared from different solvent (nPA: H2O) ratios are investigated. While Pt/Vu is not a state-of-the-art material, its high Pt site accessibility (i.e., lack of particles buried in the carbon pores) makes it ideal for studying catalyst/ionomer interactions. Ionomer coverage and electrochemical performance trends are discussed along with supplemental characterization of MEAs and ink-level properties to elucidate the origins of the solvent effects observed here and elsewhere. While these studies are performed on PEFC electrodes, the effects and conclusions are relevant for other electrochemical systems (e.g., electrochemical CO<sub>2</sub> reduction, alkaline fuel cells, and electrolysis)

and should facilitate future material (catalyst/ionomer) development and incorporation strategies.

#### **EXPERIMENTAL METHODS**

Fabrication of Catalyst-Coated Membranes. All catalyst inks were prepared using an established protocol.<sup>16,22</sup> Specifically, 50 wt % Pt/Vu (TKK, TEC10V50E) was dispersed in a mixture of deionized water (DI) and *n*-propanol (*n*-PA), resulting in a final concentration of 1.85 mg<sub>Pt</sub> mL<sup>-1</sup> solvent. Three different solvent ratios were investigated, such that the final Pt/Vu cathode inks were prepared with 24, 62, and 83 wt % water in solvent corresponding to the lowmoderate-, and high-water content inks, respectively, referenced throughout this study. The Dupont D2020 ionomer was then added to the ink solution to give the desired ionomer to carbon (I/C) mass ratio of  $0.6^{31}$  Catalyst inks were dispersed with 20 s of horn sonication followed by 20 min of bath sonication in ice water.<sup>16</sup> The cathode catalyst layer was ultrasonically sprayed onto Nafion NR211 membranes (IonPower) using a Sono-Tek spray station with a 25 kHz accumist nozzle, targeting catalyst loadings of either 0.05 mg<sub>Pt</sub> cm<sup>-2</sup> (for 5 cm<sup>2</sup> testing), 0.10 mg<sub>Pt</sub> cm<sup>-2</sup> (for 50 cm<sup>2</sup> testing), or 0.30 mg<sub>Pt</sub> cm<sup>-2</sup> [for Electrochemical impedance spectroscopy (EIS) measurements]. Platinum loadings on individual electrodes were determined by X-ray fluorescence (XRF) (Fisher XDV-SDD). Anode electrodes were fabricated with Pt/HSC (TKK, TEC10E50E) dispersed in DI/n-PA (62 wt % water) with a 0.9 I/C and a 0.10  $mg_{Pt}\ cm^{-2}$  loading.

Membrane Electrode Assembly - In Situ Electrochemical Diagnostics. Once fabricated, MEAs with cathode loadings of 0.10 and 0.30 mgp, cm<sup>-2</sup> were tested using a 50 cm<sup>2</sup> double/triple (an/cath) serpentine flow field to acquire mass/specific activities, electrochemical surface area (ECSA), and ionomer coverage via CO displacement and EIS experiments. Catalyst-coated membranes (CCMs) with a cathode loading of 0.05 mgp, cm<sup>-2</sup> were utilized in 5 cm<sup>2</sup> differential cells to obtain oxygen limiting current and the resulting oxygen transport resistances.<sup>22,46,47</sup> The CCMs were sandwiched between either (i) two 50 cm<sup>2</sup> SGL29 BC gas diffusion layers (GDLs), at 25% compression (more detail provided in Supporting Information). The CCMs, GDLs, and polytetrafluoroethylene gaskets were then placed between the flow fields and the bolts tightened to 40 in-pounds.

Break-In Procedures. The break-in procedures begin by heating the cell to 80 °C and holding the cell at an open circuit potential (load equivalent flow rates of 0.8/2.5 =  $H_2/air L_{std} min^{-1}$ ), followed by a series of 5/10/5 voltage cycles in the fuel cell regime of 0.60–0.9 V for 4 min.<sup>48</sup>

Voltage Recovery. The voltage recovery (VR) step exposed the cell to 0.1 V under H2/air (950/500 sccm) for 2 h at 40 °C and 150% RH. This procedure was previously described<sup>48</sup> and shown to be a valuable step for the removal of sulfate, resulting in improved electrochemical performance across the entire potential range after the MEA had undergone significant degradation.<sup>49</sup>

 $H_2/O_2$  Polarization Curves. The test protocol involved measuring the I-V curves from 0.4 V to OCV at 80 °C at 100 kPa O<sub>2</sub> partial pressure (150 kPa total pressure) and 100% RH for 4 min per point (average of last 1 min used) in the anodic direction. The ORR mass activities were reported at 0.90 V after applying high-frequency resistance (HFR) and hydrogen cross-over corrections.  $H_2/Air Polarization Curves$ . The test protocol involved measuring

 $H_2$ /Air Polarization Curves. The test protocol involved measuring the I-V curves from 0.3 V to OCV at 80 °C and at 150 kPa total pressure with 75% RH for 4 min per point (average of last 1 min used) in the anodic direction. Currents were only normalized by metal loading determined by XRF.

CO Displacement Chronoamperometry. The test protocol involved measuring the transient current response (I-t) resulting from the introduction of CO to an equilibrated electrode held at a constant potential.<sup>32</sup> During this process, adsorbed cationic/anionic species are displaced through oxidative/reductive process and the resulting displacement charge  $(q_{dis})$  corresponds to the amount of charged surface species present at a specific potential. Experiments

### Conclusion to Dictating Pt-Based Electrocatalyst Performance in Polymer Electrolyte Fuel Cells, from Formulation to Application

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Figure 11. Proposed structure and orientation of ionomer/Pt interface leading to differences in  $O_2$  transport across different Pt/Vu MEAs.

large ionomer aggregates are present and the hydrophobic backbone is exposed, as is the case for alcohol rich MEAs, the aggregates create thicker barriers adjacent to Pt sites, resulting in higher transport resistances despite minimal interfacial resistance because of weak ionomer/Pt interaction. On the other hand, when the sulfonate moieties are exposed to the surrounding solvent, sulfonate adsorption on Pt sites increases and leads to additional barriers caused by interfacial effects. However, the more open structure for both 62 and 83 wt % inks, gleaned earlier from ink-level experiments, leads to a reduction in the MW-dependent component (Figure 10b) and lowers overall transport rates relative to the 24 wt % ink.<sup>45</sup> In addition, as shown in Figure 10b, the increase in sulfonate adsorption from 62 to 83 wt % does not increase the interfacial resistance, but the MW-dependent transport contribution, suggesting thickening of the ionomer film and/or an increase in ionomer confinement.<sup>26,61</sup>

#### CONCLUSIONS

results

Insights from the ex situ characterization of catalyst inks comprised Nafion 1000 EW, 50 wt % Pt/Vu, and n-PA/H2O, complete value rote two solutions in the extensive in situ electrochemical testing of conditioned MEAs clearly demonstrates that ink water (alcohol) content has a significant impact on the distribution of the ionomer and its interaction with both Pt and C. CO displacement revealed a monotonic increase in anion (SO3<sup>-</sup>) adsorption with increasing ink water content because of changes in ionomer orientation. In water rich inks (62 and 83 w %) the increase in sulfonate adsorption and ionomer orientation leads to the emergence of an interfacial resistance at the ionomer/Pt interface. Despite the onset of this additional resistance, the water rich inks resulted in electrodes with lower overall oxygen transport resistance because of both the decreasing size of ionomer aggregates and the changes in mer structure and distribution on Pt. Using  $H_2/D_2$ limiting current measurements, this reduction in oxygen transport resistance, relative to electrodes prepared from the low water content (24 wt %) inks, was shown to correlate with a decrease in the molecular weight-dependent portion of local resistance derived from pores and thin ionomer films. Overall, high current density performance was shown to be a no monotonic function of ink water content, where 62 > 83 24 wt %, scaling predominantly with transport resistance through pores and thin films. HCDP optimal 627 H20 drops @ While the current study focuses only on the Nafion 1000 EW ionomer and Pt/Vu-based electrodes, future work aims to investigate the role of ionomer chemistry, ionomer loading,

and electrocatalyst/carbon-support on electrode structure and performance. In general, similar trends are expected between , avoid changes that add other resistances

Alming to find Solvent ratio Research Article Bolymers from clumping solvent ratio and performance, where optimal formulations minimize ionomer aggregation without leading to substantial interfacial and/or film resistances. These results suggest future ionomer development, and incorporation should not solely focus on kinetic effects (weaker interactions between ionomer and electrocatalyst) but rather on how modifications to ionomer chemistry impacts ionomer confinement (densification) and the local distribution of ionomer on Pt and the resulting electrode microstructure, as these factors impact device-level performance, especially during operation at higher

current densities. Important to control how ionomer affects behavior @ structural level ASSOCIATED CONTENT

#### Supporting Information

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acsami.9b17614.

MEA conditioning protocol, GDL compression calculation, ECA, mass activity, specific activity, and sulfonate coverage as a function of conditioning,  $\zeta$ -potential,  $Z_{svg}$ diameter, and pH of inks with added salt, HAADF/ STEM/EDS maps (Pt/F/C) of MEAs, CO displacements as a function of potential, Nyquist and  $-1/\omega Z_{ung}$ plots,  $C_{\rm cli}$  of various interfaces,  $R_{\rm ari}$  and ionomer coverage versus ink water content, DLS particles sizes (10–1000 nm), fractional contributions to  $R_{\rm Hy}$ , changes in gas transport resistances, and list of symbols (PDF)

#### AUTHOR INFORMATION

Corresponding Author \*E-mail: kenneth.neyerlin@nrel.gov.

ORCID • Tim Van Cleve: 0000-0001-7233-5844 Sunilkumar Khandavalli: 0000-0003-3179-5718 Svitlana Pylypenko: 0000-0001-7982-734X Min Wang: 0000-0002-5051-9199 Adam Z. Weber: 0000-0002-7749-1624 Scott A. Mauger: 0000-0003-2787-5029 K. C. Neyerlin: 0000-0002-6753-9698 Notes

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✓ Intro to Tailoring electrode microstructure via ink content to enable improved rated power performance for platinum cobalt/high surface area carbon based polymer electrolyte fuel cells

#### T. Van Cleve et al.

#### 1. Introduction

Over the past several decades, significant advances in polymer electrolyte fuel cell (PEFC) performance and durability have enabled companies such as Toyota, Honda, and Hyundai to begin introducing hydrogen PEFC-powered vehicles into select markets. However, widespread commercialization is still impeded by the high cost of electrode components necessitating the development of cheaper and more efficient PEFCs. To spur further technological developments, the U.S. Department of Energy (DOE) has established ambitious performance targets for low-Pt loading PEFCs; i) mass activity >0.44 A/mgPt, ii) > 300 mA/cm<sup>2</sup><sub>elec</sub> at 0.8 V for H<sub>2</sub>/air operation, iii) > 1.8 W/cm<sup>2</sup><sub>elec</sub> at rated power, all in an MEA with less than 0.125 mg/cm<sup>2</sup> total Pt loading

To achieve these targets, three primary research pathways have emerged: (i) improved catalyst mass activity (A/mgPt) through electrocatalyst synthesis and/or post processing conditions [2-9], (ii) decreased oxygen transport resistance [10-13], occurring at or near the Pt reaction sites by improving Pt site location and accessibility, and (iii) incorporation of ionomers that improve conductivity (e.g. low EW ionomers) or modify the local electrocatalyst environment to enhance specific and mass activity [14-16]. While advancements have been plentiful, both in scientific understanding as well as PEFC performance, material improvements relating to any one of these focus areas tend to be discussed relative to their targeted focus, rather than in a broader context with membrane-electrode assembly (MEA) fabrication-related variables such as catalyst ink formulation and processing and subsequent electrode deposition, cell assembly, and electrode conditioning, all of which have been previously demonstrated to greatly impact performance [17-31].

Proper integration of materials to enable high performing PEFC operation has never been more crucial to realizing the individual improvements in electrocatalysts [32,33], supports [13,34-36], and ion-Notes and solvent ratios), processing method, ionomer chemistry, carbon omers [37,38]. Variables such as ink formulation (i.e., solvent identity morphology/porosity and even metal loading can impact the ink level in the on interactions of the materials set and subsequently alter the final electrode structure [20,21,23,39]. The resulting electrode structure can in turn influence active site accessibility and ORR activity as well as oxygen transport resistance and electrode proton conductivity. Optimiza-tion of ink formulation and electrode structure is often an iterative process in which conclusions from in situ performance/diagnostics and ex situ characterization (e.g., microscopy and tomography) establish structure-property relationships and inform future developments.

Previous reports have shown how changes in the ink solvent ratio impact ionomer-catalyst-solvent interactions leading to different rheological, morphological, and interfacial phenomena, which impact electrode microstructure and performance. For Pt/Vulcan carbon (Pt/Vu)containing MEAs fabricated with a low equivalent weight (EW) perfluorosulfonic acid (PFSA) ionomer, Orfanidi et al. [40] observed that smaller ionomer aggregate structures and high alcohol content exhibited superior ORR and O2-transport performance. Takahashi et al. [21] reported larger Pt/high surface area carbon (Pt/HSC) (TKK) catalyst aggregates present in higher water content inks correlated with increased heterogeneity of Nafion<sup>™</sup> (D1020/D2020) ionomer in the electrode microstructure which led to improved bulk O2 transport compared to alcohol-rich ink MEAs. Van Cleve et al. [26] demonstrated increasing ink water content leads to increased coverage on Pt/Vu, but local O2

TH20

better heatlyst agglomerate break-up and stronger catalyst-ionomer in-formation for the stronger catalyst-ionomer intransport trends have a complex relationship due to competing effects of study on the impact of ink content on the bulk-electrode transport resistance (i.e., through plane gas transport) of electrocatalyst layers containing platinum group metal (PGM)-free catalysts highlighted that changes in ionomer/electrocatalyst interactions and aggregation are strongly dependent on ink water content [41,42]. Generally, optimized

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ink formulations are specific to a particular set of materials (electrocatalyst, support, and ionomer), and it remains unclear how these process variables lead to enhanced performance across various electrode In this work, the effect of ink water content, *n*-propanol to water ratio systems.

(n-PA:water), on electrode microstructure and performance of MEAs containing state-of-the-art commercial catalyst (30 wt% PtCo/HSC, Umicore), D2020 (1000EW) ionomer, and Nafion™ 211 membrane (Ion Power) are examined. In situ and ex situ characterization of catalyst inks and MEAs describes how ink water content affects ionomer-catalyst interactions leading to morphological changes across multiple length scales. Specifically, CO displacement chronoamperometry and electrochemical impedance spectroscopy (EIS) experiments were utilized to directly measure ionomer coverage on various electrodes and describe the ionomer-catalyst interface at relevant conditions (80 °C, 150 kPa). These in situ electrochemical techniques have distinct advantages over more indirect, spatially-limited techniques like energy-dispersed X-ray spectroscopy (EDS) elemental maps generated by high resolution electron microscopy, which only provide detail about select regions of the electrode at one time. Additionally, X-ray scattering (USAXS and SAXS) echnique and nano-scale resolution X-ray computed tomography (nano-CT) ex- for periments provide complementary information about the electrode morphology at larger length scales describing PtCo catalyst particles, C info particles, and aggregate size distributions (nm to 10s of µm). Ultimately, the superior performance of water-rich formulations can be attributed to the enhanced O2 transport resulting from a more porous electrode microstructure with smaller aggregate particles.

#### 2. Experimental Methods

#### 2.1. Fabrication of Catalyst Coated Membranes (CCMs)

All catalyst inks were prepared using an established protocol [20, 43]. Specifically, 30 wt% PtCo/HSC (Umicore) was dispersed in a mixture of deionized water (DI) and n-propanol (n-PA), resulting in a final concentration of 2.0 mgPt mL-1 solvent. Five different solvent ratios were investigated, such that the final PtCo/HSC cathode inks were prepared with 30, 50, 60, 70, and 80 wt% water in solvent. As a shorthand, samples will be defined by their ink solvent ratio using the notation nXwY, where X and Y correspond to the mass ratio of n-PA and H<sub>2</sub>O, respectively. Dupont D2020 ionomer was then added to the ink solution to give the desired ionomer to carbon (I/C) mass ratio of 0.9 [25]. Catalyst inks were dispersed using 20 s of horn sonication followed by 20 min of bath sonication in ice water [20]. The cathode catalyst layer was ultrasonically sprayed onto Nafion<sup>™</sup> NR211 membranes (Ion Power) heated to 80 °C on a porous vacuum plate using a Sono-Tek spray station with 25 kHz accumist nozzle, targeting catalyst loadings of either  $0.04 \text{ mg}_{Pt} \text{ cm}^{-2}$  (for O<sub>2</sub> limiting current and 5 cm<sup>2</sup> H<sub>2</sub>/Air experiments),  $0.10 \text{ mg}_{Pt} \text{ cm}^{-2}$  (for ECA and CO displacement experiments), and 0.30mg<sub>Pt</sub> cm<sup>-2</sup> (for EIS measurements). Platinum loadings on individual electrodes were determined by XRF (Fisher XDV-SDD) are reported in supporting information. Anode electrodes were fabricated with Pt/HSC (TKK, TEC10E50E) dispersed in n-PA:water (62 wt% water) with a 0.9 I/C and a 0.10  $mg_{Pt}\ cm^{-2}$  loading.

#### 2.2. Membrane electrode assembly

Once fabricated, MEAs with a cathode loading of 0.10 and 0.30 mgPt  $cm^{-2}$  were tested using a 50  $cm^2$  double/triple (anode/cathode) serpentine flow field to acquire mass and electrode area-specific oxygen reduction reaction (ORR) activities, electrochemically-active surface areas (ECA), and ionomer coverage via CO displacement and EIS experiments. High metals loadings are typical for ionomer loading measurements since both EIS and CO displacement experiments are very sensitive and higher ECA improves data reliability and reproducibility. Catalyst-coated membranes with cathode loadings of 0.04 mgPt cm

Conclusion to Tailoring electrode microstructure via ink content to enable improved

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rated power performance for platinum cobalt/high surface area carbon based polymer electrolyte fuel cells



Fig. 5. Enclosed regions show the distribution of aggregate diameters ( $d_{Agg}$ ) and aspect ratios of the middle 5 and 10% (a), 30% (b), and 50% (c) of PICO/HSC aggregates extracted from segmented nano-CT data on electrodes prepared from 30 (black), 50 (red), and 70 wt% (blue) H<sub>2</sub>O inks using watershed separation technique. (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)



Fig. 6. (a) H<sub>2</sub>/Air polarization curves measured for high-performance PtCo/HSC MEAs (H23C8 GDLs) with various ink water content (60 wt%, 70 wt%, and 80 wt% H<sub>2</sub>O) and cathode loading of 0.08 mg<sub>9</sub>/cm<sup>3</sup> at standard saturated conditions (80 °C, 150 kPa). (b) H<sub>2</sub>/Air performance of 50 cm<sup>3</sup> PtCo/HSC MEAs measured under hear rejection conditions (94 °C, 65% HR1, and 250 kPa). Gases were fed at stoichiometric ratios of 1.5 and 2.0 at anode and cathode, respectively. Error bars correspond with the standard deviation of 3 experiments performed on different MEAs.

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conditions. While our particular catalyst ink formulation (catalyst, ionomer, While our particular catalyst ink formulation (catalyst, ionomer, solvent combination) may not exhibit the best PEFC performance ever reported, this study illustrates that significant improvements in power density and efficiency can be achieved by understanding the effect of process variables such as ink solvent ratio on electrode structure and performance. Such insights will help facilitate rapid incorporation of promising materials (catalysts, ionomers, membranes, diffusion media,

etc.) into high performance PEFC architectures.

4. Conclusion

Ex situ characterization of catalyst inks (comprising Nafion™ D2020 ionomer, 30 wt% PtCo/HSC, and n-PA/H<sub>2</sub>O) and electrode layers along with in situ electrochemical testing of MEAs demonstrated that ink water (and alcohol) content has a significant impact on electrode

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#### Table 1

Comparison of PEFC performance with state-of-the-art MEAs.

Catalyst	Ink Content nPa:H <sub>2</sub> O	Pt Content  g/kW (rated)	Cathode Loading mg/cm <sup>2</sup>	Total Pt Loading mg/cm <sup>2</sup>	Activity A/mg <sub>Pt</sub> <sup>b</sup> 0.9 V	Activity at 0.8 V (80 °C, 100% RH 150kPA <sub>abs</sub> ) A/cm <sup>2</sup>	Power Density (0.67 V, 94 °C, 65% RH 250kPa <sub>abs</sub> )	Reference
							W/cm <sup>2</sup>	
PtCo/HSC	4:6	0.118	0.077	0.107	1.26 <sup>a,b</sup>	0.274	0.932	This Work
PtCo/HSC	3:7	0.107	0.078	0.108	1.27 <sup>a</sup>	0.321	1.013	This Work
PtCo/HSC	2:8	0.122	0.077	0.107	1.19 <sup>a</sup>	0.267	0.900	This Work
L1 <sub>0</sub> -PtCo/ Vu		0.171	0.10	0.2	0.67 <sup>d</sup>	0.32 <sup>d</sup>	1.17 <sup>d,e</sup>	[75]
PtCo/HSC		0.234	0.08	0.230	0.6°	0.245 <sup>c</sup>	0.981 <sup>c</sup>	[14]
PtCo/Vu		0.124	0.10	0.125	0.62	0.2	1.005	[76]
PtCo/KB		0.124	0.1	0.125	0.7	0.385	1.005	[11]
PtCo/HSC- f		0.063	0.06	0.125	0.7	0.4	1.34	[11]
PtCo/HSC-		0.098	0.1	0.125	0.65	0.3	1.275	[77]

<sup>a</sup> Measured during anodic sweep.

<sup>b</sup> Mass activity measured during cathodic sweep around 0.9 A/mg<sub>Pt</sub> [43].

<sup>c</sup> Stoichiometric flows of 2/2 instead of 1.5/2 typical for other measurements and 10 cm<sup>2</sup> cell area.

<sup>d</sup> Obtained from differential cell measurements (5 cm<sup>2</sup>).

 $^{\rm e}\,$  Obtained from differential cell measurements 0.67 V, 75% RH, 250 kPa, 80 °C.

### need to find optimal ratio

microstructure and cell performance. X-ray scattering and X-ray nano-CT results revealed that water-rich inks lead to smaller average aggregate/agglomerate size and a more porous electrode structure, which improves O<sub>2</sub> transport within the aggregate and through the catalyst layer, respectively. While *in situ* electrochemical techniques identified stronger sulfonate adsorption on Pt with increasing water content along with moderate differences in ionomer coverage on Pt and C, neither effect alters local oxygen transport for electrocatalysts where Pt is located within the pores of the support.

Using a commercially available electrocatalyst and jonomer, modi-



fying only the ink formulation,  $50 \text{ cm}^2$  MEAs prepared with a 70 wt% H<sub>2</sub>O ink exhibited similar performance compared to state-of-the-art electrodes containing novel catalysts [75,76], ionomers [14], and C supports [11,77]. This work illustrates the importance of catalyst ink formulation in determining overall fuel cell performance. The insights from this study provide useful guidelines to facilitate the rapid incorporation and optimization of novel high-performance materials for future PEFC advances. Such considerations are also critical for the development of heavy-duty PEFC applications where fuel efficiency and durability are key performance metrics.

#### Supporting information

The Supporting Information is available free of charge on the Publications website at DOI:

Metal loadings determined by XRF, Tafel plots, ECA measured by CO stripping voltammetry, sulfonate and ionomer coverages, average catalyst particle and aggregate sizes from X-ray scattering, X-ray scattering profiles of catalyst inks and electrode layers, pore volume distribution and effective diffusion coefficients calculated from the reconstructions of phase-contrast nano-CT images, absorption-contrast images and ionomer distributions from nano-CT, mass activities for different MEA loadings, MEA performance comparisons to DOE targets.

#### **CRediT** authorship contribution statement

Tim Van Cleve: Conceptualization, Formal analysis, Investigation, Writing - original draft, Writing - review & editing, Visualization, Project administration. Guanxiong Wang: Formal analysis, Investigation, Writing - review & editing, Visualization. Mason Mooney: Formal analysis, Investigation, Writing - review & editing. C. Firat Cetinbas: Formal analysis, Investigation, Writing - review & editing, Visualization. Nancy Kariuki: Formal analysis, Investigation, Writing - review & editing, Visualization. Jaehyung Park: Investigation. Ahmed Farghaly: Investigation. Deborah Myers: Writing - review & editing, Supervision, Funding acquisition. K.C. Neyerlin: Conceptualization, Writing - original draft, Writing - review & editing, Supervision, Project administration, Funding acquisition.

#### Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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**REVIEW ARTICLE** 



# The Controllable Design of Catalyst Inks to Enhance PEMFC Performance: A Review

Yuqing Guo<sup>1</sup> · Fengwen Pan<sup>2</sup> · Wenmiao Chen<sup>2</sup> · Zhiqiang Ding<sup>1</sup> · Daijun Yang<sup>1</sup> · Bing Li<sup>1</sup> · Pingwen Ming<sup>1</sup> · Cunman Zhang<sup>1</sup>

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#### Abstract

Typical catalyst inks in proton exchange membrane fuel cells (PEMFCs) are composed of a catalyst, its support, an ionomer and a solvent and are used with solution processing approaches to manufacture conventional catalyst layers (CLs). Because of this, catalyst ink formulation and deposition processes are closely related to CL structure and performance. However, catalyst inks with ideal rheology and optimized electrochemical performances remain lacking in the large-scale application of PEMFCs. To address this, this review will summarize current progress in the formulation, characterization, modeling and deposition of catalyst inks. In addition, this review will highlight recent advancements in catalyst ink materials and discuss corresponding complex interactions. This review will also present various catalyst ink dispersion methods with insights into their stability and introduce the application of small-angle scattering and cryogenic transmission electron microscopy (cryo-TEM) technologies in the characterization of catalyst ink microstructures. Finally, recent studies in the kinetic modeling and deposition of catalyst inks will be analyzed.

Keywords Catalyst ink  $\cdot$  Ink formulation  $\cdot$  Ink modeling  $\cdot$  Ink deposition process  $\cdot$  Proton exchange membrane fuel cell  $\cdot$  Catalyst layer

#### **1** Introduction



Proton exchange membrane fuel cells (PEMFCs) are devices that can convert chemical energy into electrical energy without combustion. PEMFCs are also promising energy conversion technologies in many applications such as vehicles as well as stationary and portable power generation systems due to unrivaled efficiency and environmental friendliness. At the core of PEMFCs is the membrane electrode assembly (MEA), which consists of a gas diffusion layer (GDL), a microporous layer (MPL), a catalyst layer (CL) and a proton exchange membrane (PEM). Of these components, the CL is where reactions occur and is therefore key in PEMFCs [1]. WIOST (mportant part of CL

🖂 Bing Li

libing210@tongji.edu.cn

Pingwen Ming pwming@tongji.edu.cn

<sup>1</sup> School of Automotive Studies and Clean Energy Automotive Engineering Center, Tongji University, Shanghai 201804, China

<sup>2</sup> WeiChai Power Co., Ltd., Weifang, Shandong 261016, China

And to achieve optimal performances, CLs generally need to simultaneously facilitate several conditions [2-7], including the rapid transport of reactants to catalytic sites, the rapid transport of protons to catalytic sites from CL/PEM interfaces, the unhindered movement of electrons entering current collectors from CLs through conductive media and the timely removal of water from CLs. However, the coupling of transport phenomena in CLs in limited space is extremely complex and the microstructures of CLs are heterogeneous. Despite this, the development of high-performance and stable CLs is key in the reduction of PEMFC cost and the currently, the formation of conventional CLs involves various ink-based fabrication methods in which catalyst inks are deposited onto solid materials (PEM or GDL) (Fig. 1). Here, typical catalyst inks consist of catalysts/supports, solvents and ionomers in which the structure and performance of resulting CLs usually depend on the catalyst ink based on corresponding suspension systems because all active materials are dispersed in the ink. As a result, the formulation and deposition of catalyst inks can determine the component distribution, aggregate size, catalyst/support and ionomer

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Fig. 1 Illustrations of the fabrication processes of conventional CLs

### important to performance

interface, pore structure and performance of CLs [3, 8, 9]. Despite this, current optimizations of ink formulations are mainly based on experience and research into catalyst inks is mainly focused on the innovation and optimization of ink components with research into the interactions between ink components being lacking. In addition, the manufacture of MEA through low-cost, simple and scalable ink processes dremains challenging and corresponding ink formulations

need to be adjusted to match given deposition techniques or equipment. Because of this, the in-depth understanding of catalyst inks is crucial in the design and optimization of ink formulation and processing to design CLs with optimal structures and performance.

Overall, catalyst inks are complex fluids and corresponding ink formulations have been extensively explored to reduce electrode costs and improve electrode performances formulation. Based on this, researchers have developed a variety of catalysts, supports and ionomers to receive the support of variety of catalysts, supports and ionomers to greatly impact PEMFCs in recent years. And to ensure the optimal performance of these materials, numerous studies have been conducted on the relative ratio of ink constituents, especially the ionomer/carbon (I/C) ratio. Currently, however, the two critical parameters of platinum/carbon (Pt/C) ratio and I/C Not testing, which can be inaccurate and time-consuming [5]. ratio for inks are usually based on experience or repeated In essence, the ratio of ink constituents depends on corresponding interactions within inks. And because catalyst inks are complex multiscale systems with micro- and nanoscale interactions, these interactions (ionomer/particle, particle/ solvent and ionomer/solvent) can affect not only ink microstructures, but macroscale properties, including rheology, stability and coatability [10]. Because of this, the study of these interactions is helpful in the understanding and optimization of catalyst ink formulations, which are of great significance in the preparation of CLs and electrodes. In addition, the modeling of catalyst inks can provide in-depth understandings of these interactions despite its immature development [10-12]. And although the scalable manufacturing of CLs remains challenging in the commercialization

### ink deposition methods

deposition methods such as ultrasonic spraying [13], electrospray deposition [14], electrospinning [15], slot dying [16], inkjet printing [17], doctor blade [18], screen printing [19], brush printing [20] and gravure [21]. Here, although each technology possesses unique advantages, the low-cost and continuous production of corresponding MEA on a large scale remains challenging. In this context, this review will summarize the progress of catalyst inks based on formulation, characterization, modeling and deposition to provide a reference for future ink research.

content of papers

### **2** Ink Formulations

#### 2.1 Ink Constituents

#### 2.1.1 Catalysts

As a major component of catalyst inks, the cost and performance of catalysts have always been principal factors restricting commercial application [22, 23]. Here, Pt catalysts have widely been used in PEMFCs, especially as cathode catalysts because of their good catalytic activity and stability for both hydrogen and oxygen. And because the catalytic performance of nanoparticle catalysts is usually controlled by their chemical composition, atomic coordination and top surface layer strain, the size, facets, morphology and composition of Pt are important in the rational design and synthesis of high-performance catalysts [23-26]. The particle size of Pt can also affect the specific activity and mass activity of corresponding catalysts [27-30] in which specific activity can increase with increasing catalyst particle diameter and maximum mass activity appears within 2-4 nm [31]. In addition, commercial Pt/C catalysts are generally bound by low-index facets such as (100), (111) and (110), and numerous studies have shown that oxygen reduction reaction (ORR) activity is in the order of Pt (100) < Pt (111) Pt < (110) in weakly adsorbed electrolytes and Pt (111) < Pt(110) < Pt (100) in strongly adsorbed electrolytes [24].

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of PEMFCs, significant efforts have been made toward ink

## Conclusion to The Controllable Design of Catalyst Inks to Enhance PEMFC

#### Electrochemical Energy Reviews (2021) 4:67-100

processes with a focus on ink deposition requirements and technologies to optimize CLs. Now to make 1t better As a new type of green energy source, PEMFCs have

huge developmental prospects in the fields of automobiles,

power supply equipment, public transportation, power sta-



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celationships are important



ships between the constituents and rheological properties of catalyst inks can also lead to optimization. In addition, it is necessary to adjust ink materials and rheology to be compatible with different ink deposition techniques. Overall, focus should be placed on the quantitative understanding of links between internal ink interactions, ink microstructures, deposition processes and CL structures and performances in the future research of catalyst inks.

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#### **Compliance with Ethical Standards**

**Conflict of interest** The authors declare that they have no conflict of interest.

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inkjet printing. Here, continuous inkjet printing involves a continuous flow of liquid that is ejected from a nozzle under the effects of surface tension, whereas drop-on-demand inkjet printing involves the ejection of ink from printing nozzles on-demand [256]. Inkjet printing processes used for PEMFC inks mainly include ink atomization, wet film formation, solvent evaporation and CL formation. Among these, the most critical factor involves ink jettability, which can generally be defined by the Z number and is the inverse of the Ohnesorge number (Oh) [257]. Here, the Z number is related to the viscosity, surface tension and density of inks as well as the diameter of inkjet nozzles, and in general, Z values between 1 and 14 can ensure the fluent jetting of single droplets for inkjet printing [255]. In terms of limitations, ink particle sizes in general should not exceed 200 nm to avoid nozzle clogging and solvent vapor pressures in inks should generally not be higher than that of water to prevent the drying of inks in nozzles [218]. Inkjet printing was first used in PEMFC ink deposition to prepare CLs in 2007 [258, 259] and has since been extensively used in the manufacturing of PEMFC CLs. For example, Saha et al. [260] prepared CCMs with thin CLs (1-5 µm) and corresponding ultralow Pt loadings (0.02–0.10 mg cm<sup>-2</sup>) through inkjet printing and obtained mass activities at 900 mV that were 2.5 times higher than those for CCMs fabricated through conventional spraving methods. Malevich et al. [261] also found that the geometry of patterns affected the polarization behavior and electrochemically active surface area of patterned CLs. Despite this, Shukla et al. [262] suggested that the performance differences of patterned and non-patterned electrodes prepared through inkjet printing were small. Yazdanpour et al. [263] further deposited Pt/MWCNTs inks (as a catalyst ink) directly onto substrates (Nafion membrane or decal substrate) to form MEA through inkjet printing and suggested that MEA fabricated through the CCM method possessed better performances than ones prepared through conventional decal transfer methods. In another study, Saha et al. [264] studied the effects of cathode CL (CCL) structures prepared by using different coating techniques on fuel cell performance and found that inkjet-printed CCLs possessed more homogeneous distributions of both carbon supports and ionomers as well as better utilizations of Pt catalysts as compared with decaled CCLs. Shukla et al. [265] also fabricated thin, low Pt loading CCMs using inkjet printing and reported that the Pt mass activity of inkjet-printed CCMs at ambient pressure was 10 times higher than that of spray-coated CCMs. These researchers further fabricated inkjet-printed electrodes with different Pt loadings and CL thicknesses to investigate the relationship between Pt loading and PEMFC electrode performance as manufactured by inkjet printing and reported that Pt loadings exceeding thresholds greatly reduced fuel cell performances [231, 266]. In addition, Bezerra et al. [17] found that different deposited substrates possessed different effects on inkjet-printed CLs for PEMFCs (Fig. 14) and suggested that the power density of hot-pressed GDE-based MEA was higher than those of hot-pressed CCM-based MEA and hot-pressed bilateral sandwich MEA with a CCM and a GDE.

Overall, inkjet printing technologies possess good application prospects in the deposition of PEMFC catalyst inks. First, inkjet printing has high flexibility to precisely control Nafion and Pt loading distributions in CLs. Second, inkjet printing can improve catalyst utilization and reduce the complexity of overall processes to some extent. Despite advantages of improving product quality and reducing manufacturing costs however, inkjet printing faces many difficulties in practical application for PEMFC inks. For example, inkjet printing requires the high dispersion of inks to prevent nozzle clogging. Moreover, the coffee ring effect produced during the drying process of inkjet printing can result in thicker edges and thinner middles for resulting CLs [255].

Screen printing and gravure printing are also considered to be promising printing technologies. However, these printing methods are not as flexible. Overall, further efforts are needed in the development of catalyst ink deposition technologies to improve the automation and large-scale production of electrodes. Related solvents, solid contents, Pt loadings, power density and deposition methods of mentioned catalyst inks are summarized in Table 2.

#### 6 Conclusions and Outlook

The scalable and economical manufacturing of CLs or MEA can allow for commercialization of PEMFCs in which conventional CLs are prepared through the solution treatment of catalyst inks involving a suspension of catalysts/supports and ionomers mixed in a dispersion medium. Based on this, this review provided an overview of PEMFC catalyst inks with a focus on the effects of ink constituents and potential internal interactions between constituents on the microstructure and stability of catalyst inks. Currently, there is a lack of comprehensive understanding of the formation process and internal interaction of catalyst inks, resulting in ink formulation optimizations being predominantly empirical. To address this, model and numerical simulations for particle aggregation and interactions between catalyst ink constitu- experiments ents are necessary in which detailed and accurate ink modto turner eling can allow for the elucidation of complex multiphase research ink systems as well as the optimization of ink formulations to effectively improve CL designs. In addition, continuous and efficient ink dispersion technologies are necessary for the large-scale production of CLs and MEA and indirect characterization and visualization techniques are needed to provide quantitative information on the microstructural features of inks. This review has also introduced ink deposition

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Intro to Recent progress in understanding the dispersion stability of catalyst ink for

### proton exchange membrane fuel cell and water electrolyzer

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Recent progress in understanding the dispersion stability of catalyst ink for proton exchange membrane fuel cell and water electrolyzer

#### Dhinesh Kumar Murugaiah, Samaneh Shahgaldi

Institute for Hydrogen Research (IHR), University of Quebec at Trois-Rivieres (UQTR), G8Z 4M3, QC, G8Z 4M3, Canada

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### ABSTRACT

A cell with a superior performance and durable catalyst layer can be achieved by optimizing the catalyst ink formulation. A typical commercial catalyst layer for both proton exchange membrane fuel cells and water electrolyzers is prepared via dispersion-based catalyst inks. Generally, ink dispersion composed of supported catalyst, ionomer, and solvent. The ink formulation governs physical properties such as homogeneity, the interaction between ink components, ability to store the ink (shelf-life) for an extended period and reproducibility. This is pivotal in optimizing the catalyst ink formulation for high performance, extended durability, and reproducibility, particularly in large-scale industrial manufacturing in polymer electrolyte membrane (PEM) fuel cells and electrolyzers. Despite the substantial progress on synthesis of different catalysts and ionomers, there is a limited understanding of the colloidal stability of the catalyst ink. The novelty of this review is to provide a guide to understand the importance of catalyst ink dispersion stability for manufacturing MEAs at scale-up level. This is addressed through targeting fundamental interaction behavior and physical properties of the ink materials. Further, this review covers the effect of particle surface, effect of solvent composition, and the effect of ionomer concentration that ensures a homogenized catalyst ink. In addition, this review covers the influence of different dispersion methodologies and the relevant characterization techniques for better understanding the dispersion stability.

#### 1. Introduction



from fossil fuels to renewable energies. Global renewable power generation has seen rapid growth from 1560 GW at the end of 2013-2838 GW at the end of 2020 [1]. The concept of the hydrogen (H2) economy is gaining momentum as it offers a different approach to address the minimal dependency on fossil fuels. Hydrogen is looked upon as a vital energy carrier due to its high mass gravimetric energy density compared to all types of fuels (120 MJ/kg, in low heat value) [2]. To successfully implement the hydrogen-based energy economy, fuel cells, and electrolyzers are considered potential suitors. Proton exchange membrane fuel cell (PEMFC) is a matured technology with over 30 years of research and development that converts chemical energy stored both in hydrogen and oxygen into electrical energy by electrocatalytic reduction of oxygen at the cathode and electrocatalytic oxidation of hydrogen at the anode [3]. Whereas, in proton exchange membrane water electrolyzers (PEMWE) electrocatalytic decomposition of water at the anode produces oxygen as a secondary product and hydrogen as a primary product at the

The world is moving towards clean energy for a smooth transition

\* Corresponding author. E-mail address: samaneh.shahgaldi@uqtr.ca (S. Shahgaldi).

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### alternate form of clean energy

cathode. The PEMWE system provides a distinctive advantage in the ability to operate at higher operating current densities (above 2 A/cm<sup>2</sup>), rapid system response, dynamic operation, and above all, to produce ultrapure hydrogen. Nevertheless, both PEMFC and PEMWE are oper- ether ated at low temperatures (<100 °C) [4] at the commercial industrial can be level. Additionally, hydrogen is considered as a green fuel, if the electricity is produced from a renewable source (such as solar, and wind power). Renewable hydrogen can be instrumental in combating climate change and decarbonization of industrial sectors, either by replacing fossil hydrogen in refineries, manufacturing fertilizer, or in the transportation sector as an e-fuel. However, the reliability of renewable energy sources is often indecisive when considered for commercial use due to their intermittent availability (for example, dependency on wind, and

sun) [5]. Arguback to renewate cnergy Addressing this challenge has been part of current research trends to provide maximum flexibility. Nonetheless, these forthcoming demands for hydrogen are based on the urge to address clean transportation. reducing carbon dioxide (CO2) emissions, and strict governmental regulations [6,7]. The expensive traits of both fuel cells and electrolyzers



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operated at low temperatures are due to the components of the membrane electrode assembly (MEA). The membrane electrode assembly is considered as the heart of the respective devices. A single MEA constitutes two catalyst layers separated by a thin solid polymer electrolyte membrane. Commonly, these solids electrolytes (proton conducting membranes) are made of perfluorosulfonated (PFSA) membranes. PFSA membranes allow cell operation at higher pressure with increased proton conductivity by selective transport of ion species and result in minimized gas permeability (less gas cross-over) [8]. The catalyst layers, however, consist of a catalyst, catalyst support, and ionomer. The state-of-the-art catalyst constitutes, platinum (Pt) on carbon based support material (in both the anode and cathode of PEMFC for both hydrogen oxidation reaction (HOR) and oxygen reduction reaction 1055 (ORR) catalysts. Likewise, in PEMWE, the state-of-the-art catalyst, is Iridium-based catalyst which is suitable for oxygen evolution reaction (OER) and Pt supported on carbon is utilized as a hydrogen evolution reaction (HER) catalyst [3,4]. The simplest mechanism (as presented in the equations below) for OER can be explained through the partial oxidation of water molecules as a first step, resulting in the deprotonation of  $H_2O$  molecules into the adsorption of  $OH_{ads}$  at the electrode surface (eq. (1)). In the second step, additional electron transfer and deprotonation lead to adsorption of Oads (eq. (2)) and O2 as a result of chemical recombination in the final step (eq. (3)).

 $M + H_2O \rightarrow M - OH_{ads} + H^+ + e^-$ (1)

 $M - OH_{ads} \rightarrow M - O_{ads} + H^+ + e^-$ (2)

 $2M - O_{ads} \rightarrow 2M + O_2 \tag{3}$ 

The above set of equations, 'M' refers to the catalytically active sites of the anode electrocatalyst [9,10]. Similarly, the oxygen reduction reaction (ORR) involves the electroreduction of  $O_2$  via 4 e<sup>-</sup> reduction pathways, completing the cycle by producing H<sub>2</sub>O (by-product). The mechanistic hypothesis on the ORR pathway starts with the adsorption of  $O_2$  species to the catalyst's active surface, which is followed by reduction to superoxide which spontaneously protonates to form peroxide radicals and yields H<sub>2</sub>O after sequential proton and electron transfer (as presented in the reactions below).

$$O_2 + e^- + L \leftrightarrow O_2^-$$

 $O_{2,ads}^- + H^+ \rightarrow HO_{2,ads}$ 

 $HO_{2.ads} + H^+ + e^- \rightarrow H_2O + O_{ads}$ 

#### $O_{ads} + H^+ + e^- \rightarrow HO_{ads}$

 $HO_{ads} + H^+ + e^- \rightarrow H_2O + L$ (8)

The above set of equations 'L' refers to the catalytically active sites of the cathode electrocatalyst [11]. This general reaction pathway for ORR in PEMFC and OER in PEMWE is a rate-limiting step due to the slow kinetics and complex reaction pathways of the oxygen electrode, ultimately leading to large overpotentials. Hence, the choice of precious metals as an electrocatalyst is crucial. Subsequently, the catalyst support provides an electron pathway along with electrical conductivity, whereas the ionomer enhances protonic conductivity and acts as a binder for mechanical stability. The electrochemical reaction takes place at the intersection of the electrolyte-reactant-catalyst and is commonly referred to as the triple-phase boundary. Thus, a rational architecture can enable the catalyst layer (CL) to transfer reactants to active sites and enhance gas evolution quickly [12–14].

Among the ink constituents, there are both primary and secondary catalyst agglomerates, along with the ionomers. These ionomers are present both in adsorbed and nonadsorbed (free ionomer) states concerning different ink formulations (i.e., the rate of ionomer adsorption varies for different solvent systems, ionomers, and catalyst

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compositions). During the process of catalyst layer (CL) preparation through coating and drying, these ionomers distribute and cover both primary and secondary agglomerates, assembling them into a porous structure to form a multiscale structure creating a unique catalyst layer microstructure [15]. The CL fabrication methods have a substantial influence on the microstructure. Individual materials within the catalyst layer play unique roles, such as size of agglomeration, degree of ionomer adsorption, and homogeneity of the ink dispersion. All of these are governed by the degree of hydrophobicity/hydrophilicity (effect of solvent-/alcohol-rich), ionomer concentration and mainchain/sidechain orientation.

Literature has extensively discussed different types of ionomers, catalyst morphology and functionalization of support carbon for better performance and durability [16] [-] [18]. Furthermore, extensive studies have been reported for optimizing the CL formation procedures to improve the microstructures for scale-up sizes [19-21]. The performance of PEMFCs can be highly impacted by different manufacturing processes. A study investigated by S Shahgaldi et al. [19] showed that MEAs manufactured using decal transfer method (transfer through hot press) resulted in decreased CL porosities and increased diffusion resistance, which affected the cell performances. Contrastingly, MEAs from catalyst coated membrane (CCM) without hot press resulted in a superior performance. Likewise, G Liu et al. [20] demonstrated that CL developed using doctor blade coating showed a performance that's comparable to spray coating. The performance was highlighted through better wettability and high uniformity of coated CL. Additionally, CCMs manufactured from roll-to-roll (R2R) by J Park et al. [21] demonstrated a comparable performance compared to spray coated MEAs. This performance was ascribed to proper selection of solvent system for the ink formulation that provided good dispersion, low contact angle and slow absorption of solvent by the membrane. Furthermore, R2R was considered to increase throughput by 500x when compared to laboratory spray fors \s coating. While many of the current research contributes towards in- Scoling dustrial manufacturability, still exists a limited focus towards colloidal (dispersion) stability. The necessity of catalyst ink colloidal stability is crucial as it guarantees reproducibility for coating and promotes storage of catalyst ink for a longer period without compromising structural stability. Stable catalyst ink is decisive for widespread automated industrial manufacturability. One way to optimize the CL is by understanding the interaction through macroscopic properties (generally considered as properties of constituents in bulk) of the catalyst ink, such as ink viscosity, surface charge and ink homogeneity, as they highly Sinfluence the coating process [22]. The ability of catalyst inks to have an extended shelf-life ensures significant flexibility in reducing the operating cost of the CLs manufacturing process and reducing ink waste. The catalyst's ink stability is further categorized into material and colloidal stability. The former is directly due to the individual components of the ink materials (support material, ionomer, solvent, and catalyst itself). The latter, however, reflects how well these materials interact within the ink constituents, starting with agglomeration characteristics. This is a result of the aggregate's van-der-Waals force exceeding the repulsive force causing it to form a larger agglomerate. As the size of the agglomerates increases, sedimentation due to gravity takes place, resulting in inhomogeneous catalyst ink [23,24].

In recent years, there have been multiple scientific papers reviewing the effect of ink components interactions influencing the catalyst layer formation and their effect on performance and durability of CLs [25–27]. Zhang et al. [25] probed into the effects of solvents on the catalyst layer microstructure in PEMFCs. Alternate to the conventional dual solvent system, the author used two-step-three solvent (water, methanol, 2-propanol) for ink preparation. Developed CLs exhibited a uniform distribution of ionomer and aggregates that lead to superior performance at high current densities, i.e cell performance improved from 0.55 5 V to 0.615 at 2 A cm<sup>-2</sup>. Likewise, D. Wu et al. [26] reported a study on the effect of alcohol content on ionomer adsorption, where ink containing water-rich solvent showed a stable dispersion after 14

(4)

(5)

(6)

(7)

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Fig. 1. (A.) Schematic diagram of interactions in the catalyst ink through xDLVO theory, (B.) Interaction energies as a function of particle separation distances [30] (Reprinted from Ref. [30], Copyright (2018), with permission from IOP Science).

#### previous studies

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days of storage, compared to alcohol-rich due to flocculation. This was attributed to strong adsorption of ionomer backbone to carbon surface and higher dissociation of sulfonic group in Nafion in water-rich system. Further, polybenzimidazole (PBI) coated on carbon allowed adsorption of negatively charged sulfonic (side) chains onto the positively charged PBI surface. A second layer of ionomer was made possible through hydrophobic (ionomer backbone-backbone) interaction ensuring a stable dispersion (stable ink after 14 days for both alcohol- and water-rich solvents). Also, in a study by B. Li et al. [27] used Lattice Boltzmann method to simulate the dynamic behavior of the ink dispersion process through particle agglomerations. The study showed that higher shear Sorce does not necessarily guarantee proper dispersion (de-agglomeration) but result in increased particles agglomerate sizes. The study showed ink stability in the following order: low shear < excessive shear < moderate shear. This was concluded to be due to aggregation forces between particles in large agglomerates that could offset electrostatic forces of repulsion, resulting in stronger van der Waals attraction force (could result in unstable ink dispersion).

Currently, the scope of review papers published in this domine contribute towards improving overall cell performance. Majority of the published papers are focused on development of ink formulation, different characterization techniques, simulations & model-based studies and also development of MEA fabrication techniques. For example, Y Guo et al. [28] reviewed the fuel cell catalyst ink materials and their interactions as an effect of ink formulations. The author reported the prospect of CL development by various ink deposition methods in a detailed manner. In addition, characterization tools to analyze catalyst ink microstructure, catalyst ink dispersion and stability were discussed in a brief context. Likewise, H Liu et al. [29] extensively reviewed the effect of ink composition, formulation, and preparation of CLs for PEM fuel cells. Authors emphasized the importance of ink optimization for coating and drying processes to achieve well-defined CLs. The review papers that are currently available investigate the relationship between freshly prepared catalyst ink and developed CL microstructure. Nevertheless, a deep insight into ink materials interaction impacting dispersion stability and subsequent CL development for both fuel cell and electrolyzer would add an extra edge to an industrial manufacturability. The purpose and the novelty of this work are to bridge the literature gap in establishing a fundamental interaction behavior of the catalyst ink on dispersion stability. This review guides through the factors that are decisive for these interaction behaviors aimed at proper ink formulation, which includes the effect of particle surface, the effect of solvent composition, and the effect of ionomer (Section 2.1). Further, this work will discuss the establishment of an underlying relationship between the catalyst ink dispersion stability and its dependencies on various metrics like Zeta potential, ink rheology, settling dynamics, and relevant characterization methodologies (Section 3) that are involved in ensuring a well-dispersed catalyst ink.

focus of paper

#### 2. Catalyst ink microstructure

Scalable manufacturing of highly stable and durable catalyst layers can be optimized by understanding the microstructure and macroscopic properties of the catalyst ink. As stated in the previous section, microstructure portrays the catalyst layer architecture, while the macroscopic properties of ink components govern the nano-scale interactions. These interactions include ionomer | solvent, ionomer | particle (includes catalyst on support material), and particle | solvent, eventually reflecting on the agglomeration and sedimentation of catalyst material [30]. This interaction between particles in the ink is usually governed by three forces, namely van-der-Waals, double laver, and steric repulsion. Both van-der-Waals and double-layer interaction forces are considered when evaluating the suspension stability in the absence of ionomer (general DLVO theory). However, the inclusion of polymers in the ink contributes to an additional repulsive force called steric repulsion, known as "non-DLVO theory or xDLVO theory," deviating from general DLVO theory for particle interaction. The steric repulsion between the catalyst particles is due to an adsorbed layer of ionomer on the catalyst surface, which hinders the attractive forces (enhancing the interparticle interaction) (Fig. 1A). This repulsive force slows down the formation of agglomerates, making it a decisive characteristic for colloidal dispersion stability [31].

Interpreting this behavior as a function of particle separation distances between two adjacent particles (represented as r, total energy represented as U in Fig. 1 B) transcribes that particles experience a weak van-der-Waals attraction at long separation distances. However, particles moving closer to each other undergo steric interaction, which is due to the ionomer layer adsorbed on the catalyst (particle) surface. The particles thus repel each other at a shorter distance, maintaining a state of dispersion [31,32].

#### 2.1. Catalyst ink formulation

Elucidating macro-scale ink descriptors can help in understanding the targeted material interaction within the ink constituents. Catalyst ink formulation holds a crucial role in defining the microstructure for highly active sites for catalysts, homogeneously distributed ionomers, and advanced catalyst layer architecture [33]. Within the ink constituents, polymer | solvent interactions control the formation of interfaces through ionomer stretching, chain mobilities, and orientations (which will be discussed in the upcoming section). This facilitates a homogeneous distribution of ionomers at a preferential adsorption site on the catalyst surface, contributing to a better ionomer network and allowing greater catalyst utilization and catalyst layer porosity [34]. Furthermore, catalysts interaction with both solvent and polymer (particle | polymer and particle | solvent) governs the agglomeration behavior through particle mobility (self-assembly by Brownian motion) [35,36]. The phenomena of catalyst agglomeration are caused by the collision of small (catalyst) aggregates due to a relative motion (the likes of

First draft background research:

The global transition to renewable energy has recently accelerated significantly due to growing concerns about climate change, energy security, and the impacts of fossil fuel use. Countries around the world are adopting various clean energy technologies, such as solar and wind, to reduce their reliance on fossil fuels, control greenhouse gas emissions, and promote sustainability. In 2015, 196 countries signed the Paris Agreement, which, according to the United Nations Framework Convention on Climate Change, aims to strengthen the global response to climate change by keeping the rise in temperatures less than 1.5 degrees Celsius this century. Another goal of the Paris Agreement is to reach net-zero emissions by 2050, meaning that the amount of greenhouse gases produced and removed from the atmosphere needs to be equal.

According to the International Energy Agency (IEA), renewable energies will account for nearly 50% of all global power by 2030 due to government policy and technology. Despite this, there are many challenges to reaching the targets set by the Paris Agreement. The demand for fossil fuels is still significant, especially in developing countries. Additionally, although the costs of renewable energy sources have been declining, there are challenges to technology and infrastructure that make it difficult to make them affordable. Finding ways to overcome these challenges is important to create a sustainable future that aligns with the goals of almost 200 countries worldwide.

## October 08, 2024:

Rewrite background section of RP with proper citations and follow flow suggested.

The global transition to renewable energy has recently accelerated significantly due to growing concerns about climate change, energy security, and the impacts of fossil fuel use. Fossil fuels such as coal, oil, and natural gas account for over 75% of global greenhouse gas emissions and almost 90% of carbon dioxide emissions globally (United Nations, n.d.). Processes that require the burning of fossil fuels, such as generating power and manufacturing goods, are some of the most common causes of global climate change. The greenhouse effect is the primary driver of climate change, and human activities are responsible for increasing the concentration of greenhouse gases released into the atmosphere ("Causes of Climate Change," n.d.). As a result of the increasing emissions, 196 countries signed the Paris Agreement," n.d.). Countries that signed onto the Paris Agreement each proposed commitments to reduce emissions. Some examples of these commitments include the European Union reducing emissions through domestic measures and India increasing electric power in the form of non-fossil fuel energy resources ("The Paris Agreement on Climate Change," n.d.).

In the United States, three economic sectors—transportation, electric power, and industry—contribute over 20% of greenhouse gas emissions. Transportation is the largest sector, making up 28% of all greenhouse gas emissions because petroleum-based fuels are most commonly used for transportation (Us Epa 2015). The best way to minimize the emissions of greenhouse gases would be to limit the amount of emissions released in the transportation sector, and the best way to achieve this is to curtail the amount of fossil fuels burned and instead find alternative sources of clean energy. Clean energy is a form of energy that comes from renewable, net-zero sources that do not pollute the atmosphere. Proton-exchange membrane fuel cells,

PEMFCs, are a promising alternative to fuel cells due to their efficiency and environmental benefits. The advantages of using a PEM are the high power density and low operating temperature, which makes it suitable for commercial applications (Baroutaji et al. 2016). The use of PEMFCs in cars is not currently being explored due to the rise of electric vehicles. Hydrogen gas-powered PEMFCs were simulated in heavy-duty vehicles, and the study found that the metrics used to determine performance standards were not only met but also exceeded (Ogungbemi et al. 2021), showing great promise in the use of PEMFCs in the transportation sector. The cost of PEMFCs is no longer the most significant issue. Instead, the durability and performance of a fuel cell in commercial applications are the causes of concern amongst researchers.

### ☑ Role of PEMFC for background research

For the PEMFC to perform effectively, the catalyst layer must activate oxygen effectively, remove the water produced from the catalyst surface, and be stable in corrosive operating conditions [8]. Additionally, it must facilitate the efficient transport of reactants, products, electrons, and heat. The catalyst layer is also a significant cost factor, accounting for about 42% of the total cost of mass-produced PEMFCs. The two ways to reduce the cost are to improve the fuel cell's performance and durability and lower the amount of expensive catalyst, platinum, used in the catalyst layer. However, these improvements tend to trade off against each other, making it challenging to find the optimal balance. The structure of the catalyst layer is very important because it impacts the short- and long-term performance of the fuel cell. However, there is still no clear consensus on the best structure for the catalyst layer [8].

### October 10, 2024:

✓ Work on the role of the catalyst layer function and importance section of the RP intro.

Current efforts to address the challenges in the catalyst layer (CL) design focus both on reducing the use of platinum and improving the structure of the CL [8]. While platinum is the most effective catalyst for the oxygen reduction reaction (ORR), its high cost makes it difficult to mass-produce PEMFCs for commercial applications. To address this, researchers are exploring platinum alloys and alternative non-precious metal (NPM) catalysts to reduce platinum content without sacrificing performance. However, while NPM catalysts are more cost-effective, they are not as efficient or durable as CLs made with platinum, resulting in more frequent replacements that increase long-term costs [8].

In addition to catalyst materials, the structure of the CL is being optimized through advancements in fabrication techniques, such as the creation of ultra-thin CLs [8]. These techniques allow for more efficient use of expensive catalyst materials by reducing catalyst loading while maintaining effective reactant transport and overall performance. Researchers are exploring three main thin-film methods for applying the catalyst ink: coating the gas diffusion layer (GDL), coating the membrane, and using the decal transfer method. Coating the GDL involves applying the catalyst directly to the GDL, coating the membrane places the catalyst ink directly onto the membrane for greater contact, and the decal transfer method transfers the catalyst ink from a decal substrate to the membrane. Each method has challenges, such as controlling the catalyst penetration into the gas diffusion layer and balancing performance and durability. Nanostructured thin-film CLs have also gained attention due to their potential to reduce the amount of platinum used – thereby reducing the cost of platinum – but they face issues with water buildup and reduced durability [8].

### October 15, 2024:

### $\square$ RP Intro $\rightarrow$ role of the CL: Challenges

One of the significant challenges in the catalyst layer design is water management [8]. During the operation of a PEMFC, water is produced as a byproduct of the ORR at the cathode, and this water must be removed to prevent water buildup, which can block reaction sites and reduce the fuel cell's overall performance. This issue is known as water flooding and significantly impacts the efficiency of the fuel cell. Poor water management can lead to hydrogen peroxide ( $H_2O_2$ ) forming, which accelerates the degradation of the fuel cell components, shortening its lifespan. Designing a catalyst layer that not only manages water buildup but also maintains long-term durability and performance is essential to improve the functionality of PEMFCs [8].

### October 16, 2024:

### ☑ Edits to research proposal

The global transition to renewable energy has recently accelerated significantly due to growing concerns about climate change, energy security, and the impacts of fossil fuel use. Fossil fuels such as coal, oil, and natural gas account for over 75% of global greenhouse gas emissions and almost 90% of carbon dioxide emissions globally [1]. Processes that require the burning of fossil fuels, such as generating power and manufacturing goods, are some of the most common causes of global climate change. The greenhouse effect is the primary driver of climate change,

and human activities are responsible for increasing the concentration of greenhouse gases released into the atmosphere [2]. As a result of the increasing emissions, 196 countries signed the Paris Agreement, which aims to limit global warming to 1.5°C by the end of the century [3]. Countries that signed onto the Paris Agreement each proposed commitments to reduce emissions. Some examples of these commitments include the European Union reducing emissions through domestic measures and India increasing electric power in the form of non-fossil fuel energy resources [4].

In the United States, three economic sectors-transportation, electric power, and industry-contribute over 20% of greenhouse gas emissions. Transportation is the largest sector, making up 28% of all greenhouse gas emissions because petroleum-based fuels are most commonly used for transportation [5]. The best way to minimize the emissions of greenhouse gases would be to limit the amount of emissions released in the transportation sector, and the best way to achieve this is to curtail the amount of fossil fuels burned and instead find alternative sources of clean energy. Clean energy is a form of energy that comes from renewable, net-zero sources that do not pollute the atmosphere. Proton-exchange membrane fuel cells, PEMFCs, are a promising alternative to internal combustion engines due to their efficiency and environmental benefits. The advantages of using a PEM are the high power density and low operating temperature, which makes it suitable for commercial applications [6]. The focus of PEMFCs is no longer on light-duty vehicles due to the fact that electric vehicles (EVs) have been around for longer, the cost of EVs is significantly lower than vehicles using PEMFCs, and charging infrastructure has been expanded. Hydrogen-powered PEMFCs were simulated in heavy-duty vehicles, and the study found that the metrics used to determine performance standards were not

only met but also exceeded [7], showing great promise in the use of PEMFCs in the transportation sector. Although there is room to reduce the cost of PEMFCs further, it is no longer the most significant issue. Instead, the durability and performance of a fuel cell in commercial applications are the causes of concern amongst researchers.

### October 19, 2024:

Dr. Garcia's edits to RP intro

The global transition to renewable energy has recently accelerated significantly due to growing concerns about climate change, energy security, and the impacts of fossil fuel use. Fossil fuels such as coal, oil, and natural gas account for over 75% of global greenhouse gas emissions and almost 90% of carbon dioxide emissions globally [1]. Processes that require the burning of fossil fuels, such as generating power and manufacturing goods, are some of the most common causes of global climate change. The greenhouse effect is the primary driver of climate change, and human activities are responsible for increasing the concentration of greenhouse gases released into the atmosphere [2]. As a result of the increasing emissions, 196 countries signed the Paris Agreement, which aims to limit global warming to 1.5°C by the year 2050 [3]. Each country that signed onto the Paris Agreement proposed commitments to reduce emissions. Some examples of these commitments include the European Union reducing emissions through domestic measures and India increasing electric power in the form of non-fossil fuel energy resources [4].

In the United States, three economic sectors—transportation, electric power, and industry—contribute over 20% of greenhouse gas emissions. Transportation is the largest sector, making up 28% of all greenhouse gas emissions because petroleum-based fuels are most

commonly used for transportation [5]. The best way to minimize the emissions of greenhouse gases would be to limit the amount of emissions released in the transportation sector, and the best way to achieve this is to curtail the amount of fossil fuels burned and instead find alternative sources of clean energy. Clean energy is a form of energy that comes from renewable, net-zero sources that do not pollute the atmosphere. Proton-exchange membrane fuel cells, PEMFCs, are a promising alternative to internal combustion engines due to their efficiency and environmental benefits. The advantages of using PEMFCs are the high power density and low operating temperature, which makes them suitable for commercial applications [6]. The focus of PEMFCs is no longer on light-duty vehicles due to the fact that electric vehicles (EVs) have been around for longer, the cost of EVs is significantly lower than vehicles using PEMFCs, and charging infrastructure has been expanded. Instead, the focus has been on making PEMFCs durable enough for heavy-duty vehicles. Hydrogen-powered PEMFCs were simulated in heavy-duty vehicles, and the study found that the metrics used to determine performance standards were not only met but also exceeded [7], showing great promise in the use of PEMFCs in the transportation sector. Although there is room to further reduce the cost of PEMFCs, it is no longer the most significant issue. Instead, the durability and performance of a fuel cell in commercial applications are the causes of concern amongst researchers.

In a proton-exchange membrane fuel cell (PEMFC), hydrogen and oxygen are supplied into flow channels, gas diffusion layers, and the catalyst layer [8]. At the anode, hydrogen splits into protons and electrons through the hydrogen oxidation reaction (HOR). The electrons are transported through electron-conducting components, such as carbon paper, while protons pass through the membrane via the ionomer. Protons are transported through the membrane to the catalyst layer while electrons travel through an external circuit, generating electricity as they move. At the cathode, absorbed oxygen reacts with the protons and electrons in the catalyst layer, forming water in the oxygen reduction reaction (ORR). The ORR is slower and more complex than the HOR, which limits the overall performance of the fuel cell [8].
## **November Background Research**

### November 15, 2024:

intro to Effect of Catalyst Ink Properties on the Performance of Proton Exchange Membrane Fuel Cell and Water Electrolyzer: A Mini Review

Korean Journal of Chemical Engineering https://doi.org/10.1007/s11814-024-00221-2

**REVIEW ARTICLE** 

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#### Effect of Catalyst Ink Properties on the Performance of Proton Exchange Membrane Fuel Cell and Water Electrolyzer: A Mini Review

Won-Jong Choi<sup>1,2</sup> · Inku Kang<sup>1,3</sup> · Duk Man Yu<sup>1</sup> · Sang Jun Yoon<sup>1</sup> · Soonyong So<sup>1</sup> · Keun-Hwan Oh<sup>1</sup>

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#### Abstract

The usual way to create the catalyst layer in electrochemical energy conversion cells involves combining catalyst, ionomer dispersion, and solvents. When this ink dispersion is processed, the resulting microstructure and rheological properties of the catalyst ink are influenced by the components composition and how they interact each other. Once the catalyst ink is dried, it forms the microstructure of the catalyst layer (CL), which includes agglomerates and pores that can impact the catalyst activity and the mass transport performance. As a result, examining the correlation between the catalyst ink characteristics and the CL structure is highly valuable. Recently, numerous studies have explored the relationship among the rheological properties of the catalyst ink, the structure of the CL, and the performance of the cell. In this review, we examine how the composition and rheological properties of the catalyst ink influence cell performance and compare the findings of these studies to provide insights into creating high-performance catalyst ink

Keywords Rheology · Catalyst ink · Catalyst layer · Fuel cell · Water electrolyzer · Performance

#### Introduction

perform

For electrochemical energy conversion cells such as fuel cells and water electrolyzers, a membrane-electrode assembly (MEA) consisting of a catalyst layers (CLs), mass transport layers (MTLs), and proton exchange membrane (PEM) is a key compartment primarily affecting cell performance. Particularly, the CLs, which are made up of carbon-sup-

Soonyong So syso@krict.re.kr

- 🖂 Keun-Hwan Oh khoh@krict.re.ki
- Hydrogen Energy Research Center, Korea Research Institute of Chemical Technology, 141 Gajeong-ro, Yuseong-gu, Daejeon 34114, Republic of Korea
- Program in Environmental and Polymer Engineering, Department of Polymer Science and Engineering, Inha University, Incheon 22212, Republic of Korea
- Department of Chemical Engineering, Hanyang University, Seoul 04763, Republic of Korea

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cell performance. For example, the oxygen transport through the cathode CL in PEM fuel cells (PEMFCs) is significantly performa governed by their pore size and distribution [1-8]. Likewise, the redox kinetics in PEM water electrolyzers (PEMWE) are strongly influenced by microstructure of the CL and play Celin an important role in the charge and mass transport [9-14]. CLs are typically produced by employing a solution pro-

S cessing of a catalyst containing ink, which is prepared by ported catalyst and ionomers, are important components of the single of a catalyst, dispersint, and additives MEAs, because they impact both charge transport and mass in a solvent mixture. The catalyst ink is deposited on a subtransport during oxidation/reduction reactions. Thus, the strate or on a PEM by different methods, such as bar-coating, microstructure of CL should be optimized to exhibit high coating to maintain their uniformity of wet-layer [15–19]. After drying, a continuous 3D interconnected network of S catalyst, ionomer, and pore is formed. For the higher cell performance, the 3D structure of CL should be optimized by factors affecting the formation of catalyst-ionomer interface for efficient catalyst utilization and proton conductivity, and lotes proper porous structure for the efficient mass transport of reactants and products. The controllable factors for the CL Sa optimization are the microstructure, dispersion and coating

method, and drying processes of the catalyst inks. Therefore, numerous studies have focused on examining the interactions in the catalyst inks between solid particles, charged ionomers, and organic solvents, as well as their impact

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#### All have an impact on overall performance

Rheological Properties

on dispersion microstructure [20, 21]. Under the multiple attractive and repulsive interactions in the inks, catalyst/ ionomer agglomerates can exhibit either stabilization or flocculation, resulting in different controllable microstructures that significantly influence the rheological properties of ink dispersions.

Rheology is considered as a sensitive technique for analyzing the overall microstructure of various materials, and serves as a strong predictor of inks behavior during the manufacturing process of CL. Specifically, the rheological properties play a crucial role in determining coating characteristics, including uniformity, thickness, sedimentation, and stacking during the drying process. Therefore, it is critical to characterize the rheological properties to establish relationships between ink formulation, processing methods, ink structure, CL microstructure, and performance.

Meanwhile, PEM fuel cells and water electrolyzers generally employ expensive precious metal catalysts (typically platinum), fluorine-based polymer electrolyte membranes, and bipolar plates with anti-corrosion coatings. In contrast, anion exchange membrane (AEM) fuel cells and water electrolyzers utilize relatively inexpensive catalysts, such as silver, cobalt, nickel, iron, and their alloys, along with hydrocarbon-based PEMs and uncoated stainless steel bipolar plates. However, AEM systems have a lower ability to respond to load fluctuations and significantly reduced longterm durability compared to PEM systems. Consequently, many issues must be addressed before AEM systems can be used industrially. Additionally, because the PEM system is more influenced by the mass transfer characteristics within the CL than the AEM system, it is crucial to analyze the rheological properties of the ink, the structure of the CL, and the cell performance based on the ink composition. Particularly, research on how the CL structure changes with different ink compositions is important, and many studies have been conducted on this topic. Therefore, this review aims to enhance our understanding of how catalyst ink components and dispersion methods affect the rheological properties of catalyst ink and subsequently impact the electrochemical performance of PEM fuel cell and water electrolyzer. Furthermore, the insights gained from this review can guide the ink formulation that can achieve the desired performance in other electrochemical devices.

emphasis on ink formulation

#### Factors Affecting the Rheological Properties of Catalyst Inks and the Microstructure of CL

#### **Constituents, Composition, and Concentration**

A catalyst ink is a catalyst (or supported catalysts) dispersed fluid in a solvent mixture. Since the catalyst particles are not self-dispersive in a solvent, amphiphilic ionomers are generally W.-J. Choi et al.

added into a catalyst ink as dispersant [22]. Once a catalyst ink is prepared, coating and drying processes are required to be followed for the catalyst layer deposition on a PEM, a diffusion layer, or a substrate [19]. In the resulting CL, a three-dimensional interconnected structure of catalyst, ionomer, and pore is formed after the solvent evaporation, and it is required to be optimized to maximize the catalytic activity, the mass transportation of reactants and products, and the proton conductance [20]. The ink compositions used in PEMFCs, selected from existing literature, are presented in Table 1.

Considering that the solvent mixtures, such as aqueous solvents with isopropanol (IPA) or *n*-propanol (NPA), are Newtonian fluids, the rheological properties of a catalyst ink, a multi-phase fluid, are mainly governed by the ink formulation—constituents, composition, and concentration—and the interaction between the components [23]. The content of each component needs to be determined for various catalytic systems, but the solid content in ink commonly depends on the flowability for a specific coating process of the ink for the uniform quality and defect-free catalyst layer. The coating process of the ink can be categorized into a viscous and a low viscous coating process; doctor blade or roll-to-roll coating requires a higher solid content, > 5 wt%, whereas spray coating requires a lower solid content commonly less than 3 wt% [24, 25].

In all catalyst inks, catalytic agglomerates, composed of catalysts (or supported catalysts) and ionomers, are suspended in the solvent medium in the form of relatively small primary aggregates (a few hundred nm) and large secondary agglomerate particles (>400 nm in size), which are assembled from aggregates by weak van der Waals forces. Under shear, the weakly assembled large agglomerates break down into smaller agglomerates and aggregates. This behavior induces the non-Newtonian shear-thinning behavior observed in most catalyst inks at various solid concentrations, which is characterized by the Herschel-Bulkley model.

#### $\tau = \eta \times \dot{\gamma} = \tau_0 + \kappa \times \dot{\gamma}^n,$

where  $\tau$  is the shear stress,  $\eta$  is the viscosity,  $\tau_0$  is the yield shear stress,  $\kappa$  is the consistency index,  $\dot{\gamma}$  is the shear rate, and *n* is the shear-thinning index. In general, the catalyst ink under shear flow exhibits n < 1, representing a shear-thinning fluid. Noted that at low-shear rates where Brownian motion dominates the hydrodynamic motion, some catalyst inks show Newtonian plateau in steady-shear viscosities. Therefore, generally, in the course of the coating procedure, the catalyst ink displays low viscosity under the application of high shear rate; however, during the subsequent resting and drying stages where the shear force is eliminated (low-shear rate), the catalyst ink shows high viscosity.

As mentioned above, the rheological characteristics of a catalyst ink are highly influenced by factors, such as the solid content, composition, and interactions among

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catalyst and ionomer in the solvent, and enhance the interaction between the catalyst and ionomer, which are crucial for improving the utilization of catalyst. The methods for ink dispersion include ultrasonication, mechanical stirring, hydrodynamic cavitation, and ball milling [1, 23, 68-76]. Ultrasonication and ball milling are the most common techniques for ink dispersion. Tip sonication, bath sonication, or a combination of both, along with ball milling, are suitable for inks with low viscosity or low solid concentration. However, for viscous inks or inks with high solid concentration, ball milling is often more appropriate [73]. Recently, additional methods, such as hydrodynamic cavitation, planetary mixers, and high-pressure homogenization, have been employed for dispersing catalyst ink. A recent review provides a comprehensive summary of ball milling, mechanical stirring, ultrasonication, and their respective advantages and disadvantages [23, 74]. This particular review primarily focuses on the impact of the dispersion process on the rheological and macroscopic properties of the ink, as well as the resulting CLs and performance.

Ultrasonic dispersion is thought to be an environmentally friendly and convenient way for maintaining purity when using volatile dispersion media. There are two primary types of ultrasonication methods: bath ultrasonication and tip ultrasonication. Between them, tip ultrasonication is found to be more effective at achieving dispersion when operating under the same conditions [70–72].

Ball milling is a method used for batch processing, where metal balls, ceramics, or other types of grinding media are combined with catalyst inks. This process relies primarily on intense collisions, extrusion, and friction between the ball grinding media, catalyst inks, and the walls of the ball grinding tank. These interactions transfer mechanical energy from the ball milling media to the catalyst inks, facilitating dispersion [75-77]. Ball milling offers several advantages, including cost-effectiveness, high efficiency, and suitability for large-scale production. However, it is important to note that ball milling can result in wear during the impact and grinding processes, potentially leading to ink contamination. Currently, there are numerous studies available that explore the treatment of catalyst inks for PEMFC using ball milling methods [20, 78, 79]. In a study conducted by S. Du et al., a catalyst ink was prepared using both ultrasonication and ball mill mixing techniques to examine the impact of the dispersion method on the viscosity and thixotropy of the ink. In terms of viscosity, the average viscosity of the ink produced through ball milling was higher compared to that obtained through sonication (Fig. 7). Furthermore, the ink exhibited a more pronounced thixotropic recovery as a result of ball milling. This characteristic is advantageous for effectively coating the ink on a surface [73]. Additionally, the effects of viscosity and dispersity on ink were studied, and the process parameters affecting cracks and performance of CL were

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Fig. 7 The change of viscosity during 3ITT of ball milling and sonication dispersion processes. Reproduced from Ref. [73], Copyright (2020), with permission from the the Elsevier

investigated [80]. The results obtained using Pt-high surface area carbon at an ionomer/carbon weight ratio of 0.8 indicated that the dispersity of the ink is highly influenced by the mixing method employed. It was observed that, after sonication, the ink formed large agglomerates.

#### Summary and Outlook

#### properties that better improve performance

The development of catalyst ink, its rheological characteristics, and the overall structure of the ink state are essential for improving the performance and durability of the electrode in electrochemical devices. The CL consists of catalyst and ionomer that are interconnected to form a porous multiscale structure. The transportation of reactants and products to and from the active sites is governed by the structure of the CL. CL is typically manufactured via an ink-based process, with the ink consists of catalyst/ionomer agglomerates, additive/ionomer/catalyst agglomerates, non-adsorbed ionomer, and solvent. These agglomerates consolidate to form the CL during the drying process. Consequently, the microstructure of the CL, which have a direct effect on the performance and durability of MEAs, is determined by the cluster size, catalyst and ionomer con-tent, solvent type, additives (or dispersants), and disper-sion method for catalyst ink. Particularly, the ink formulation-constituents, composition, and concentration-and the interaction between the components have a direct effect on the rheological properties of catalyst ink, such as viscosity, viscoelasticity, and thixotropy.

When it comes to commercialization and mass production using roll-to-roll ink deposition technology, it is essential to design the rheology of the ink in a logical and careful manner. Various factors, including ink rheology and coating

to optimize fuel Cell properties process parameters, influence the formation of CLs during the ink deposition procedure. Therefore, it is crucial to investigate the effects of ink rheology on each stage of deposition. Understanding the relationship between the constituents and rheological properties of catalyst inks can also contribute to their optimization.

#### To gain a better understanding of the correlation between ink rheological properties, the macroscopic structure of catalyst ink, and the overall cell performance and durability, it is necessary to consider certain challenges and future directions. These include investigating the microstructure of catalyst inks and CLs, ensuring that catalyst inks have a wide range of solid concentrations, and investigating the coating

and drying processes. **Important to both PEM & AEM** Meanwhile, similar to the PEM system, it is crucial to investigate how the ink composition and dispersion method impact the rheological properties of the ink, electrode structure, and overall performance in AEM fuel cells and water electrolyzers. Although research on the AEM system has been limited thus far, it is essential to analyze these factors as more studies are conducted in the future.

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## November 27, 2024:

#### CYSF portal research edits

The global transition to renewable energy has recently accelerated significantly due to growing concerns about climate change, energy security, and the impacts of fossil fuel use. Fossil fuels such as coal, oil, and natural gas account for over 75% of global greenhouse gas emissions and almost 90% of carbon dioxide emissions globally [1]. Processes that require the burning of fossil fuels, such as generating power and manufacturing goods, are key causes of greenhouse gas emissions. The greenhouse effect is the primary driver of climate change, and human activities are responsible for increasing the concentration of greenhouse gases released into the atmosphere [2]. As a result of the increasing carbon emissions, 196 countries signed the Paris Agreement, which aims to limit global warming to 1.5°C by the year 2050 [3]. Each country that signed onto the Paris Agreement proposed commitments to reduce emissions. Some examples of these commitments include the European Union reducing emissions through domestic measures and India increasing electric power from non-fossil fuel energy resources [4].

In the United States, three economic sectors — transportation, electric power, and industry — contribute to over 75% of all greenhouse gas emissions [5]. Transportation is the largest sector, making up 28% of all greenhouse gas emissions because petroleum-based fuels are most commonly used for transportation [5]. In Canada, oil and gas, transportation, and buildings are the top three economic sectors contributing to over 60% of emissions in the country (Share of greenhouse gas emissions in ...). Therefore, a significant reduction in overall greenhouse gas emissions can be achieved by limiting the emissions from the transportation sector [6]. This has led to the adoption of clean energy sources and clean energy transportation solutions. Accordingly, there has been a global push for zero-emission vehicles, including battery-electric and hydrogen fuel cell-powered vehicles [6].

Both electric batteries and proton-exchange membrane fuel cells (PEMFCs) are promising alternatives to internal combustion engines due to their efficiency and environmental benefits. The application focus of PEMFCs is no longer on light-duty vehicles due to the fact that electric vehicles (EVs) have been around for longer, the cost of EVs is significantly lower than PEMFC-powered vehicles in consideration to small vehicles, and charging infrastructure has been expanded [7]. However, because all the energy is stored in batteries, for long-distance heavy-duty vehicles (e.g., trucks), the weight of the battery required for long operations is a huge limitation. Thus, there has been immense interest in PEMFCs' zero-emissions power source for heavy-duty vehicles. For heavy-duty vehicle applications, a key technological challenge is improving the durability of PEMFCs [7], [8]. Hydrogen-powered PEMFCs were simulated in heavy-duty vehicles, and a study found that the metrics used to determine performance standards were not only met but also exceeded [9], showing great promise in the use of PEMFCs in the transportation sector.

In a PEMFC, hydrogen and oxygen are supplied into flow channels, gas diffusion layers (GDLs), and the catalyst layer (CL) [10]. At the anode, hydrogen splits into protons and electrons through the hydrogen oxidation reaction (HOR). The electrons are transported through electron-conducting components, such as carbon paper. At the same time, protons are conducted through the ionic polymer (ionomer) in the anode catalyst layer through the polymer electrolyte membrane to the cathode catalyst layer. Protons are transported through the membrane to the catalyst layer.

move. At the cathode, oxygen reacts with the protons and electrons at the catalyst surface to produce water via the oxygen reduction reaction (ORR). The ORR is slower and more complex than the HOR, which limits the overall performance of the fuel cell. A simplified model of these processes has been described in the literature [11], [12] and can be seen in Figure 1 and Figure 2. Over 40% of the total cost of mass-produced PEMFCs is attributed to the catalyst layer. To address this, researchers are exploring platinum alloys and alternative non-precious metal (NPM) catalysts to reduce platinum content without sacrificing performance. However, while NPM catalysts are more cost-effective, they are not as efficient or durable as CLs made with platinum, resulting in more frequent replacements that increase long-term costs [10]. Thus, in the near term, the PEMFC technology is expected to continue to use platinum-based catalysts.



Figure 1. Schematic depiction of a PEM electrolyzer and fuel cell: The fuel cell combines hydrogen and oxygen to produce electricity and water [11].



Figure 2. Schematic depiction of a PEMFC showing the different layers, compositions, and reactant transport pathways [12]. Black structures are the carbon supports, purple represents the ionomer, red is the polytetrafluoroethylene (PTFE), and green is the catalysts. Note the figure is not drawn to scale, and the catalyst layer, GDL, and MPL have different porosities and support material sizes.

Since performance and durability are higher-priority challenges for PEMFC application in heavy-duty vehicles, current efforts are directed to the catalyst layer (CL) design with the aim of both reducing the use of platinum and improving the CL structure [10]. The catalyst layer structure is very important because it impacts the fuel cell's short- and long-term performance. For the PEMFC to perform effectively, the catalyst layer must facilitate the efficient transport of the reactants (oxygen or hydrogen, protons, and electrons) of the electrochemical reactions, as well as the removal of product water and heat. The CL structure must have sufficient porosity and large pores for easy transport of oxygen gas in the cathode catalyst layer and hydrogen gas in the anode catalyst layer. The catalyst layer must have a well-connected network of ionomers coating the catalyst to ensure protons can reach the reaction sites for electrochemical reactions to occur. The catalyst layer must have enough ionomer to ensure ionic connectivity but not too much to isolate the catalyst/carbon-support particles electronically. The catalyst layer structure is controlled by the catalyst ink formulation as well as the catalyst ink coating method for the fabrication of the catalyst layer [10].

The formulation of the catalyst ink plays a crucial role in enhancing the performance and durability of PEMFCs [13]. Figure 3 below shows the workflow from constituent materials to the final catalyst layer formation [14]. The catalyst layer constituent materials, the catalyst and ionomer, are added to a solvent, which is typically a mixture of water and alcohol. The complex mixture is homogenized by mixing using ultrasonic and ball milling to make a uniform suspension called the catalyst ink. The ink is sprayed on a substrate made of a Teflon-like material known as polytetrafluoroethylene (PTFE), and upon evaporation of the solvent, the catalyst and ionomer create a nanoporous composite catalyst structure [14].



Figure 3. Schematic depiction of the process of creating the catalyst ink and fabricating the catalyst layer from the catalyst ink [14]. Materials, including the ionomer, catalyst, and solvent, are combined and mixed in a dispersion step. The resulting catalyst ink is deposited onto a substrate — the catalyst layer forms on the substrate to be used in fuel cells.

It has been discovered that adjusting the ratio between water and isopropyl alcohol in the catalyst ink allows researchers to improve the viscosity of the ink, which may be important for spray deposition of the ink onto the substrate and adhesion of catalyst-ionomer aggregates to the substrate [13]. The size of the catalyst-ionomer aggregates in the ink can control the pores in the final catalyst layer structure. The ratio of ionomer and catalyst can control whether all catalysts

are effectively utilized by providing protonic access. The link between catalyst ink properties and the final catalyst layer structure is not currently well understood. As a result, there is a lack of a rational approach to designing the optimum catalyst layer structure that yields high performance [13].

New research on ink composition and application methods aims to maximize the total utilization of the catalyst while also balancing durability and reactant transport [13]. This contributes to the development of PEMFCs for commercial applications, especially in the heavy-duty vehicle sector [13].

# **December Background Research**

## December 5th, 2024

Research with APA style citations for the CYSF Portal :

The global transition to renewable energy has recently accelerated significantly due to growing concerns about climate change, energy security, and the impacts of fossil fuel use. Fossil fuels such as coal, oil, and natural gas account for over 75% of global greenhouse gas emissions and almost 90% of carbon dioxide emissions globally (United Nations, n.d.). Processes that require the burning of fossil fuels, such as generating power and manufacturing goods, are key causes of greenhouse gas emissions. The greenhouse effect is the primary driver of climate change, and human activities are responsible for increasing the concentration of greenhouse gases released into the atmosphere (*Causes of Climate Change*, n.d.). As a result of the increasing carbon emissions, 196 countries signed the Paris Agreement, which aims to limit global warming to 1.5°C by the year 2050 (*The Paris Agreement*, n.d.). Each country that signed onto the Paris Agreement proposed commitments to reduce emissions through domestic measures and India increasing electric power from non-fossil fuel energy resources (*The Paris Agreement on Climate Change*, n.d.).

In the United States, three economic sectors — transportation, electric power, and industry — contribute to over 75% of all greenhouse gas emissions (Us Epa, 2015). Transportation is the largest sector, making up 28% of all greenhouse gas emissions because petroleum-based fuels are most commonly used for transportation (Us Epa, 2015). In Canada, oil and gas, transportation, and buildings are the top three economic sectors contributing to over 60% of emissions in the country (*Share of Greenhouse Gas Emissions in Canada 2023, by Sector*, n.d.). Therefore, a significant reduction in overall greenhouse gas emissions can be achieved by limiting the emissions from the transportation sector (Baroutaji et al., 2016). This has led to the adoption of clean energy sources and clean energy transportation solutions. Accordingly, there has been a global push for zero-emission vehicles, including battery-electric and hydrogen-fuel cell-powered vehicles (Baroutaji et al., 2016).

Both electric batteries and proton-exchange membrane fuel cells (PEMFCs) are

promising alternatives to internal combustion engines due to their efficiency and environmental benefits. The application focus of PEMFCs is no longer on light-duty vehicles due to the fact that electric vehicles (EVs) have been around for longer, the cost of EVs is significantly lower than PEMFC-powered vehicles in consideration to small vehicles, and charging infrastructure has been expanded (Cullen et al., 2021). However, because all the energy is stored in batteries, for long-distance heavy-duty vehicles (e.g., trucks), the weight of the battery required for long operations is a huge limitation. Thus, there has been immense interest in PEMFCs' zero-emissions power source for heavy-duty vehicles. For heavy-duty vehicle applications, a key technological challenge is improving the durability of PEMFCs (Cullen et al., 2021), (Meeting, n.d.). Hydrogen-powered PEMFCs were simulated in heavy-duty vehicles, and a study found that the metrics used to determine performance standards were not only met but also exceeded (Ogungbemi et al., 2021), showing great promise in the use of PEMFCs in the transportation sector.

In a PEMFC, hydrogen and oxygen are supplied into flow channels, gas diffusion layers (GDLs), and the catalyst layer (CL) (Zhao et al., 2023). At the anode, hydrogen splits into protons and electrons through the hydrogen oxidation reaction (HOR). The electrons are transported through electron-conducting components, such as carbon paper. At the same time, protons are conducted through the ionic polymer (ionomer) in the anode catalyst layer through the polymer electrolyte membrane to the cathode catalyst layer. Protons are transported through the membrane to the catalyst layer while electrons travel through an external circuit, generating electricity as they move. At the cathode, oxygen reacts with the protons and electrons at the catalyst surface to produce water via the oxygen reduction reaction (ORR). The ORR is slower and more complex than the HOR, which limits the overall performance of the fuel cell. A simplified model of these processes has been described in the literature (Escobar-Yonoff et al., 2021), (Suter et al., 2021) and can be seen in Figure 1 and Figure 2. Over 40% of the total cost of mass-produced PEMFCs is attributed to the catalyst layer. To address this, researchers are exploring platinum alloys and alternative non-precious metal (NPM) catalysts to reduce platinum content without sacrificing performance. However, while NPM catalysts are more cost-effective, they are not as efficient or durable as CLs made with platinum, resulting in more frequent replacements that increase long-term costs (Zhao et al., 2023). Thus, in the near term, the PEMFC technology is expected to continue to use platinum-based catalysts.



Figure 1. Schematic depiction of a PEM electrolyzer and fuel cell: The fuel cell combines hydrogen and oxygen to produce electricity and water (Escobar-Yonoff et al., 2021).



Figure 2. Schematic depiction of a PEMFC showing the different layers, compositions, and reactant transport pathways (Suter et al., 2021). Black structures are the carbon supports, purple represents the ionomer, red is the polytetrafluoroethylene (PTFE), and green is the catalysts. Note the figure is not drawn to scale, and the catalyst layer, GDL, and MPL have different porosities and support material sizes.

Since performance and durability are higher-priority challenges for PEMFC application in heavy-duty vehicles, current efforts are directed to the catalyst layer (CL) design with the aim of both reducing the use of platinum and improving the CL structure (Zhao et al., 2023). The catalyst layer structure is very important because it impacts the fuel cell's short- and long-term performance. For the PEMFC to perform effectively, the catalyst layer must facilitate the efficient transport of the reactants (oxygen or hydrogen, protons, and electrons) of the electrochemical reactions, as well as the removal of product water and heat. The CL structure must have sufficient porosity and large pores for easy transport of oxygen gas in the cathode catalyst layer and hydrogen gas in the anode catalyst layer. The catalyst layer must have a well-connected network of ionomer coating the catalyst to ensure protons can reach the reaction sites for electrochemical reactions to occur. The catalyst layer must have enough ionomer to ensure ionic connectivity but not too much to isolate the catalyst/carbon-support particles electronically. The catalyst layer structure is controlled by the catalyst ink formulation as well as the catalyst ink coating method for the fabrication of the catalyst layer (Zhao et al., 2023).

The formulation of the catalyst ink plays a crucial role in enhancing the performance and durability of PEMFCs (Van Cleve et al., 2019). Figure 3 below shows the workflow from constituent materials to the final catalyst layer formation (Guo et al., 2020). The catalyst layer constituent materials, the catalyst and ionomer, are added to a solvent, which is typically a mixture of water and alcohol. The complex mixture is homogenized by mixing using ultrasonic and ball milling to make a uniform suspension called the catalyst ink. The ink is sprayed on a substrate made of a Teflon-like material known as polytetrafluoroethylene (PTFE), and upon evaporation of the solvent, the catalyst and ionomer create a nanoporous composite catalyst structure (Guo et al., 2020).

Figure 3. Schematic depiction of the process of creating the catalyst ink and fabricating the catalyst layer from the catalyst ink (Guo et al., 2020). Materials, including the ionomer, catalyst, and solvent, are combined and mixed in a dispersion step. The resulting catalyst ink is deposited onto a substrate — the catalyst layer forms on the substrate to be used in fuel cells.



It has been discovered that adjusting the ratio between water and isopropyl alcohol in the catalyst ink allows researchers to improve the viscosity of the ink, which may be important for spray deposition of the ink onto the substrate and adhesion of catalyst-ionomer aggregates to the substrate (Van Cleve et al., 2019). The size of the catalyst-ionomer aggregates in the ink can control the pores in the final catalyst layer structure. The ratio of ionomer and catalyst can control whether all catalysts are effectively utilized by providing protonic access. The link between catalyst ink properties and the final catalyst layer structure is not currently well understood. As a result, there is a lack of a rational approach to designing the optimum catalyst layer structure that yields high performance (Van Cleve et al., 2019).

New research on ink composition and application methods aims to maximize the total utilization of the catalyst while also balancing durability and reactant transport (Van Cleve et al., 2019). This contributes to the development of PEMFCs for commercial applications, especially in the heavy-duty vehicle sector (Van Cleve et al., 2019).

## **January Background Research**

### January 28, 2025:

The global transition to renewable energy has significantly accelerated recently due to growing concerns about climate change, energy security, and the impacts of fossil fuel use. Fossil fuels such as coal, oil, and natural gases account for over 75% of global greenhouse gas emissions and almost 90% of carbon dioxide emissions globally [1]. Processes that require the burning of fossil fuels, such as generating power and manufacturing goods, are key causes of greenhouse gas emissions. The greenhouse effect primarily drives climate change, and human activities are responsible for increasing the concentration of greenhouse gases released into the atmosphere [2]. As a result of rising carbon emissions, 196 countries signed the Paris Agreement, which aims to limit global warming to 1.5°C by the year 2050 [3]. Each country that signed the Paris Agreement proposed commitments to reduce greenhouse gas emissions. Some examples of these commitments include India increasing electrical power generated from non-fossil fuel energy resources and the European Union reducing emissions through domestic measures [4].

In the United States, three economic sectors — transportation, electrical power, and industry — contribute to over 75% of all greenhouse gas emissions [5]. Transportation is the largest sector, making up 28% of all greenhouse gas emissions. This is because petroleum-based fuels are most commonly used for transportation [5]. As of 2023, in Canada, oil and gas, transportation, and buildings are the top three economic sectors contributing to over 60% of all greenhouse gas emissions in the country [6]. A significant reduction in overall greenhouse gas

emissions can be achieved by limiting the emissions from the transportation sector because, as seen in the data from the United States and Canada, the majority of the greenhouse gas emissions come from the transportation sector [7]. This has led to the adoption of clean energy sources and clean energy transportation solutions. Accordingly, there has been a global push for zero-emission vehicles, including battery-electric and hydrogen fuel cell-powered vehicles [7].

Both electric batteries and proton-exchange membrane fuel cells (PEMFCs) are promising alternatives to internal combustion engines due to their efficiency and environmental benefits. The application focus of PEMFCs is no longer on light-duty vehicles due to the fact that electric vehicles (EVs) have been around for longer [8]. This has resulted in the cost of EVs being significantly lower than PEMFC-powered vehicles in consideration to small vehicles, and charging infrastructure has been expanded [8]. However, because all of the energy is stored in batteries, for long-distance heavy-duty vehicles (e.g., trucks), the weight of the battery required for long operation periods is a huge limitation. Thus, there has been an immense interest in PEMFCs' zero-emissions power source for heavy-duty vehicles. For heavy-duty vehicle applications, a key technological challenge is improving the durability of PEMFCs [8], [9]. Hydrogen-powered PEMFCs were simulated in heavy-duty vehicles, and a study found that the metrics used to determine performance standards were not only met but also exceeded [10]PEMFCs in the transportation sector.

In a PEMFC, hydrogen and oxygen are supplied into flow channels, gas diffusion layers (GDLs), and the catalyst layer (CL) [11]. At the anode, hydrogen splits into protons and electrons through the hydrogen oxidation reaction (HOR). The electrons are transported through electron-conduction components, such as carbon paper.

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### January 30, 2025:

At the same time, protons are conducted through the ionic polymer, also known as the

ionomer, in the anode catalyst layer through the polymer electrolyte membrane to the cathode

catalyst layer. Protons are transported through the membrane to the catalyst layer while electrons

travel through an external circuit, generating electricity as they move. At the cathode, oxygen

reacts with the protons and electrons at the catalyst surface to produce water via the oxygen

reduction reaction (ORR). The ORR occurs slower than the HOR because it is more complex, limiting the overall performance of the fuel cell. A simplified model of these processes has been described in the literature [12], [13] and can be seen in Figure 1 and Figure 2. Over 40% of the total cost of mass-produced PEMFCs is attributed to the catalyst layer. To address this, researchers are exploring platinum alloys and alternative non-precious metal (NPM) catalysts to reduce platinum content without sacrificing performance. However, while NPM catalysts are more cost-effective, they are less efficient and durable than CLs made with platinum, resulting in more frequent replacements that increase long-term costs [11]. Thus, in the near future, the PEMFC technology is expected to continue to use platinum-based catalysts.



Figure 1. Schematic depiction of a PEM electrolyzer and fuel cell: The fuel cell combines hydrogen and oxygen to produce electricity and water [12]



Figure 2. Schematic depiction of a PEMFC showing the different layers, compositions, and reactant transport pathways [13]. Black structures are the carbon supports, purple represents the ionomer, red is the polytetrafluoroethylene (PTFE), and green is the catalysts. Note: the figure is not drawn to scale, and the catalyst layer, GDP, and MPL have different porosities and support material sizes.

Since the performance and durability are higher-priority challenges for PEMFC application in heavy-duty vehicles, current efforts are directed to the catalyst layer (CL) design with the aim of both reducing the use of platinum and improving the CL structure [11]. The catalyst layer structure is very important because it impacts both the short and long-term performance of the fuel cell. For the PEMFC to perform effectively, the catalyst layer must facilitate the efficient transport of the reactants (oxygen or hydrogen, protons, and electrons) of the electrochemical reactions, as well as the removal of product water and heat. The CL structure must have sufficient porosity and large pores for easy transport of oxygen gas in the cathode catalyst layer and hydrogen gas in the anode catalyst layer. The catalyst layer must have a well-connected network of ionomer coating the catalyst to ensure protons can reach the reduction sites for electrochemical reactions to occur. The catalyst layer must have enough ionomer to ensure ionic conductivity but not too much to isolate the catalyst/carbon-support particles electronically. The catalyst layer structure is controlled by the catalyst ink formulation as well as the catalyst ink coating method for the fabrication of the catalyst layer [11].

The formulation of the catalyst ink plays a crucial role in enhancing the performance and durability of PEMFCs [14]. Figure 3 below shows the workflow from constituent materials to the final catalyst layer formation. [15]. The catalyst layer constituent materials – the catalyst and ionomer – are added to a solvent, which is typically a mixture of water and alcohol. This complex mixture is homogenized using ultrasonication and ball milling to make a uniform suspension called the catalyst ink. The ink is sprayed onto a substrate made of a Teflon-like material known as polytetrafluoroethylene (PTFE). Upon evaporation of the solvent, the catalyst and ionomer create a nanoporous composite catalyst structure [15]



Figure 3. Schematic depiction of the process of creating the catalyst ink and fabricating the catalyst layer from the catalyst ink [15]erials, including the ionomer, catalyst, and solvent, are combined and mixed in a dispersion step. The resulting catalyst ink is deposited onto a substrate — the catalyst layer forms on the substrate to be used in fuel cells.

It has been discovered that adjusting the ratio between water and isopropyl alcohol in the catalyst ink allows researchers to improve the viscosity of the ink, which may be important for spray deposition of the ink onto the substrate and adhesion of catalyst-ionomer aggregates to the substrates [14]. The size of the catalyst-ionomer aggregates in the ink can control the pores in the final catalyst layer structure. The ratio of ionomer and catalyst can control whether all catalysts

are effectively utilized by providing protonic access. The link between catalyst ink properties and the final catalyst layer structure is not well understood currently. As a result, researchers lack a rational approach to designing the optimum catalyst structure that yields high performance [14].

New research on ink composition and application methods aims to maximize the total utilization of the catalyst while also balancing durability and reactant transport [14]. This contributes to the development of PEMFCs for commercial applications, especially in the heavy-duty vehicle sector [14]. This project aims to understand how varying isopropyl alcohol concentrations in the water-isopropyl alcohol solvent mixture affect the properties of the catalyst layer, aggregate size, coverage, and ionic resistance to optimize the fuel cell's durability and efficiency. The short-term objectives of this project are to investigate the impact of solvent composition on ink properties, including viscosity and catalyst-ionomer aggregate size; investigate the impact of solvent composition of the catalyst ink on catalyst layer properties such as ionic resistance, electronic resistance, and pore size; and to determine the optimum ink composition that results in high-performing PEMFCs. The long-term, future goals of this project are to design a set of manufacturing parameters for applying the ink to the catalyst layer with an optimized concentration of isopropyl alcohol in PEMFCs, especially for applications in heavy-duty vehicles and to help large-scale production of PEMFCs as a sustainable alternative to internal combustion engines in the transportation sector.

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## **February Background Research**

## February 03, 2024:

New research on ink composition and application methods aims to maximize the total utilization of the catalyst while also balancing durability and reactant transport [14]. This contributes to the development of PEMFCs for commercial applications, especially in the heavy-duty vehicle sector [14]. This project aims to understand how varying isopropyl alcohol concentrations in the water-isopropyl alcohol solvent mixture affect the properties of the catalyst layer, aggregate size, coverage, and ionic resistance to optimize the fuel cell's durability and efficiency. The short-term objectives of this project are to investigate the impact of solvent composition on ink properties, including viscosity and catalyst-ionomer aggregate size; investigate the impact of solvent composition of the catalyst ink on catalyst layer properties such as ionic resistance, electronic resistance, and pore size; and to determine the optimum ink composition that results in high-performing PEMFCs. The long-term, future goals of this project are to design a set of manufacturing parameters for applying the ink to the catalyst layer with an optimized concentration of isopropyl alcohol in PEMFCs, especially for applications in heavy-duty vehicles and to help large-scale production of PEMFCs as a sustainable alternative to internal combustion engines in the transportation sector. Ultimately, this research seeks to answer the question: how do catalyst ink parameters affect ink properties, and subsequently, how do ink properties impact the catalyst layer structure and thereby affect the performance of a PEMFC?

## February 05, 2025:

New research on ink composition and application methods aims to maximize the total utilization of the catalyst while also balancing durability and reactant transport [14]. This contributes to the development of PEMFCs for commercial applications, especially in the heavy-duty vehicle sector [14]. This study aims to determine how varying isopropyl alcohol concentrations in the water-isopropyl alcohol solvent mixture affect the properties of the catalyst layer, aggregate size, coverage, and ionic resistance to optimize the fuel cell's durability and efficiency. The short-term objectives of this research are to investigate the impact of solvent composition on ink properties (viscosity, catalyst-ionomer aggregate size) and catalyst layer properties (ionic resistance, electronic resistance, pore size) and to determine the optimum ink composition that results in high-performing PEMFCs. The long-term, future goals of this project are to design a set of manufacturing parameters for applying the ink to the catalyst layer with an optimized concentration of isopropyl alcohol in PEMFCs, especially for applications in heavy-duty vehicles and to help large-scale production of PEMFCs as a sustainable alternative to internal combustion engines in the transportation sector.

## March 13, 2025:

☑ Background edits for CYSF

The global transition to renewable energy has recently accelerated significantly due to growing concerns about climate change, energy security, and the impacts of fossil fuel use. Fossil fuels such as coal, oil, and natural gas account for over 75% of global greenhouse gas emissions and almost 90% of carbon dioxide emissions globally (United Nations, n.d.). Processes that require the burning of fossil fuels, such as generating power and manufacturing goods, are key causes of greenhouse gas emissions. The greenhouse effect is the primary driver of climate change, and human activities are responsible for increasing the concentration of greenhouse gases released into the atmosphere (*Causes of Climate Change*, n.d.). As a result of the increasing carbon emissions, 196 countries signed the Paris Agreement, which aims to limit global warming to 1.5°C by the year 2050 (*The Paris Agreement*, n.d.). Each country that signed onto the Paris Agreement proposed commitments to reduce emissions. Some examples of these commitments include the European Union reducing emissions through domestic measures and India increasing electric power from non-fossil fuel energy resources (*The Paris Agreement on Climate Change*, n.d.).

In the United States, three economic sectors — transportation, electric power, and industry — contribute to over 75% of all greenhouse gas emissions (Us Epa, 2015). Transportation is the largest sector, making up 28% of all greenhouse gas emissions because petroleum-based fuels are most commonly used for transportation (Us Epa, 2015). In Canada, oil and gas, transportation, and buildings are the top three economic sectors contributing to over 60% of emissions in the country (*Share of Greenhouse Gas Emissions in Canada 2023, by Sector*, n.d.). Therefore, a significant reduction in overall greenhouse gas emissions can be achieved by limiting the emissions from the transportation sector (Baroutaji et al., 2016). This has led to the adoption of clean energy sources and clean energy transportation solutions. Accordingly, there has been a global push for zero-emission vehicles, including battery-electric and hydrogen-fuel cell-powered vehicles (Baroutaji et al., 2016).

Both electric batteries and proton-exchange membrane fuel cells (PEMFCs) are promising alternatives to internal combustion engines due to their efficiency and environmental benefits. The application focus of PEMFCs is no longer on light-duty vehicles due to the fact that electric vehicles (EVs) have been around for longer, the cost of EVs is significantly lower than PEMFC-powered vehicles in consideration to small vehicles, and charging infrastructure has been expanded (Cullen et al., 2021). However, because all the energy is stored in batteries, for long-distance heavy-duty vehicles (e.g., trucks), the weight of the battery required for long operations is a huge limitation. Thus, there has been immense interest in PEMFCs' zero-emissions power source for heavy-duty vehicles. For heavy-duty vehicle applications, a key technological challenge is improving the durability of PEMFCs (Cullen et al., 2021), (Meeting, n.d.). Hydrogen-powered PEMFCs were simulated in heavy-duty vehicles, and a study found that the metrics used to determine performance standards were not only met but also exceeded (Ogungbemi et al., 2021), showing great promise in the use of PEMFCs in the transportation sector.

In a PEMFC, hydrogen and oxygen are supplied into flow channels, gas diffusion layers (GDLs), and the catalyst layer (CL) (Zhao et al., 2023). At the anode, hydrogen splits into protons and electrons through the hydrogen oxidation reaction (HOR). The electrons are transported through electron-conducting components, such as carbon paper. At the same time, protons are conducted through the ionic polymer (ionomer) in the anode catalyst layer through the polymer electrolyte membrane to the cathode catalyst layer. Protons are transported through the membrane to the catalyst layer while electrons travel through an external circuit, generating electricity as they move. At the cathode, oxygen reacts with the protons and electrons at the catalyst surface to produce water via the oxygen reduction reaction (ORR). The ORR is slower and more complex than the HOR, which limits the overall performance of the fuel cell. A simplified model of these processes has been described in the literature (Escobar-Yonoff et al., 2021), (Suter et al., 2021) and can be seen in Figure 1 and Figure 2. Over 40% of the total cost of mass-produced PEMFCs is attributed to the catalyst layer. To address this, researchers are exploring platinum alloys and alternative non-precious metal (NPM) catalysts to reduce platinum content without sacrificing performance. However, while NPM catalysts are more cost-effective, they are not as efficient or durable as CLs made with platinum, resulting in more frequent replacements that increase long-term costs (Zhao et al., 2023). Thus, in the near term, the PEMFC technology is expected to continue to use platinum-based catalysts.



Figure 1. Schematic depiction of a PEM electrolyzer and fuel cell: The fuel cell combines hydrogen and oxygen to produce electricity and water (Escobar-Yonoff et al., 2021).



Figure 2. Schematic depiction of a PEMFC showing the different layers, compositions, and reactant transport pathways (Suter et al., 2021). Black structures are the carbon supports, purple represents the ionomer, red is the polytetrafluoroethylene (PTFE), and green is the catalysts. Note the figure is not drawn to scale, and the catalyst layer, GDL, and MPL have different porosities and support material sizes.

Since performance and durability are higher-priority challenges for PEMFC application in heavy-duty vehicles, current efforts are directed to the catalyst layer (CL) design with the aim of both reducing the use of platinum and improving the CL structure (Zhao et al., 2023). The catalyst layer structure is very important because it impacts the fuel cell's short- and long-term performance. For the PEMFC to perform effectively, the catalyst layer must facilitate the efficient transport of the reactants (oxygen or hydrogen, protons, and electrons) of the electrochemical reactions, as well as the removal of product water and heat. The CL structure must have sufficient porosity and large pores for easy transport of oxygen gas in the cathode catalyst layer and hydrogen gas in the anode catalyst layer. The catalyst layer must have a well-connected network of ionomer coating the catalyst to ensure protons can reach the reaction sites for electrochemical reactions to occur. The catalyst layer must have enough ionomer to ensure ionic connectivity but not too much to isolate the catalyst/carbon-support particles electronically. The catalyst layer structure is controlled by the catalyst ink formulation as well as the catalyst ink coating method for the fabrication of the catalyst layer (Zhao et al., 2023).

The formulation of the catalyst ink plays a crucial role in enhancing the performance and durability of PEMFCs (Van Cleve et al., 2019). Figure 3 below shows the workflow from constituent materials to the final catalyst layer formation (Guo et al., 2020). The catalyst layer constituent materials, the catalyst and ionomer, are added to a solvent, which is typically a mixture of water and alcohol. The complex mixture is homogenized by mixing using ultrasonic and ball milling to make a uniform suspension called the catalyst ink. The ink is sprayed on a substrate made of a Teflon-like material known as polytetrafluoroethylene (PTFE), and upon evaporation of the solvent, the catalyst and ionomer create a nanoporous composite catalyst structure (Guo et al., 2020).

Figure 3. Schematic depiction of the process of creating the catalyst ink and fabricating the catalyst layer from the catalyst ink (Guo et al., 2020). Materials, including the ionomer, catalyst, and solvent, are combined and mixed in a dispersion step. The resulting catalyst ink is deposited onto a substrate — the catalyst layer forms on the substrate to be used in fuel cells.



It has been discovered that adjusting the ratio between water and isopropyl alcohol in the catalyst ink allows researchers to improve the viscosity of the ink, which may be important for spray deposition of the ink onto the substrate and adhesion of catalyst-ionomer aggregates to the substrate (Van Cleve et al., 2019). The size of the catalyst-ionomer aggregates in the ink can control the pores in the final catalyst layer structure. The ratio of ionomer and catalyst can control whether all catalysts are effectively utilized by providing protonic access. The link between catalyst ink properties and the final catalyst layer structure is not currently well understood. As a result, there is a lack of a rational approach to designing the optimum catalyst layer structure that yields high performance (Van Cleve et al., 2019).

New research on ink composition and application methods aims to maximize the total utilization of the catalyst while also balancing durability and reactant transport (Van Cleve et al., 2019). This contributes to the development of PEMFCs for commercial applications, especially in the heavy-duty vehicle sector (Van Cleve et al., 2019).

# BACKGROUND RESEARCH SUMMARY NOTES

This section contains all the notes I have written summarizing the papers I have read and annotated in the background research section.

# September Background Research Summary Notes

## September 30, 2024:

- ✓ Structure, Property, and Performance of Catalyst Layer in Proton Exchange Membrane Fuel Cells Section 1
  - Proton exchange membrane fuel cells (PEMFCs) face significant challenges in cost, performance, and durability, especially in the catalyst layers (CLs)
  - CLs make up about 42% of the cost of mass-produced PEMFCs
  - Two ways to reduce costs are
    - Improve performance and durability
    - Lower amount of expensive catalyst used (ex. Platinum)
  - These improvements trade off against each other, making it hard to find an optimal balance.
  - In PEMFCs
    - Hydrogen splits into protons and electrons in the anode
    - Electrons generate electricity by moving through an external circuit
    - Protons move to the cathode, where they react with oxygen to form water
  - The  $O_2$  reduction reaction (ORR) at the cathode is slower and more complicated than the hydrogen oxidation (HOR) at the anode.
  - Water buildup can block reactions, causing a problem known as 'water flooding.'
  - If the CL design is poor, hydrogen peroxide (H<sub>2</sub>O<sub>2</sub>) can form and damage components.
  - Platinum is the most common catalyst because it has been proven effective but is very expensive.
  - Researches are exploring
    - Pt alloys to reduce the amount of Pt needed (therefore reducing cost) and improve performance.
    - Using non-precious metal catalysts  $\rightarrow$  not as reliable or efficient
  - An effective CL should
    - Activate O<sub>2</sub> effectively

- Remove water easily
- Be stable in corrosive conditions
- Transport reactants, products, electrons, and heat efficiently
- There is no agreement on the best CL structure
- The structure is very important because it impacts short and long-term performance.
- CL structure spans from nanometer to micron levels
  - Including CL thickness, pore size, and arrangement of catalyst particles
- A better understanding of CL structure and performance is needed to improve fuel cells.
- Despite progress, more improvements are needed to enhance mass transport and catalyst usage in PEM fuel cells.
- Long-term use degrades CL structure, leading to performance loss over time.
- The article reviews the current understanding of CL structure and performance and discusses the experimental techniques used to study them.

## Structure, Property, and Performance of Catalyst Layer in Proton Exchange Membrane Fuel Cells Section 2.1

- **The catalyst layer (CL)** is formed during the fuel cell production process and is affected by ingredients, methods, and conditions.
- Early fuel cells used a lot of platinum, making them incredibly expensive
- **PTFE** is added to make the CL waterproof and stabilize catalysts, but too much can reduce efficiency by covering the catalyst surface.
- **Carbon-supported platinum (Pt/C)** was introduced to reduce platinum usage. Pt loading was cut down to 0.35mg/cm<sup>2</sup> without a change in performance levels.
- **Nafion polymer** replaced PTFE, improving cell performance by enhancing proton transport and increasing surface area for reactions.
- Three thin-film methods
  - **Catalyst coated on gas diffusion layer (GDL)** known as CCS, the catalyst is coated on a gas diffusion layer.
  - **Catalyst coated on membrane** known as CCM, the catalyst is coated directly on the membrane for better contact.
  - **Decal transfer method** known as DTM, the catalyst is transferred from a decal substrate to the membrane.

- **Challenges** include minimizing catalyst penetration into gas diffusion layers and maintaining a balance between performance and durability.
- **Ultra-thin CLs**: new methods of applying catalyst ink have created thin layers of catalysts using even less platinum.
- **Nanostructured thin-film (NSTF) CLs** are super thin layers that have gained attention for reducing the cost of platinum, but they have issues like water buildup and low durability.
- Focus on efficiency: There is ongoing work to improve methods for making these layers thinner, cheaper, and more durable for industrial use.
- Structure, Property, and Performance of Catalyst Layer in Proton Exchange Membrane Fuel Cells Section 2.4
  - The way that CLs are made can change depending on things such as the materials, composition, methods, and procedures used.
  - PTFE-bonded CLs are super strong because they use a lot of platinum, but platinum is expensive, so this method isn't used much in industries.
  - While Pt is very expensive, CLs made with little platinum are cheaper, but the methods are tricky and challenging to implement for mass production.
  - The ionomer-bonded method (thin-film method) is an excellent middle ground because it is both durable and affordable. This method could get even better with improvements in how the CLs are structured.
  - To see the microstructures of CLs, scientists use different types of microscopes (SEM, TEM, optical, etc.), which show the surface in varying details)
  - To see the inside of CLs, 3D X-ray CT and other techniques are used.
  - Advanced 4D microscopy can be used to look at stuff like chemical composition, temperature, or how CLs change over time.
  - The pore structure (how many and how large they are) is measured using various techniques, such as a densimeter.
  - The solid structure can be studied using methods like Raman spectroscopy.

Structure, Property, and Performance of Catalyst Layer in Proton Exchange Membrane Fuel Cells Section 4.6

- Researchers use a bunch of methods and models to study the electrochemical properties of CLs
- Key properties include exchange current density, charge transfer coefficient, surface area, electrode roughness, and both electronic and protonic conductivities.
- These properties help us understand how electrodes work and how well

they perform in FCs.

- Measuring these electrochemical properties is complicated; sometimes, they must be measured indirectly.
- It is incredibly important to check how accurate these methods are.
- There is not a lot of experimental data for some properties, so reliable models are rare.
- A few models exist for protonic and electronic conductivity, but more testing is required to ensure they are valid.

# October Background Research Summary Notes

## October 04, 2024:

- Dictating Pt Based Electrocatalyst Performance in Polymer Electrolyte Fuel Cells, from Formulation to Application Intro
  - Advantages of PEMFCs:
    - Higher efficiency + lower emissions than combustion engine
    - Only produces water as a byproduct
  - Challenges in Pt use:
    - Higher loading than desired for cost-effectiveness
    - Current loading exceeds the DOE 2020 target (0.125 gPGM/kW)
    - Reducing Pt loading is essential for long-term cost and efficiency targets
  - Strategies for Improvement:
    - Novel electrode fabrication methods
    - Conditioning protocols to boost performance
    - Advancements in specific reactions like ORR, which impact electrode structure and performance
  - Ionomer chemistry and catalyst accessibility
    - Influence by ionomer properties, Pt accessibility, ionomer thickness, ionomer distribution
    - Imaging techniques have helped visualize distribution in membrane linking structure to performance.
  - Research insights
    - Ionomer aggregate size and distribution impact ORR efficiency and transport
    - Adjusting the ionomer-to-carbon ratio affects the coverage
    - Research required to connect ionomer-catalyst interactions with performance
- Dictating Pt-Based Electrocatalyst Performance in Polymer Electrolyte Fuel Cells, from Formulation to Application – Conclusion
  - Ink composition and testing
- A mix of n-proponal (n-PA) and water
- Testing reveals that water/alcohol content influences ionomer distribution and Pt/carbon interactions.
- Water content affects
  - Increased anion absorption
  - Water-rich ink reduces oxygen transport resistance  $\rightarrow$  smaller ionomer aggregates, and improves ionomer distribution on Pt.
- Implications
  - Research suggests that prioritizing ionomer properties is important as it affects electrode microstructures and density performance.
  - Ionomer chemistry considers impacts on ionomer densification and distribution beyond kinetic effects.

☑ Intro to Tailoring electrode microstructure via ink content to enable improved rated power performance for platinum cobalt/high surface area carbon based polymer electrolyte fuel cells

- Advances in PEMFCs:
  - Progress has led to the release of hydrogen–fueled vehicles by companies such as Toyota, Hyundai, and Honda
  - High costs of electrode components still limit widespread use of PEMFCs, promoting research for more efficient fuel cells
- DOE targets for PEMFC performance:
  - Mass activity > 0.44 A/mgPt
  - $300 \text{ mA/cm}^2$  at 0.8 V for H<sub>2</sub>/air operation
  - 1.8 W/cm<sup>2</sup> at rated power with low Pt loading
- Primary research areas
  - Improving catalyst mass activity: enhancing electrocatalyst synthesis and post-processing
  - Reducing oxygen transport resistance: better Pt site location and accessibility
  - Incorporating conductive ionomers: low equivalent weight ionomers boost conductivity and improve the electrocatalyst environment
- Challenges in material inegration
  - Focus on individual aspects without fully integrating MEA processes
  - Includes catalyst ink formulation, cell assembly, processing, and electrode conditioning  $\rightarrow$  all impact performance
- Importance of materials and electrode structure
  - Variables such as ink formulation (solvent ratio and ionomer chemistry) and processing methods affect the following
    - Electrode structure
    - Active site accessibility

- Oxygen transport resistance
- Proton conductivity
- Optimization is a iterative process
- Influence of ink solven ratio on electrode performance
  - Solvent ratio affect ionomer-catalyst and electrode microstructure
  - Water rich inks create more porous structures with smaller particle aggregates enhancing oxygen transport and overall performance
- In situ and ex sity characterization
  - Methods such as CO displacement chronomperometry, electrochemical impedance spectroscopy, and nano-CT provide insights into
    - Ionomer catalyst interface
    - Electrode morphology
    - Oxygen transport pathways
  - Establish structure property relationships guiding future PEMFC development
- Conclusion to Tailoring electrode microstructure via ink content to enable improved rated power performance for platinum cobalt/high surface area carbon based polymer electrolyte fuel cells
  - Effect of ink composition on electrode microstructure and performance
    - There are significant impacts from water and alcohol content in ink.
    - Water rich inks
      - Smaller aggregate sizes
      - More porous
      - Enhance O<sub>2</sub> transport within aggregates and through catalyst layer
  - Characterization techniques and findings
    - X-ray scattering and nano-ct
      - Smaller aggregate sizes
      - Increased porosity in water-rich inks
    - In situ electrochemical testing
      - Stronger sulfonate absorption of Pt with higher water content
      - Moderate differences in ionomer coverage on Pt and carbon
      - No significant impact on local O<sub>2</sub> tranport where Pt is located in support pores
  - Performance of water-rich MEAs:
    - 70 wt% water content performance comprably to advanced materials with novel catalysts, ionomers, and supports
    - Highlighted crucial role of ink formulation on overall performance
  - Implications for development
    - Guidelines for optimization of high-performance materials
    - Very important for heavy-duty applications prioritizing efficiency and durability

- Supporting data
  - Details on metal loading, sulfonate coverages, catalyst particle size, pore distribution, diffusion coefficients, MEA performance compared to DOE targets

## October 06, 2024:

- ☑ Intro to The Controllable Design of Catalyst Inks to Enhance PEMFC Performance: A Review
  - Overview of PEMFCs
    - Convert chemical energy to electrical energy without combustion
    - Efficient, environmentally friendly, suitable for vehicle, stationary, and portable power system applications.
    - Core of PEMFCs in the MEA, consists of GDL, microporous layer, CL, and PEM.
    - Catalyst layer is crucial because it is the site of electrochemical reactions
  - Catalyst layer requirements
    - Efficient transport of reactants to catalytic sites
    - Quick transport of protons and electrons to catalytic sites
    - Effective water removal from CL
    - CL microstructure is complex
      - Heterogeneous transport properties that affect cost, power density, and lifespan
  - Formation of CLs
    - Depositing catalyst ink onto solid supports (PEM or GDL)
    - Catalyst ink consists of catalysts/supports, solvents, and ionomers
    - Affecting factors fo PEMFC efficiency
      - Component distribution
      - Aggregate size
      - Pore structure
    - Optimizing ink formulation is challenging  $\rightarrow$  based on experience not study of interactions
  - Ink formualtion
    - ionomer/carbon ratio and platinum/carbon ratio crutial for optimization
    - Catalyst ink is very complex made up of interactions between ionomer, particle, and solvent
    - Understanding these interactions helps design a CI with optimized performance
  - Modeling and manufacturing CI
    - Modeling is in the early stages but can provide insitghts into design of efficient CL

- Deposition methods:
  - Ultrasonic spraying
  - Electrospray deposition
  - Electrospinning
  - Slot die coating
  - Inkjet printing
  - Doctor blade
  - Screen printing
  - Brush painting
  - Gravure
- Each technique has benefits but scaling up to be cost-efficient is difficult
- Future
  - Continue reserch into ink formulation is important for further development
  - Critical for commercial use of PEMFCs
- Conclusion to *The Controllable Design of Catalyst Inks to Enhance PEMFC Performance: A Review* 
  - Challenges in scaling CLs
    - Scalable and economical manufacturing is crutial
    - CLs are produced using CI where catalysts and ionomers are mixed
    - Optimizing ink formulation is difficult due to limited understanding of CI formulation
  - Importance of modeling
    - Makes it a lot easier to understand
    - Accurate ink modeling aids in creating an omptimal ink formulation and improved CL design
  - Continuous ink dispertion needs
    - Efficient and continues dispertion technologies essential for large-scale production of CL
    - Indirect characterization and visualization needed for quantitative assessment of ink microstructures
  - Review ink deposition techniques
    - Various techniques have been discussed for their effects on ink formulation and CL performance
    - Scaling up while keeping costs low is challenging
  - PEMFC development and cost-perfomance challenges
    - Hold potential for automotive, public transport, power equiptment, etc.
    - Cost, performance, and lifespan limit commercialization
  - Role of Ink component
    - Interactions during ink dispersion, storage, and deposition affect microstructure and effectiveness of CL

- Optimizing three-phase interfaces in CL enhances MEA performance
- Interaction control for enhanced CL
  - Reducing catalyst-ionomer interactions and increasing ionomer-support interactions
  - High-density ionomer films near catalyst surfaces redure ORR activity.
- Advancements and limitations in ink characterization
  - In situ, non destructive, and visual characterization of CI is complex
  - Current models rely on DLVO theory and don't fully capture non-DLVO forces
- Future
  - Understanding of how internal ink interactions influence CL performance
  - Research should focus on quantitative understandings and optimization of relationships between ink formulation, microstructures, and CL properties
- ☑ Intro to Recent progress in understanding the dispersion stability of catalyst ink for proton exchange membrane fuel cell and water electrolyzer
  - Global shift
    - Movement to hydrogen as sustainable energy carrier
    - Aligns with global goal to reduce reliance of fossil fuels
    - Reduces carbon emissions across sectors
  - Key technologies
    - PEMFCs: convert chemical energy from hydrogen and oxygen into electricity. Suitable for low-temp operation and long-term applications
    - PEMWEs: produce hydrogen by decomposing water at anode. Creates ultrapure hydrogen product. Beneficial for high current density requirements
  - Core component membrane electrode assembly (MEA)
    - Comprises of two catalyst layers and solid polymer electrolyte membrane
    - Essential for PEMFC and PEMWE performance
    - Catalyst like Pt utilized in these sustems for reactions involving hydrogen and oxygen.
    - High catalytic efficiency is crucial for both HOR and ORR in PEMFCs and OER and HER in PEMWEs.
  - Challenges in manufacturing and performance optimization
    - Optimizing CL strucutre through ink formulation and processing techniques essential to improve performance
    - Focused on understanding role of CI components in CL formation, dispertion stability, and microstructure
      - Vital for large-scale production

- Research and development needs
  - Colloidal stability necessary for effective coating processes
  - Interaction between materials in CI is complex and require better characterization methods
  - Industrial scale manufacturing are promising but require more refinement to optimize CL coating
- Conclusion to Recent progress in understanding the dispersion stability of catalyst ink for proton exchange membrane fuel cell and water electrolyzer
  - Catalyst ink stability in manufacturing
    - Crucial for industrial scalability
    - Instabilities compromise ink's effectiveness
    - Key factors for dispersion stability
      - Ionomer absoption
        - Binding catalyst particles is crutial for stable dispersion
        - Ensures and ideal film thickness, stronger forces that keep particles evenly dispersed
        - Essential for maintaining a conductive network supporting transport and performance
      - Interaction of ink components
        - Ionomers, solvens, and particles influence ink stability
        - Optimizing interactions prevent aggregation and maintain
          - dispersion  $\rightarrow$  essential for high-quality catalyst layers
  - Research gaps

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- Model based approaches
  - Research focuses on experimental results limiting model-based approaches
  - Simulation complements experimental methods
    - Deeper understanding of how particles aggregate and interact with ink
- Non-destructive characterization
  - Current methods are indirect with limitations
  - Future studies could develop combined techniques
- Rheology and visualization
  - Insights into structure-property relationship of ink components
  - Establish clearer links between ink formulation and microstructure of CL
- Reversing agglomeration
  - Reverse agglomeration and sedimentation
  - Quick efficient techniques to re-disperse catalyst inks for improved ability to be manufactured

# November Background Research Summary Notes

## November 15, 2024:

- ☑ Intro to Effect of Catalyst Ink Properties on the Performance of Proton Exchange Membrane Fuel Cell and Water Electrolyzer: A Mini Review
  - Importance of CL
    - Composed of carbon-supported catalysts and ionomers
    - Pivotal to cell performance due to influence on charge and mass transport
    - Oxygen transport governed by pore size and distribution within CL
  - Catalyst ink and application methods
    - Ink is formulated by dispersing components such as ionomer, catalyst, and solvent. The ink is then deposited onto the substrate or PEM using a coating method.
    - After application, an interconnected network forms within CL, combining catalyst, ionomer, and pores → essential for high cell performance. Controlling the catalyst-ionomer interface to enhance proton conductivity and creating a porous structure for mass transport efficiency involved.
  - Role of rheology
    - Key technique for analyzing catalyst ink microstructure
    - Offers insights into drying
    - Helps connect ink formulation, processing methods, and CL microstructure to overall performance
  - Cost and material differences in AEM systems
    - PEM systems use expensive catalysts such as Pt
    - Anion exchange membrane fuel cells use more cost-effective catalysts but are not as durable.
  - Impact of ink composition on performance
    - PEM is sensitive to mass transfer characteristics within CL, which is critical to studying the influence of different ink compositions on CL structure
    - Refine ink formulations to enhance electrochemical performance in PEMFCs
- Conclusion to Effect of Catalyst Ink Properties on the Performance of Proton Exchange Membrane Fuel Cell and Water Electrolyzer: A Mini Review
  - Catalyst layer structure and formation
    - CL is a multiscale porous structure consisting of interconnected catalysts and ionomers.

- Critical for effective transport of reactants and products to and from active sites
- Catalyst inks contain agglomerates of catalysts, ionomers, and solvents
- While drying, these form the CL microstructure, which directly impacts the performance and durability of MEA
- Key factors influencing CL microstructure
  - Shaped by several factors that can be controlled
    - Cluster size
    - Catalyst and ionomer content
    - Solvent type
    - Additives and dispersants
    - Dispersion method
  - Affect rheological properties, which are essential for creating a stable CL.
    - Viscosity
    - Viscoelasticity
    - Thixotropy
- Rheological design for commercialization
  - Careful rheological design is essential for large-scale, commercial applications.
  - Both ink rheology and coating process parameters affect CL formation at each deposition stage.
  - The relationships help enable optimization and achieve consistent high-performing electrodes when scaled.
- Challenges and the future
  - Future should focus on exploring the microstructure of catalyst ink and CLs, maintaining a range of solid concentrations, and refining coating and drying processes.
  - Research on AEM systems is important to understanding ink composition and dispersion methods and their effects on rheological properties, electrode structure, and performance.
  - Research on AEM is limited, but advances this will be key to developing efficient alternatives to PEM-based devices.

# **EXPERIMENTAL PROCEDURES**

This section contains a list and description of all materials and equipment that are being used in this experiment. Each material will be described along with its source. Procedures will be recorded in detail.

# **October Experimental Procedures**

## October 19, 2024:

✓ Write the variables into the proposal

Independent Variable: The ratio of isopropyl alcohol in the solvent used to mix the catalyst ink.

<u>Responding Variable</u>: The size of the aggregates in the catalyst ink and the properties of the catalyst layer: coverage, ionic resistance, electronic resistance, and pore size.

<u>Controlled variables</u>: The thickness of the catalyst layer, the concentration of other components in the catalyst ink, and the temperature of the environment during the making and application of the catalyst ink.

#### Confounding Variables:

- I am not sure what a confounding variable is or what the confounding variables would be for the experiment happening at the University of Calgary so I will ask Dr. Karan about this during our meeting on Monday.

## October 20, 2024:

☑ Write the hypothesis for the research proposal

If the ratio of isopropyl alcohol in the catalyst ink solvent is increased, then the size of the aggregates in the catalyst ink will decrease, leading to improved catalyst layer coverage and reduced ionic resistance. This is because a higher concentration of isopropyl alcohol allows particles to spread uniformly across the catalyst surface and promotes better interactions with the membrane.

## October 25, 2024:

#### ☑ RP confounding variables

### Confounding Variables:

- The mixing technique: could have an affect particle dispersion and aggregate size
- The application technique: could have an impact on the uniformity of the catalyst ink on the catalyst layer

# **November Experimental Procedures**

# November 21, 2024:

- ☑ <del>CYSF hypothesis:</del>
  - If the ratio of isopropyl alcohol in the catalyst ink solvent is increased, then the size of the aggregates in the catalyst ink will decrease, leading to improved catalyst layer coverage and reduced ionic resistance. This is because a higher concentration of isopropyl alcohol allows particles to spread uniformly across the catalyst surface and promotes better interactions with the membrane.
- ✓ CYSF variables:

### Independent Variable:

• The ratio of isopropyl alcohol in the water-isopropyl alcohol solvent mixture used to disperse the ionomer and catalyst in the catalyst ink.

#### Responding Variable:

- Catalyst ink properties: catalyst-ionomer aggregate size, viscosity
- Catalyst layer properties: pore size, electronic resistance, ionic resistance, and ionomer coverage of the catalyst.

### Controlled Variables:

- The concentration of other components in the catalyst ink.
- The temperature of the environment during the making and application of the catalyst ink.
- The thickness of the catalyst layer.

### Confounding Variables:

- The mixing technique could have an effect on particle dispersion and aggregate size.
- The application technique could have an impact on the uniformity of the catalyst ink on the catalyst layer.

☑ <del>CYSF procedure</del>

This study will follow the procedure described in sources [15], [16]. A brief explanation of the methodology is as follows.

The first step to be completed is preparing the catalyst ink. Different mixtures of isopropyl alcohol and water in known ratios are prepared by weighing the required amounts of deionized water and high-purity isopropyl alcohol. The catalyst ink is then prepared carefully by measuring the required amounts of materials in a beaker and mixing them using ultrasonication for thirty minutes, followed by ball milling for 24 hours.

Following the preparation of the catalyst ink, the particle size distribution is determined using the dynamic light scattering (DLS) instrument, specifically the Malvern Zetasizer Nano ZS. Additionally, the inks' viscosities are measured using the Anton Paar MCR702 Rheometer. The pore size distribution of the catalyst layer is determined using the nitrogen adoption technique and BET analyses.

A commercial four-point probe instrument is utilized to measure the catalyst layer's electrical resistance. In this setup, two probes apply an electrical potential while the other two probes measure the current. The resistance is calculated from the measured potential and current, along with known geometric parameters, such as the distance between the probes.

The catalyst layer ionic resistance is measured within a fuel cell device. First, a membrane electrode assembly (MEA) is prepared, consisting of a membrane coated with a catalyst layer on each side. The coating of the membrane with the catalyst layer is achieved through a process called decal transfer. In this process, the catalyst layer deposited on a substrate, as shown in Figure 2 above, is transferred to the polymer electrolyte membrane using a hot-pressing method. The resistance of the catalyst layer is measured using a specialized electrochemical technique.

The ionomer coverage of the catalysts is inferred from the double-layer capacitance of the catalyst layer. This double-layer capacitance is determined through an electrochemical technique known as cyclic voltammetry, which is performed in a fuel cell device for the membrane electrode assembly.

### November 27, 2024:

CYSF edits to variables

Independent Variable:

• The ratio of isopropyl alcohol in the water-isopropyl alcohol solvent mixture used to disperse the ionomer and catalyst in the catalyst ink (changed in 5% increments).

### Responding Variables:

- Catalyst ink properties: catalyst-ionomer aggregate size, viscosity
- Catalyst layer properties: pore size, electronic resistance, ionic resistance, and ionomer coverage of the catalyst.

#### Controlled Variables

- The concentration of other components (ionomer and catalyst) in the catalyst ink.
- The temperature of the environment during the making and application of the catalyst ink (20°C 22°C).
- The thickness of the catalyst layer (10-20 μm).
- The application technique (slot die coating)
- The mixing technique (ultrasonication and ball milling)
- CYSF edits to procedure (I can't switch the citation to APA because my Paperpile is not working at the moment)

This study will follow the procedure described in sources [15] and [16]. A brief explanation of the methodology is as follows.

The first step to be completed is preparing the catalyst ink. Different mixtures of isopropyl alcohol and water in known ratios are prepared by measuring the required volumes of deionized water and high-purity isopropyl alcohol. The catalyst ink is then prepared carefully by measuring the required amounts of materials (ionomer, solvent, and catalyst) in a beaker and mixing them using ultrasonication for thirty minutes, followed by ball milling for 24 hours.

Following the preparation of the catalyst ink, the particle size distribution is determined using the dynamic light scattering (DLS) instrument, Zetasizer Nano ZS (Malvern Panalytical, UK). Additionally, the inks' viscosities are measured using a rheometer (Anton Paar MCR702). The pore size distribution of the catalyst layer is determined using the nitrogen adoption technique and BET analyses.

A commercial four-point probe instrument is utilized to measure the catalyst layer's electrical resistance. In this setup, two probes apply an electrical potential while the other two probes measure the current. The resistance is calculated from the measured potential and current, along with known geometric parameters, such as the distance between the probes.

The catalyst layer ionic resistance is measured within a fuel cell device. First, a membrane electrode assembly (MEA) is prepared, consisting of a membrane coated with a catalyst layer on each side. The coating of the membrane with the catalyst layer is achieved through a process called decal transfer. In this process, the catalyst layer deposited on a substrate, as shown in Figure 3 above, is transferred to the polymer electrolyte membrane using a hot-pressing method. The resistance of the catalyst layer is measured using a specialized electrochemical technique – cyclic voltammetry.

The ionomer coverage of the catalysts is inferred from the double-layer capacitance of the catalyst layer. This double-layer capacitance is determined through an electrochemical technique known as cyclic voltammetry, which is performed in a fuel cell device. This measurement is conducted within the MEA, a key component of a fuel cell where electrochemical reactions occur, consisting of the proton exchange membrane, catalyst layers, and gas diffusion layers.

# **December Experimental Procedures**

## December 05, 2024:

☑ Updated procedure for CYSF portal

Procedure:

This study will follow the procedure described in (Islam et al., 2022) and (Poojary et al., 2020). A brief explanation of the methodology is as follows.

The first step to be completed is preparing the catalyst ink. Different mixtures of isopropyl alcohol and water in known ratios were prepared by measuring the required volumes of deionized water and high-purity isopropyl alcohol. The catalyst ink was then prepared carefully by measuring the required amounts of materials (ionomer, solvent, and catalyst) in a beaker and mixing them using ultrasonication for thirty minutes, followed by ball milling for 24 hours.

Following the preparation of the catalyst ink, the particle size distribution was determined using the dynamic light scattering (DLS) instrument, Zetasizer Nano ZS (Malvern Panalytical, UK). Additionally, the inks' viscosities were measured using a rheometer (Anton Paar MCR702). The pore size distribution of the catalyst layer was determined using the nitrogen adoption technique and BET analyses.

A commercial four-point probe instrument was utilized to measure the catalyst layer's electrical resistance. In this setup, two probes apply an electrical potential while the other two probes measure the current. The resistance was calculated from the measured potential and current, along with known geometric parameters, such as the distance between the probes.

The catalyst layer ionic resistance was measured within a fuel cell device. First, a membrane electrode assembly (MEA) is prepared, consisting of a membrane coated with a catalyst layer on each side. The coating of the membrane with the catalyst layer was achieved through a process called decal transfer. In this process, the catalyst layer deposited on a substrate, as shown in Figure 3 above, was transferred to the polymer electrolyte membrane using a hot-pressing method. The resistance of the catalyst layer was measured using a specialized electrochemical technique – cyclic voltammetry.

The ionomer coverage of the catalysts was inferred from the double-layer capacitance of the catalyst layer. This double-layer capacitance was determined through an electrochemical technique known as cyclic voltammetry, which was performed in a fuel cell device. This measurement was conducted within the MEA, a key component of a fuel cell where electrochemical reactions occur, consisting of the proton exchange membrane, catalyst layers, and gas diffusion layers.

# **February Experimental Procedures**

### February 07, 2025:

To investigate the effect of solvent composition on catalyst ink and catalyst layer properties, the ratio of isopropyl alcohol (IPA) in the water-IPA alcohol solvent mixture used to disperse the ionomer and catalyst in the catalyst ink was varied in 5% increments. While the ratio of water to IPA changed in different tests, the properties of the catalyst ink (catalyst-ionomer aggregate size and viscosity) and the catalyst layer properties (pore size, electronic resistance, ionic resistance, and ionomer coverage of the catalyst) were measured and analyzed using various instruments. To ensure that the changes in these properties were solely due to the water-to-IPA ratio in the catalyst ink, many key factors were kept constant: the concentration of ionomer and catalyst in the catalyst ink, the environmental temperature (maintained at 20°C and 22°C), the thickness of the catalyst layer (10-20 µm), the application technique of the catalyst ink (slot die coating), and the mixing technique of the catalyst ink (ultrasonication and ball milling). This experiment was based on the hypothesis that increasing the concentration of IPA in the catalyst ink solvent would decrease the aggregate size in the ink, leading to improved catalyst layer coverage and reduced ionic resistance. This is because a higher concentration of IPA allows particles to spread uniformly across the catalyst surface and promotes better interactions with the membrane.

### February 13, 2025:

✓ Notes on DLS

- Measures the Brownian motion of particles in a dispersion
- uses info to determine hydrodynamic size
- Brownian motion is the random movement of particles that results from their collision with solvent molecules such as water
  - Smaller molecules move/diffuse faster
  - The rate of Brownian motion is quantified as the translational diffusion coefficient  $\rightarrow$  D
- Hydrodynamic size is the size of a sphere that diffuses at the same rate as the particle being measured
  - The sphere contains the core particle plus anything bound to its surface (ex. Ions, absorbed polymers)
- Measuring diffusion rates
  - Particles are illuminated using a laser, and they scatter some of the light that hits them.
  - If the particles were completely still, there would be a constant intensity of scattered light
  - In a dispersion, dispersion causes the intensity of light scattered by the particles to fluctuate over time (it's dynamic)
  - The detected light combines to create a fluctuating intensity signal
  - The fluctuations are caused by the interference of light scattered by each individual particle
  - Intensity changes over time as the particles continue to diffuse
  - The speed of the fluctuations depends on the particle diffusion rate
  - Smaller particles, faster diffusion, more rapid fluctuations in scattered light
- How particle size is measured using this info
  - Snapshots of the light scattering signal are taken rapidly one after another always compared back to the original signal
  - Between consecutive snapshots, the intensity signals are very similar
  - Snapshots further apart in time have a decrease in similarities between them
  - Eventually intensity signal changes completely until there is no correlation with the original  $\rightarrow$  autocorrelation
  - Larger the particles, slower diffusion, longer for a complete loss of the correlation to og signal
  - Small particle, fast diffusion, fast degradation of correlation to og

signal

- How do we calculate size?
  - Auto correlation enables us to extract the translational diffusion coefficients
  - The values are used in the stokes einstein equation to obtain size information  $d_{\rm H}$  = kT/3 $\pi\eta D$ 
    - $dH \rightarrow hydrodynamic diameter$
    - K = boltzmann's constant
    - T = absolute temperature
    - H = viscosity
    - D = diffusion coefficient
  - Using DLS the size of all the particles can be quickly determined
    - The size distribution measured is shown as intensity distribution
    - This is the primary result and shows intensity of scattered light from each size population present in sample
    - Results can be converted into volume or number-sized distribution if needed
- Malvern Panalytical DLS can
  - Measure particle size distributions to less than a nanometer up to several microns in size
  - Rapid non invasive technique that is extremely versatile and used in thousands of applications
    - Characterize pigments used in paints, dyes, inks
    - Advance research into drug delivery systems
    - Improve formulation of emulsions and colloidal systems
    - Investigate and improve vaccine and drug formulations
    - And many more
- ✓ Paragraph on ink preperation

This study will follow the procedure described in sources [1] and [2]. A brief explanation of the methodology is as follows.

The first step to be completed is the preparation of the carbon ionomer dispersion catalyst

ink. Different inks were prepared by mixing carbon black (Vulcan XC-72, Cabot Corp., place of

origin) with a surface area of 223m<sup>2</sup>/g [3], water, and a mix of isopropyl alcohol (IPA) (make,

Sigma Aldrich, place of origin) and deionized water in known ratios, which acts as the dispersion media. A 20 wt% Nafion ionomer dispersion (Nafion, Ion Power Inc., place of origin) was used to control the water content in the ink. Both the target ionomer-to-carbon ratio (I/C) of 0.8 and a solid-to-liquid (S/L) ratio of 0.05 were maintained while preparing the catalyst ink for all dispersions. Before using the Nafion ionomer, it was homogenized for 24 hours at room temperature, and that homogenization was followed by 30 minutes of sonication. Following this, the components of the ink were added in a set order: carbon first, then water, followed by IPA, and ending with the Nafion ionomer. The mixture was then probe-sonicated for a total of two minutes in four-second on/off cycles. After that, 16.5g of zirconia balls were added to the vial for every 200mg of carbon in the ink. The vial was sealed to prevent evaporation of the solvent and mixed on a roller mixer at 70 rpm for 15 hours.

#### ✓ Paragraph on DLS and average particle size

Following the preparation of the catalyst ink, its average particle size was determined using the dynamic light scattering (DLS) instrument (Zetasizer Nano ZS, Malvern Panalytical, UK), which measures the Brownian motion of particles in a dispersion [4]. Brownian motion is the random movement of particles that results from their collisions with solvent molecules, such as water. DLS quantified this movement of particles using the translational diffusion coefficient (D) and calculated the hydrodynamic size – the size of a sphere that diffuses at the same rate as the particle being measured, including anything bound to the surface of the particle (ions, absorbed polymers, etc.). When a laser beam is directed at the ink sample, the particles scatter light, and due to the dynamic nature of the sample, the intensity of light scattered by the particles fluctuates over time. Autocorrelation tracks these fluctuations by comparing the intensity signals at different time intervals to determine how long it takes for the signal to lose all correlation with the original signal, and from this, the translational diffusion coefficient can be found to use in the Stokes-Einstein equation, which related the diffusion coefficient to the particle size, temperature, and viscosity of the solvent. The Stokes-Einstein equation states that  $d_H = kT/3\pi\eta D$  where  $d_H$  is the hydrodynamic diameter, *k* is Boltzmann's constant, *T* is the absolute temperature,  $\eta$  is viscosity, and *D* is the diffusion coefficient. The Malvern Panalytical DLS can measure particle size distribution down to the nanometer scale, which makes this technique useful in applications such as the formulation of catalyst ink for proton-exchange membrane fuel cells [4]. Each ink sample underwent three trials using the Malvern Panlytical DLS system and calculations using the Stokes-Einstein equation and the results were averaged to determine the average particle size of each ink sample.

#### February 15, 2025:

#### ☑ Write a paragraph on electrical conductivity for procedures

After the catalyst ink was deposited onto the Teflon substrate and the solvent evaporated to create the CL structure, the electrical conductivity of the layer was determined. To do this, the electrical resistance first needs to be determined using a two-probe multimeter (Fluke 177 True-RMS Digital Multimeter, Fluke, place of origin). A small sample (2cm x 5cm) of the CL was cut, and its thickness was measured using calipers. The CL was deposited on a Teflon substrate 52 microns thick, so the thickness of the CL was found by subtracting the thickness of the Teflon substrate from the total thickness of the CL and the Teflon substrate. The process of finding the thickness of the CL was repeated in three different spots on the same sample. This is because the thickness at three different points of the sample may not be exactly the same since

the sample may not be perfectly even although a good sample should be. The average of the thicknesses of the CL was taken to be used in the electrical conductivity calculation. To measure the resistance of the CL, the sample is placed face down on two copper strips, which are good conductors of electricity. The two probes of the multimeter were placed on either copper strip and the multimeter returned the resistance of the CL. Once the electronic resistance of the layer was determined, the electrical conductivity ( $\sigma$ ) was calculated using the formula  $\sigma = L/(RA)$  where L is the thickness of the sample, R is the resistance, and A is the area of the sample. The measurements were repeated for three different cut samples from the same deposited catalyst layer, and the average of the calculated electrical conductivities was taken in order to determine the electrical conductivity of each ink sample.

#### ☑ Write a paragraph on BJH average pore width for procedures

The BJH average pore width of the CL was determined using nitrogen (N<sub>2</sub>)-sorption analysis. The dried deposited CL prepared to find the electrical conductivity was scratched into powder form. Approximately 120mg of this powder was used for analysis. To remove any absorbed moisture or gases, the sample of powder was degassed at 160°C for at least 12 hours. Nitrogen adsorption and desorption isotherms were collected at 77 Kelvin using a 3FlexTM analyzer (Alberta Sulphur Research Ltd., University of Calgary Research Center), with pressure varying from 1mmHG to 760mmHG. The sample's porosity was determined using BET analysis to measure its nitrogen adsorption capacity. The pore size distribution was then determined using the Barrett-Joyner Halenda (BJH) method, which was used to analyze the pore size distribution of materials, focusing on mesopores [5]. It used nitrogen adsorption and desorption of isotherms obtained from BET analysis, applying the Kelvin equation to convert pressure values into pore diameters. By looking at the desorption branch of the isotherm, the BJH method was used to calculate the pore width distribution. This is important for understanding the performance of the CL and helps track changes in pore structure [5]. For each powder sample, this process was repeated three times, and the average was calculated in order to get the best representation of the BJH average pore width for each sample.

### February 16, 2025:

#### ☑ Write a paragraph on how the data was graphed for procedures

In order to visually represent the data collected using the above procedures, Microsoft Excel<sup>™</sup> (Excel 2024) was used to create graphs. Three tables were then created where each property measured – average particle size, electrical conductivity, and BJH average pore width – was plotted against water content (wt.%) with water content as the manipulated variable and the property as the responding variable. Each table was then converted into a graph using Excel's graphing tool. The average particle size was graphed on a bar graph, and error bars were added

using the standard deviation formula:  $\sigma = \sqrt{\frac{\Sigma(x_i - \overline{x})^2}{n-1}}$  where  $\sigma$  is the standard deviation

(nanometers),  $x_i$  is the individual particle size measurements from the three trials (nanometers),  $\overline{x}$  is the average particle size (nanometers), and n is the number of trials conducted. Both the electrical conductivity and the BJH average pore width were plotted on a discrete line graph. These visual representations made it easier to identify relationships between water content and each measured property. Examining the patterns in the data allows for the impact of solvent composition on catalyst ink and CL properties to be effectively evaluated.

#### February 18, 2025:

Lauren's edits to my paper

#### Procedures Section of Final Paper

To investigate the effect of solvent composition on catalyst ink and catalyst layer (CL) properties, the ratio of isopropyl alcohol (IPA) in the water-IPA alcohol solvent mixture used to disperse the ionomer and catalyst in the catalyst ink was varied in 5% increments. The properties of the catalyst ink and the CL were measured and analyzed using various instruments for each water-to-IPA ratio. To ensure that the changes in these properties were solely due to the water-to-IPA ratio in the catalyst ink, many key factors were kept constant: the concentration of ionomer and catalyst in the catalyst ink, the environmental temperature (maintained at 20°C and 22°C), the thickness of the CL (10-20  $\mu$ m), the application technique of the catalyst ink (slot die coating), and the mixing technique of the catalyst ink (ultrasonication and ball milling). This experiment was based on the hypothesis that increasing the concentration of IPA in the catalyst ink solvent would decrease the aggregate size in the ink, leading to improved CL coverage and reduced ionic resistance. This is because a higher concentration of IPA allows particles to spread uniformly across the catalyst surface and promotes better interactions with the membrane.

This study will follow the procedure described in sources [1] and [2]. A brief explanation of the methodology is as follows.

#### Preparation of the Catalyst Ink:

The first step that was completed was the preparation of the carbon ionomer dispersion catalyst ink. Different inks were prepared by mixing carbon black (Vulcan XC-72, Cabot Corp.,

Massachusetts) with a surface area of 223m<sup>2</sup>/g [3], water, a mix of isopropyl alcohol (IPA) (Sigma Aldrich, Missouri), and deionized water in known ratios, which acted as the dispersion media. A 20 wt% Nafion ionomer dispersion (Nafion, Ion Power Inc., Deleware) was used to control the water content in the ink. Both the target ionomer-to-carbon ratio (I/C) of 0.8 and a solid-to-liquid (S/L) ratio of 0.05 were maintained while preparing the catalyst ink for all dispersions. Before using the Nafion ionomer, it was homogenized for 24 hours at room temperature, and that homogenization was followed by 30 minutes of sonication. Following this, the components of the ink were added in a set order: carbon first, then water, followed by IPA, and ending with the Nafion ionomer. The mixture was then probe-sonicated for a total of two minutes in four-second on/off cycles. After that, 16.5g of zirconia balls were added to the vial for every 200mg of carbon in the ink. The vial was sealed to prevent evaporation of the solvent and mixed on a roller mixer at 70 rpm for 15 hours.

#### Average Particle Size:

Following the preparation of the catalyst ink, its average particle size was determined using the dynamic light scattering (DLS) instrument (Zetasizer Nano ZS, Malvern Panalytical, UK), which measured the Brownian motion of particles in a dispersion [4]. Brownian motion is the random movement of particles that results from their collisions with solvent molecules, such as water. DLS quantified this movement of particles using the translational diffusion coefficient (D) and calculated the hydrodynamic size – the size of a sphere that diffused at the same rate as the particle being measured, including anything bound to the surface of the particle (ions, absorbed polymers, etc.).

When a laser beam is directed at the ink sample, the particles scatter light, and due to the dynamic nature of the sample, the intensity of light scattered by the particles fluctuates over time. Autocorrelation tracked these fluctuations by comparing the intensity signals at different time intervals to determine how long it took for the signal to lose all correlation with the original signal. From this, the translational diffusion coefficient was determined to be used in the Stokes-Einstein equation, which relates the diffusion coefficient to the particle size, temperature, and viscosity of the solvent. The Stokes-Einstein equation states that  $d_h = \frac{kT}{3\pi\eta D}$  where  $d_H$  is the hydrodynamic diameter (nanometers), k is Boltzmann's constant (joules/Kelvin), T is the absolute temperature (Kelvin),  $\eta$  is viscosity (pascal-seconds), and D is the diffusion coefficient (meters squared per second). The Malvern Panalytical DLS can measure particle size distribution down to the nanometer scale, which makes this technique useful in applications such as the formulation of catalyst ink for proton-exchange membrane fuel cells [4]. Each ink sample underwent three trials using the Malvern Panlytical DLS system and calculations using the Stokes-Einstein equation and the results were averaged to determine the average particle size of each ink sample.

#### **Electrical Conductivity:**

After the catalyst ink was deposited onto the Teflon substrate and dried in a vacuum oven at 60°C overnight to allow the solvent to evaporate to create the CL structure, the electrical conductivity of the layer was determined. To do this, the electrical resistance first needed to be determined using a two-probe multimeter (Fluke 177 True-RMS Digital Multimeter, Fluke, Washington). A small sample (2cm x 5cm) of the CL was cut, and its thickness was measured using calipers. The CL was deposited on a Teflon substrate 52 microns thick, so the thickness of the CL was found by subtracting the thickness of the Teflon substrate from the total thickness of the CL and the Teflon substrate. The process of finding the thickness of the CL was repeated in three different spots on the same sample. This is because the thickness at three different points of the sample may not be exactly the same since the sample may not be perfectly even though a good sample should be. The average of the thicknesses of the CL was taken to be used in the electrical conductivity calculation.

To measure the resistance of the CL, the sample was placed face down on two copper strips, which are good conductors of electricity. The two probes of the multimeter were placed on either copper strip, and the multimeter returned the resistance of the CL. Once the electronic resistance of the layer was determined, the electrical conductivity ( $\sigma$ ) was calculated using the formula  $\sigma = \frac{L}{RA}$  where L is the thickness of the sample (microns), R is the resistance (ohms), and A is the area of the sample (centimeters squared). The measurements were repeated for three different cut samples from the same deposited catalyst layer, and the average of the calculated electrical conductivities was taken in order to determine the electrical conductivity of each ink sample.

#### Barrett-Joyner-Halenda (BJH) Average Pore Width:

The BJH average pore width of the CL was determined using nitrogen  $(N_2)$ -sorption analysis. The dried deposited CL prepared to find the electrical conductivity was scratched into powder form. Approximately 120mg of this powder was used for analysis. To remove any absorbed moisture or gases, the sample of powder was degassed at 160°C for at least 12 hours. Nitrogen adsorption and desorption isotherms were collected at 77 Kelvin using a 3FlexTM analyzer (Alberta Sulphur Research Ltd., University of Calgary Research Center), with pressure varying from 1mmHG to 760mmHG. The sample's porosity was determined using BET analysis to measure its nitrogen adsorption capacity. The pore size distribution was then determined using the Barrett-Joyner Halenda (BJH) method, which was used to analyze the pore size distribution of materials, focusing on mesopores [5]. It used nitrogen adsorption and desorption of isotherms obtained from BET analysis, applying the Kelvin equation to convert pressure values into pore diameters. By looking at the desorption branch of the isotherm, the BJH method was used to calculate the pore width distribution. This is important for understanding the performance of the CL and helps track changes in pore structure [5]. For each powder sample, this process was repeated three times, and the average was calculated in order to get the best representation of the BJH average pore width for each sample.

#### Graphs and Analysis:

In order to visually represent the data collected using the above procedures, Microsoft Excel<sup>™</sup> (Excel 2024) was used to create graphs. Three tables were then created where each property measured – average particle size, electrical conductivity, and BJH average pore width – was plotted against water content (wt.%) with water content as the manipulated variable and the property as the responding variable. Each table was then converted into a graph using Excel's graphing tool. The average particle size was graphed on a bar graph, and error bars were added

using the standard deviation formula:  $\sigma = \sqrt{\frac{\Sigma(x_i - \overline{x})^2}{n-1}}$  where  $\sigma$  is the standard deviation

(nanometers),  $x_i$  is the individual particle size measurements from the three trials (nanometers),  $\overline{x}$ 

is the average particle size (nanometers), and n is the number of trials conducted. Both the

electrical conductivity and the BJH average pore width were plotted on a discrete line graph.

These visual representations made it easier to identify relationships between water content and

each measured property. Examining the patterns in the data allows for the impact of solvent

composition on catalyst ink and CL properties to be effectively evaluated.

#### References

- [1] M. N. Islam, A. B. Mansoor Basha, V. O. Kollath, A. P. Soleymani, J. Jankovic, and K. Karan, "Designing fuel cell catalyst support for superior catalytic activity and low mass-transport resistance," *Nat. Commun.*, vol. 13, no. 1, p. 6157, Oct. 2022, doi: 10.1038/s41467-022-33892-8.
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# **March Experimental Procedures**

March 05, 2025:



March 07, 2025:



## March 17, 2025:

☑ Edited methods for CYSF

This diagram shows the flow of the methodology used to conduct these experiments. As outlined, the first step is the preparation of the catalyst ink. Following the preparation of the ink, the three properties of average particle size, electrical conductivity, and Barrett-Joyner-Halenda average pore width were measured. These properties are outlined in the variables section. The procedures are described in further detail below the figure.



To investigate the effect of solvent composition on catalyst ink and catalyst layer (CL) properties, the ratio of isopropyl alcohol (IPA) in the water-IPA alcohol solvent mixture used to disperse the ionomer and catalyst in the catalyst ink was varied in 5% increments. The properties of the catalyst ink and the CL were measured and analyzed using various instruments for each water-to-IPA ratio. To ensure that the changes in these properties were solely due to the water-to-IPA ratio in the catalyst ink, many key factors were kept constant: the concentration of ionomer and catalyst in the catalyst ink, the environmental temperature (maintained at 20°C and 22°C), the thickness of the CL (10-20  $\mu$ m), the application technique of the catalyst ink (slot die coating), and the mixing technique of the catalyst ink (ultrasonication and ball milling).

This study will follow the procedure described in sources (Islam et al., 2022) and (Poojary et al., 2020). A brief explanation of the methodology is as follows.

Preparation of the Catalyst Ink:

The first step that was completed was the preparation of the carbon ionomer dispersion catalyst ink. Different inks were prepared by mixing carbon black (Vulcan XC-72, Cabot Corp., Massachusetts) with a surface area of  $223m^2/g$  (Khan et al., n.d.), water, a mix of isopropyl alcohol (IPA) (Sigma Aldrich, Missouri), and deionized water in known ratios, which acted as the dispersion media. A 20 wt% Nafion ionomer dispersion (Nafion, Ion Power Inc., Delaware) was used to control the water content in the ink. Both

the target ionomer-to-carbon ratio (I/C) of 0.8 and a solid-to-liquid (S/L) ratio of 0.05 were maintained while preparing the catalyst ink for all dispersions. Before using the Nafion ionomer, it was homogenized for 24 hours at room temperature, and that homogenization was followed by 30 minutes of sonication. Following this, the components of the ink were added in a set order: carbon first, then water, followed by IPA, and ending with the Nafion ionomer. The mixture was then probe-sonicated for a total of two minutes in four-second on/off cycles. After that, 16.5g of zirconia balls were added to the vial for every 200mg of carbon in the ink. The vial was sealed to prevent evaporation of the solvent and mixed on a roller mixer at 70 rpm for 15 hours.

#### Average Particle Size:

Following the preparation of the catalyst ink, its average particle size was determined using the dynamic light scattering (DLS) instrument (Zetasizer Nano ZS, Malvern Panalytical, UK), which measured the Brownian motion of particles in a dispersion (Panalytical, 2019). Brownian motion is the random movement of particles that results from their collisions with solvent molecules, such as water. DLS quantified this movement of particles using the translational diffusion coefficient (D) and calculated the hydrodynamic size – the size of a sphere that diffused at the same rate as the particle being measured, including anything bound to the surface of the particle (ions, absorbed polymers, etc.).

When a laser beam is directed at the ink sample, the particles scatter light, and due to the dynamic nature of the sample, the intensity of light scattered by the particles fluctuates over time. Autocorrelation tracked these fluctuations by comparing the intensity signals at different time intervals to determine how long it took for the signal to lose all correlation with the original signal. From this, the translational diffusion coefficient was determined to be used in the Stokes-Einstein equation, which relates the diffusion coefficient to the particle size, temperature, and viscosity of the solvent. The Stokes-Einstein equation can be seen below where  $d_H$  is the hydrodynamic diameter (nanometers), *k* is Boltzmann's constant (joules/Kelvin), *T* is the absolute temperature (Kelvin),  $\eta$  is viscosity (pascal-seconds), and *D* is the diffusion coefficient (meters squared per second). The Malvern Panalytical DLS can measure particle size distribution down to the nanometer scale, which makes this technique useful in applications such as the formulation of catalyst ink for proton-exchange membrane fuel cells (Panalytical, 2019). Each ink sample underwent three trials using the Malvern Panlytical DLS system and calculations using the Stokes-Einstein equation and the results were averaged to

determine the average particle size of each ink sample.

Stokes-Einstein equation:

$$d_h = \frac{kT}{3\pi\eta D}$$

**Electrical Conductivity:** 

After the catalyst ink was deposited onto the Teflon substrate and dried in a vacuum oven at 60°C overnight to allow the solvent to evaporate to create the CL structure, the electrical conductivity of the layer was determined. To do this, the electrical resistance first needed to be determined using a two-probe multimeter (Fluke 177 True-RMS Digital Multimeter, Fluke, Washington). A small sample (2cm x 5cm) of the CL was cut, and its thickness was measured using calipers. The CL was deposited on a Teflon substrate 52 microns thick, so the thickness of the CL was found by subtracting the thickness of the Teflon substrate from the total thickness of the CL and the Teflon substrate. The process of finding the thickness of the CL was repeated in three different spots on the same sample. This is because the thickness at three different points of the sample may not be exactly the same since the sample may not be perfectly even, though a good sample should be. The average of the thicknesses of the CL was taken to be used in the electrical conductivity calculation.

To measure the resistance of the CL, the sample was placed face down on two copper strips, which are good conductors of electricity. The two probes of the multimeter were placed on either copper strip, and the multimeter returned the resistance of the CL. Once the electronic resistance of the layer was determined, the electrical conductivity ( $\sigma$ ) was calculated using the formula below, where L is the thickness of the sample (microns), R is the resistance (ohms), and A is the area of the sample (centimeters squared). The measurements were repeated for three different cut samples from the same deposited catalyst layer, and the average of the calculated electrical conductivities was taken in order to determine the electrical conductivity of each ink sample.

Electrical conductivity:

$$\sigma = \frac{L}{RA}$$

Barrett-Joyner-Halenda (BJH) Average Pore Width:

The BJH average pore width of the CL was determined using nitrogen (N<sub>2</sub>)-sorption analysis. The dried deposited CL prepared to find the electrical conductivity was scratched into powder form. Approximately 120mg of this powder was used for analysis. To remove any absorbed moisture or gases, the sample of powder was degassed at 160°C for at least 12 hours. Nitrogen adsorption and desorption isotherms were collected at 77 Kelvin using a 3FlexTM analyzer (Alberta Sulphur Research Ltd., University of Calgary Research Center), with pressure varying from 1mmHG to 760mmHG. The sample's porosity was determined using BET analysis to measure its nitrogen adsorption capacity. The pore size distribution was then determined using the Barrett-Joyner Halenda (BJH) method, which was used to analyze the pore size distribution of materials, focusing on mesopores (Dey et al., 2023). It used nitrogen adsorption and desorption of isotherms obtained from BET analysis, applying the Kelvin equation to convert pressure values into pore diameters. By looking at the desorption branch of the isotherm, the BJH method was used to calculate the pore width distribution. This is important for understanding the performance of the CL and helps track changes in pore structure (Dey et al., 2023). For each powder sample, this process was repeated three times, and the average was calculated in order to get the best representation of the BJH average pore width for each sample.

#### Graphs and Analysis:

In order to visually represent the data collected using the above procedures, Microsoft Excel<sup>™</sup> (Excel 2024) was used to create graphs. Three tables were then created where each property measured – average particle size, electrical conductivity, and BJH average pore width – was plotted against water content (wt.%) with water content as the manipulated variable and the property as the responding variable. Each table was then converted into a graph using Excel's graphing tool. The average particle size was graphed on a bar graph, and error bars were added using the standard deviation formula below where is the standard deviation (nanometers), x<sub>i</sub> is the individual particle size (nanometers), and n is the number of trials conducted. Both the electrical conductivity and the BJH average pore width were plotted on a discrete line graph. These visual representations made it easier to identify relationships between water content and each measured property. Examining the patterns in the data allows for the impact of solvent composition on catalyst ink and CL properties to be effectively evaluated.
Standard deviation:

$$: \sigma = \sqrt{\frac{\Sigma(x_i - x)^2}{n-1}}$$

☑ Edits to hypothesis for CYSF

If the ratio of isopropyl alcohol (IPA) to water in the catalyst ink solvent is increased, then the size of the aggregates in the catalyst ink will decrease, leading to improved catalyst layer coverage and reduced ionic resistance. This is because a higher concentration of isopropyl alcohol allows particles to spread uniformly across the catalyst surface and promotes better interactions with the membrane.

✓ Edits to variables for CYSF

Independent Variable:

- The ratio of isopropyl alcohol in the water-isopropyl alcohol solvent mixture used to disperse the ionomer and catalyst in the catalyst ink
  - wt.%: 10, 15, 25, 40, 50, 60, 80, 90

Responding Variables:

- Catalyst ink properties: catalyst-ionomer aggregate size, viscosity
- Catalyst layer properties: pore size, electronic resistance.

**Controlled Variables** 

- The concentration of other components (ionomer and catalyst) in the catalyst ink.
- The thickness of the catalyst layer.

# **DATA COLLECTION & RESULTS**

This section contains raw data, images, and tables with the data gathered. It also contains graphs, charts, tables, and pictures that I will be presenting as my results. Notes on problems encountered during the data collection and improvements made will also be contained in this section.

# **February Data Collection and Results**

### February 03, 2024:

Water Content (%)	Average Particle Size (nm)	
10	309.00	
15	261.00	
25	385.00	
30	492.00	
50	527.60	
60	896.00	
80	749.00	
90	443.00	

Water Content (%)	Electrical Conductivity (S/cm)	
10	2.97	
15	4.20	
25	3.60	
30	2.70	
50	1.73	
60	1.90	
80	3.48	
90	3.06	

Water Content (%)	Barrett-Joyner-Halenda (BJH) Average Pore Width (nm)
10	28.18
15	35.90
25	40.14
30	27.90
50	20.78
60	25.80
80	21.12
90	24.15

### February 05, 2025:

### link to Excel sheet with graphs/tables

☑ Avg particle size vs water content

Water Content (wt.%)	Average Particle Size (nm)
10	309.00
15	261.00
25	385.00
30	492.00
50	527.00
60	896.00
80	749.00

443.00



#### ☑ Electrical conductivity vs water content

Water Content (wt.%)	Electrical Conductivity (S/cm)
10	2.97
15	4.20
25	3.60
30	2.70

90

50	1.73
60	1.90
80	3.48
90	3.06



☑ Barrett-Joyner-Halenda (BJH) Avg Pore Width vs Water Content

Barrett-Joyner-Halenda (BJH) Average Pore Width Water Content (wt.%) (nm)	
10	28.18

15	35.90
25	40.14
30	27.90
50	20.78
60	25.80
80	21.12
90	24.15



#### February 07, 2025:

- ☑ Water content vs. Average Particle Size
  - There is a decrease in particle size between 10-15% from 309nm to 261nm
  - This decrease is followed by an increase in particle size between 15% and 60%. The particle size steadily increases, peaking at 896nm at 60% water content.
  - Beyond 60%, the particle size starts to decrease, dropping to 443nm at 90% water content.
    - This is not the smallest particle size of all the data
  - There is a non-linear relationship between water content and average particle size.
    - Initially, the slight increases in water content may promote dispersion, reducing particle size however, beyond a threshold, higher water content seems to lead to particle aggregation, increasing particle size until about 60% water content. After that, further dilution seems to cause the dispersion of particles again.
- ☑ Water content vs. electrical conductivity
  - There is an initial increase in conductivity between 10% and 15% water content, rising from 2.97 S/cm to 4.20 S/cm.
  - This is followed by a gradual decline in conductivity between 15% and 50% water content, where electrical conductivity decreases from 4.20 S/cm to 1.73 S/cm.
  - Conductivity increases again between 60% and 90% water content, peaking at 3.48 S/cm at 80%, then slightly decreases to 3.07 S/cm at 90%.
  - Conductivity peaks early, which gives the impression that moderate water content optimizes ion mobility. The mid-range decline could result from increased particle aggregation (seen in particle size) hindering conductivity. The rise seen towards the end of the data trend could be due to the redispersion of particles or increased ion availability in highly diluted samples.

#### February 10, 2025:

☑ Water content vs. BJH Average Pore Width

- There is an increase in pore width between 10% and 25% water content, where pore width increases from 28.18nm to 40.14nm.
- This increase is followed by a sharp decrease in pore width between 25% and 50%, where pore width drops from 40.14nm to 20.78nm.
- Between 60% to 90% water content, the pore width fluctuates between 20-25nm without a clear trend.
- The initial increase could be an indicator that water content expands pore structures up to 25%. Beyond that, pores may be collapsing, reducing the average pore size. The fluctuations at higher water contents could result from pores swelling at one point, then collapsing as more water is added.
- General patterns
  - Particle size vs. conductivity
    - Larger particle size seems to correlate with lower conductivity
      - This could imply that particle aggregation hinders ion movement
      - At 60% water content, the average particle size is 896nm (the highest recorded), and electrical conductivity is at 1.90 S/cm (the lowest recorded)
  - Pore width vs. conductivity
    - Wider pores seem to correlate with moderate levels of conductivity.
      - This being said, the highest conductivity (4.20 S/cm at 15% water content) does not correlate to the largest pore size (40.13nm at 25% water content).
        - This suggests that other factors, such as ion concentration/dispersion, play a role in this relationship.
  - Non-linear relationships
    - None of the data sampled above show a purely linear trend with water content.
    - All three variables have peaks and troughs that can be seen in the graphs, suggesting transitional spots.

#### February 19, 2025:

Average Particle Size (nm) Electrical Conductivity (S/cm)

309.00	2.97
261.00	4.20
385.00	3.60
492.00	2.70
527.00	1.73
896.00	1.90
749.00	3.48
443.00	3.06



Electrical Conductivity

Barrett-Joyner-Halenda (BJH) Average Pore Width

(S/cm)	(nm)
2.97	28.18
4.20	35.90
3.60	40.14
2.70	27.90
1.73	20.78
1.90	25.80
3.48	21.12
3.06	24.15



Average Particle Size (nm)	Barrett-Joyner-Halenda (BJH) Average Pore Width (nm)
309.00	28.18
261.00	35.90
385.00	40.14
492.00	27.90
527.00	20.78
896.00	25.80
749.00	21.12
443.00	24.15



#### February 20, 2025:

- ☑ Water content vs. average particle size
  - Not a strictly linear relationship
  - Smaller particles (ex., 261 nm) tend to have higher conductivity (4.20S/cm)
  - Larger particles (ex., 896 nm) tend to have lower conductivity (1.90S/cm)
  - There is an inverse trend: as particle size increases, conductivity decreases
  - This could be because smaller particles provide a higher surface area, enhancing charge transfer efficiency, which is important for catalyst activity in PEMFCs
- ☑ Electrical conductivity v.s BJH average pore width
  - The highest electrical conductivity (4.2S/cm) corresponds to a larger pore width (35.90nm)
  - The lowest electrical conductivity (1.73S/cm) corresponds to a smaller pore width (20.78nm)
  - General trend suggests that larger pore widths are associated with higher electrical conductivity
  - This could indicate that well-structured porosity improves ion transport, which benefits the performance of PEMFC catalysts
- Average Particle Size vs. BJH Avg pore width
  - No strict linear correlation between properties
  - Smaller particles (261nm, 309nm) have larger pores (35,90nm, 28.18nm)
  - Larger particles (896 nm) have moderate pore widths (25.80nm0
  - Mid-range particles (385nm, 443nm) correspond to the largest pore widths (40.14nm, 24.15nm)
  - This suggests that smaller particles tend to form more porous structures while larger particles pack more densely, reducing porosity
- ✓ Key takeaways
  - Smaller particles generally result in higher electrical conductivity
  - Large pore widths are associated with better conductivity, suggesting enhanced transport
  - Smaller particles tend to have larger pore widths, potentially improving catalyst efficiency

## **March Data Collection and Results**

#### March 05, 2025:

Graph with error bars



#### March 13, 2025:

The graph below shows the effect of water content on average particle size. Smaller average particle size is better for catalytic activity as it creates a higher surface area-to-volume ratio, providing more sites for reactions (Xie et al., 2021). As seen in the graph below, the optimum water content in regards to average particle size is 15wt.% because this is where average particle size is the smallest.



The graph below shows the effect of water content on electrical conductivity. High electrical conductivity is conducive to an optimal PEMFC as it is indicative of efficient electron transport during reactions. This minimizes resistive losses, enhancing overall performance of a PEMFC (Xie et al., 2021). As seen in the graph below, electrical conductivity peaks at 15wt.%, indicating that this is the most optimal water content for electrical conductivity.



The graph below shows the effect of water content on Barrett-Joyner-Halenda (BJH) average pore width. Large BJH average pore width is important for an optimal PEMFC as gases need to have enough space to diffuse throughout the cell to facilitate reactions (Xie et al., 2021). As seen in the graph below, BJH average pore width peaks at 25wt.%, indicating that this is the most optimal water content for average pore width, however, average pore width is still relatively high at 15wt.% making this a viable option.



The analysis of the ratio of isopropyl alcohol (IPA) to water in the catalyst ink solvent composition highlights many key factors that influence its performance, including water content, particle size and pore width, electrical conductivity, and overall efficiency.

Water content plays a significant role in determining the particle size, pore structure, and conductivity of the ink. The non-linear trends observed in all three graphs above indicate a complex relationship between solvent composition and ink behavior.

Electrical conductivity is affected by water levels in the ink. When water levels are low to moderate, smaller particles are formed, enhancing the conductivity of the ink as ions can flow throughout the cell with greater ease. However, excessive amounts of water cause particles to aggregate, leading to decreased conductivity as ions are unable to efficiently move throughout the proton-exchange membrane fuel cell (PEMFC). Interestingly, the data suggests that at very high water contents (between 60wt.% and 80wt.%), particles seem to redisperse, resulting in an increase in conductivity once again.

Particle size and pore width also influence conductivity. Smaller particles and larger pores increase the overall conductivity of the catalyst layer and well-structured porosity reduces ionic resistance within the cell.

Efficiency and overall performance are directly linked to conductivity and ion mobility. Higher conductivity and better ion mobility lead to increased efficiency, whereas poor dispersion and large particle aggregates create higher resistance, reducing the overall performance of a PEMFC.

Achieving an optimal balance between all three properties – particle size, average pore width, and electrical conductivity – is key for maximizing the performance of a PEMFC.

#### March 17, 2025:

Observations section of the CYSF portal

The image below shows the instrument used to spread the catalyst ink into an even layer to create the catalyst layer.



The image below shows the catalyst layer, which was prepared using catalyst ink that was dried to form the layer.



The following two images show the prepared catalyst ink after it had been fully dispersed.



The image below shows the catalyst ink on the rolling mixer, which ensures that the catalyst ink is fully dispersed.



The image below shows the two-probe multimeter that was used to find the electronic resistance of the catalyst layer, to then be used to find the electrical conductivity of the layer.



The image below shows the two-probe multimeter used to find the electrical resistance. The catalyst layer was placed face down on two copper strips, which conduct electricit,y and the multimeter returned the electronic resistance.



The image below shows the thickness of the catalyst layer being found using calipers. The thickness of the catalyst layer was found by taking the total thickness of the catalyst layer and the substrate, then subtracting the thickness of the substrate, which is a known value.



The table below shows the raw data collected, which shows the different average particle sizes of the catalyst ink for different water contents. The last column shows the error bar values, which were calculated using standard deviation.

Water Content (wt.%)	Average Particle Size (nm)	Error Bars
10	309.00	42.75156
15	261.00	9.1047
25	385.00	24.4205
40	492.00	59.69552
50	527.00	85.4321

60	896.00	35.19785
80	749.00	21.19399
90	443.00	16.09564

The table below shows the raw data collected, which shows the electrical conductivity of the catalyst layer at different water contents.

Water Content (wt.%)	Electrical Conductivity (S/cm)
10	2.97
15	4.20
25	3.60
40	2.70
50	1.73
60	1.90
80	3.48
90	3.06

The table below shows the raw data collected, which shows the Barrett-Joyner-Halenda (BJH) Average Pore Width at different water contents.

Water Content (wt.%)	Barrett-Joyner-Halenda (BJH) Average Pore Width (nm)
10	28.18

15	35.90
25	40.14
40	27.90
50	20.78
60	25.80
80	21.12
90	24.15

# **DISCUSSIONS & CONCLUSIONS**

This section contains an in-depth analysis of my results, whether or not they support my hypothesis, any recommendations for improving my project, and any further questions/experiments that have arisen from my results.

# **February Discussions and Conclusions**

### February 21, 2025:

- Determining Optimal Water Content
  - Electrical conductivity: higher conductivity is better
  - Average particle size: smaller particles better for catalytic activity
  - BJH average pore width: optimal pore size helps in water retention and gas diffusion
- ☑ The data shows that
  - Electrical conductivity: peaks at 15 wt.% (4.20S/cm)
  - Average particle size: smallest at 15 wt.% (261nm)
  - BJH average pore width: the highest at 25 wt.% (40.14 nm), but 15wt.%
    (35.90 nm) is also relatively high
- ☑ 15wt.% appears to be the best because
  - It has the highest electrical conductivity (best ion transport)
  - The smallest particle size (better catalytic performance)
  - A relatively high pore width allowing proper gas and water diffusion

# **March Discussions and Conclusions**

### March 05, 2025:

- ✓ Limitations
  - Testing period: The performance of PEMFC electrodes may change over time. Testing for durability & degradation over extended periods would better results
  - Limited range of water content tested: The study focused on specific water content values. A finer range would provide more precise optimization
- ✓ Future Directions
  - Test more water to IPA ratios to determine the most precise optimum
  - Design a set of manufacturing parameters for large-scale production of PEMFCs

### March 07, 2025:

- ☑ Redone conclusions
  - Electrical conductivity: peaks at 15 wt.% (4.20S/cm)
  - Average particle size: smallest at 15 wt.% (261nm)
  - BJH average pore width: highest at 25 wt.% (40.14 nm), but 15wt.% (35.90 nm) is also relatively high
  - 15wt.% appears to be the best
    - It has the highest electrical conductivity (best ion transport)
    - The smallest particle size (better catalytic performance)
    - A relatively high pore width allowing proper gas and water diffusion

#### March 17, 2025:

✓ Conclusions for CYSF portal

The results indicate that electrical conductivity reaches its peak at 15 wt.% with a value of 4.20 S/cm. Additionally, the smallest average particle size, measuring 261nm, is also observed at the concentration of 15 wt.%. While the BJH average pore width is the

highest at 25 wt.% (40.14 nm) the value at 15wt.% (25.90 nm) is still relatively high.

Based on these findings, 15wt.% appears to be the optimal concentration. It offers the highest electrical conductivity, which enhances ion transport. The smallest particle size at this concentration contributes to better catalytic performance. Furthermore, the relatively high pore width supports proper gas and water diffusion, making 15 wt.% the most favorable option.

- Sources of Error for CYSF portal
  - Testing period: The performance of proton-exchange membrane fuel cell (PEMFC) electrodes may change over time due to issues like water poisoning, which occurs when the cell fails to efficiently remove excess water produced in the cathode. This buildup of water hinders electrochemical reactions, reducing the overall efficiency of the fuel cell. Testing for durability and degradation over extended periods would yield better results.
  - Limited range of water content tested: The study focused on specific water content values as listed in the variables section. Expanding the range with finer intervals would allow for more precise optimization of the solvent to be used in the catalyst ink.
- ☑ Application for CYSF portal

Developing efficient proton-exchange membrane fuel cells (PEMFCs) is incredibly important to advance sustainable energy alternatives. By enhancing durability, performance, and cost-effectiveness, this research supports the creation of PEMFCs for commercial applications, helping bridge the gap in the transition to renewable energy. One of the most significant applications of efficient fuel cells is in heavy-duty vehicles, which are among the largest contributors to greenhouse gas emissions. By improving fuel cell technology, these vehicles can transition away from using fossil fuels, reducing their ecological footprint.

Future work will focus on refining the water-to-isopropyl alcohol (IPA) ratio to determine the optimal ratio for catalyst ink formulation and establishing a set of manufacturing parameters for large-scale production of PEMFCs. As these advancements continue, PEMFCs have the potential to become more affordable and widely accessible. In the long term, once they reach cost-effectiveness, fuel cells can be used globally across various industries and in regions that do not have access to a reliable source of energy, providing a clean and sustainable power source to communities in need.

### **EMAIL COMMUNICATION WITH MENTOR**

This section contains all email communication between my mentor and me.

## **May '24 Email Communication**

#### May 13, 2024:

I emailed Dr. Karan asking to set up a meeting to discuss the Applied Science Project.

Dr. Karan,

Dr. Garcia informed me that she had discussed the Applied Science Project with you. She encouraged me to reach out to set up a meeting with you. I am available to meet between May 21st and May 24th at any time between 11:45 a.m. and 12:15 p.m. I look forward to meeting with you soon. Sincerely, Andrar Krishnamurthy

#### May 21, 2024

I sent a follow-up email to my previous one asking to set up a meeting to discuss the Applied Science Project.

Dr. Karan,

Dr. Garcia informed me that she had discussed the Applied Science Project with you. She encouraged me to reach out to set up a meeting with you. I am available to meet between May 21st and May 24th at any time between 11:45 a.m. and 12:15 p.m.

I look forward to meeting with you soon.

Sincerely, Antara Krishnamurthy

### May 27, 2024:

I sent another follow-up email to my previous ones asking about setting up a meeting.

Hello Dr. Karan,

I hope you are doing well. I apologize for the multiple emails. I am following up on my previous email to see if you have any time this week for an introductory meeting. I am looking forward to hearing back from you.

Sincerely, Antara Krishnamurthy

#### May 29, 2024:

I got a response from Dr. Karan about connecting.

Dear Antara.

I am away this week and last week was very hectic. I can connect with you next week. Let me know if Tuesday would still work for you.

Talk to you soon, Dr. Karan

I replied with a date and time that worked for me.

Dr. Karan,

Tuesday works for me. Would 11:45 p.m. MST work for you?

Sincerely, Antara Krishnamurthy

#### May 30, 2024:

It had slipped my mind that I would not be in town on the day of our meeting, and I asked him whether a virtual meeting would be okay.

Dr. Karan,

I forgot to mention in my previous email, but I am not going to be in Calgary on Tuesday. I will still be able to meet with you over Zoom at whatever time is most convenient for you, but if you would prefer to meet in person, I will be back on June 8th.

Sincerely, Antara Krishnamurthy

## **April '24 Email Communication**

#### April 21, 2024:

I emailed Dr. Karan regarding my interest in working in the lab over the summer.

Dear Dr. Karan,

My name is Antara Krishnamurthy, and I am currently a grade 10 student at Webber Academy. I am writing to express my interest in working with you on your research regarding fuel cells. I have read a lot about the catalysts in fuel cells and how they are making fuel cells expensive and your research on how to make the catalysts smaller in size is very interesting to me, and I would love to learn more about them. I believe that there is a need in the world for energy sources that are reliable, clean, and affordable, and fuel cells are a step in that direction.

Although I am currently in high school, I am passionate about engineering and am eager to gain hands-on experience in a professional setting. I consider myself to be a critical thinker who is motivated, detail-oriented, and adaptable, which I believe are traits that are beneficial to a research environment like this. Recently, I have spent some time reading more about fuel cells, and I am looking for an opportunity this summer to see firsthand the concepts I have read about.

I have attached my resume for your review. I would appreciate the possibility of further discussing this opportunity with you. If you have any questions, please feel free to contact me by email at <u>antarakris30@gmail.com</u> or by phone at (403)-608-5676.

Thank you so much for your time and consideration.

Sincerely, Antara Krishnamurthy

### April 22, 2024:

I received a reply from Dr. Karan about a summer research opportunity. He also mentioned that Dr. Garcia emailed him about the Applied Science Project mentorship.

Hello Antara.

Thank you for contacting me regarding summer research opportunity. Thank you also for sending your resume; it is impressive.

I would be happy to discuss what sort of research experience you are seeking and, more importantly, how to accommodate a high school student in the university lab. I'll look into the University regulations and protocols relevant to such positions.

Also, I received an email from Beatrice from Webber.

Thanks, Dr. Karan

I sent an email back to Dr. Karan thanking him for the opportunity and telling him about the Applied Science Project.

Dr. Karan,

Thank you so much for considering me for a possible research position this summer. I applied to take the Applied Science Project course through Webber Academy for next year. I am keenly interested in using this summer to further my knowledge of fuel cells before the course starts in the fall. I would be delighted to meet with you at whatever time is most convenient for you.

Thank you, Antara Krishnamurthy

## **June '24 Email Communication**

#### June 03, 2024:

I sent Dr. Karan a Zoom link for our meeting the following day.

Dr. Karan,

I have created a Zoom meeting for tomorrow at 11.45 MST. If that time does not work for you, I am free at anytime between 8 a.m. and 5 p.m. MST. I am looking forward to meeting with you.

Antara Krishnamurthy is inviting you to a scheduled Zoom meeting.

Topic: Antara Krishnamurthy's Zoom Meeting Time: Jun 4, 2024 10:45 AM Mountain Time (US and Canada)

Join Zoom Meeting https://us04web.zoom.us/j/73197993996?pwd=DqYbRHisQgkZITbRZRGxIA8flpjC4r.1

Meeting ID: 731 9799 3996 Passcode: 5MMJ93

Sincerely, Antara Krishnamurthy

#### June 04, 2024:

Dr. Karan confirmed our meeting for later in the day.

Hello Antara.

Thanks for the zoom link. Talk to you at 11:45 am.

Dr. Karan

I send Dr. Karan a copy of my application to ASP.

#### Dr. Karan,

Here is the copy of my application to ASP that contains a literature review of what I read on fuel cells. I am looking forward to meeting with you again on June 26th. Thank you so much for your time today. I really appreciate it.

Sincerely, Antara Krishnamurthy

#### June 22, 2024:

## I sent Dr. Karan an email regarding meeting with him in person at the University of Calgary.

Good Morning Dr. Karan,

I hope this email finds you well. I am looking forward to meeting with you in person on Wednesday, June 26th . I was just wondering, what time works best for you to meet and is there a place you would like me to meet you?

Antara

#### June 25, 2024:

### I sent Dr. Karan a follow-up email to my previous one regarding meeting with him in person at the University of Calgary.

#### Good Morning Dr. Karan,

I just wanted to follow up on my previous email. I am looking forward to meeting with you on June 26th. What time works best for you to meet, and is there a specific location you would prefer to meet at?

Sincerely, Antara Krishnamurthy

He replied with a time and a location to meet.

Would 9:30 am work for you, Antara? I can also meet earlier.

Meet at ICT-Building - GoodEarth Café.

Dr. Karan

I emailed him to confirm the time and location.

#### Sounds great! See you then!

#### June 26, 2024:

He emailed me after our meeting at the University of Calgary.

Hope you got see a bunch of cool stuff and learn a lot of new things.

Sent from iPhone, pardon the typos.

Kunal

I send him an email back thanking him for showing me around.

## **August '24 Email Communication**

#### August 26, 2024:

#### Dr. Garcia sent an email to Dr. Karan about school resuming with forms to fill out.

Dear Dr. Karan,

I hope you had a great summer. School will resume here at Webber Academy on Wednesday, August 28th. I will have my first class with Antara and her classmates on Friday, August 30th and I will go over course expectations and first assignments. Antara will be able to share her school timetable and the information I provide in class.

I am not sure what is the procedure in your department for Health and Safety, but you may need access to the master legal agreement our school has with the U of C that allows our students to visit the labs. The Schedule B form is part of this legal agreement, I have completed the form for Antara and it is signed by our Vice-President.

Depending on the hazard levels of each lab, some professors have required our students to complete safety courses online before any experimental work. For that purpose, students need a UCID and the Young Persons Accessing Laboratories form completed. I have attached all these documents and forms in case you need them. Please note that many other labs/departments have not required these forms, so it is completely up to your department.

I am looking forward to a great collaboration.

Cheers,

Beatriz
## **September '24 Email Communication**

## September 03, 2024:

I sent Dr. Karan an email asking him about setting up a meeting to plan my project.

Good Afternoon Dr. Karan,

I just had my first Applied Science Project class on Friday. I was wondering whether it would be possible to meet with you to go over possible projects, literature readings, and a schedule for me to see experiments in the lab? I have added times over the next two weeks that I would be available to meet either in person or via Zoom.

Wednesday, September 4th: 12:50 pm - 1:30 pm Thursday, September 5th: 2:15pm Friday, September 6th: 10:15 am - 11:30 pm Unesday, September 10th: 10:15 am - 11:30 pm Unesday, September 11th: 12:50 pm - 1:30 pm Thursday, September 11th: 12:50 pm - 1:30 pm Friday, September 13th: 12:55 am - 1:30 am Unesday, September 13th: 10:15 am - 11:30 pm Unesday, September 13th: 10:15 am - 11:30 pm Unesday, September 18th: 10:15 am - 11:30 pm Thursday, September 18th: 10:15 am - 11:30 pm Friday, September 19th: 12:50 pm - 1:30 pm Friday, September 20th: 12:50 pm - 1:30 pm

I am also available to meet at 4:00 pm every day after school and can meet over the weekend.

Thank you, Antara Krishnamurthy

## September 06, 2024:

I sent a follow-up email to Dr. Karan about meeting to discuss my project.

Hi Dr. Karan

I just wanted to follow up on my last email. During my last ASP class on Wednesday, we were introduced to our first assignment, which is to write a research proposal for our project. Would it be possible to set up a meeting to go over possible project ideas and literature I can read for my project proposal? I am available over the next couple of weeks on these dates and times.

Monday, September 9th: 10:15 am - 11:30 pm Tuesday, September 10th: 10:15 am - 11:30 pm Wednesday, September 11th: 12:50 pm - 1:30 pm Thursday, September 12th: 12:50 pm - 1:30 pm Friday, September 12th: 21:50 m Monday, September 12th: 10:15 am - 9:30 am Tuesday, September 17th: 10:15 am - 11:30 pm Thursday, September 18th: 10:15 am - 11:30 pm Thursday, September 18th: 12:50 pm - 1:30 pm

I am also available after 4:00 pm every day after school and am available to meet over the weekend at any time. I would be happy to meet either in person or via Zoom, whichever works best for you

Sincerely, Antara Krishnamurthy

Dr. Karan sent a response back with possible dates and times.

Hello Antara.

Sorry about the late response. It is first week of classes and things have been hectic.

We can meet on the following date/time:

Wednesday, September 11th: 12:50 pm - 1:30 pm Wednesday, September 18th: 10:15 am - 11:30 pm

Can you send me calendar invite for the meeting? If you are not sure how to do that, let me know.

Talk to you soon.

Dr. Karan

### I confirmed a meeting time with him and sent a Zoom invite.

#### Hi Dr. Karan,

Thank you so much for the response. I would be happy to meet on Wednesday, September 11th at 12:50. I am not sure how to send you the calendar invite for it but I have attached the Zoom invite below.

Antara Krishnamurthy is inviting you to a scheduled Zoom meeting.

Topic: Antara Krishnamurthy's Zoom Meeting Time: Sep 11, 2024 12:50 PM Edmonton

Join Zoom Meeting https://us04web.zoom.us/j/77335516916?pwd=D9fbKU9hu3rLWjsqJL1KB0fmd8QP7V.1

Meeting ID: 773 3551 6916 Passcode: 7w0m8e

Thank you so much! Antara Krishnamurthy

## September 08, 2024:

Dr. Karan sent me a Google Calendar invite for our meeting on Wednesday.

Topic: Antara Krishnamurthy's Zoom Meeting Time: Sep 11, 2024 12:50 PM Edmonton

Join Zoom Meeting <a href="https://us04web.zoom.us/j/77335516916?pwd=D9fbKU9hu3rLWjsqJL1KB0fmd8QP7V.1">https://us04web.zoom.us/j/77335516916?pwd=D9fbKU9hu3rLWjsqJL1KB0fmd8QP7V.1</a>

Meeting ID: 773 3551 6916 Passcode: 7w0m8e

## September 11, 2024:

I sent Dr Karan an email summarizing what we discussed during our meeting.

Thank you so much for taking the time out of your busy schedule to meet with me today. I just wanted to review the main points of our meeting today.

- The project I am working on is going to be a data analysis project.
- You mentioned that I may be paired up with a graduate student sometime down the line, but for now, you will directly supervise me.
- You have a project in mind that I could work on with some results already collected that are still generating more results.
- You will be sending me papers to read on Monday following our meeting.

I hope I haven't forgotten to summarize any important items we discussed. Please let me know if I missed anything.

Sincerely, Antara Krishnamurthy

### September 15, 2024:

I sent Dr. Karan an email reminding him of our coming meeting with a Zoom link and a Google Calendar invitation to our meeting.

Hi Dr. Karan,

I apologize for the late email. Below is the Zoom meeting link for our meeting on Monday at 4:00 p.m., as well as a calendar invite.

Antara Krishnamurthy is inviting you to a scheduled Zoom meeting.

Topic: Antara Krishnamurthy's Zoom Meeting Time: Sep 16, 2024, 04:00 PM Edmonton

Join Zoom Meeting

https://us04web.zoom.us/j/78889645993?pwd=pUrfNeIPbkSqHJSJCIZFfKwhRYjR1G.1

Meeting ID: 788 8964 5993 Passcode: 2a4y2a

> Monday Meeting Sep 16, 2024, 4:00pm - Sep 16, 2024, 5:00pm (GMT-07:00) Pacific Time - Los Angeles

Sincerely, Antara Krishnamurthy

## September 16, 2024:

I emailed Dr. Karan to thank him for meeting with me and to summarize our meeting.

Thank you so much for taking the time to meet with me today. I wanted to review the things we discussed during our meeting.

We spent today reviewing some papers. You explained the visuals and key ideas in the papers so I could gain a general understanding of how fuel cells work. You will be sending me the papers we looked at today, as well as some other papers, for me to review before our meeting next Monday.

During our meeting next week, we will be narrowing down the research question I will be using in my research proposal as well as be discussing some goals I have for the project

I hope I haven't forgotten to include anything important we have discussed. Please let me know if I missed anything.

I am looking forward to seeing you again next week!

Sincerely, Antara Krishnamurthy

## September 20, 2024:

I sent Dr. Karan an email reminding him of our upcoming meeting and including things I wanted to discuss. I also asked him to send me the papers we were looking at during our last meeting.

Hi Dr. Karan,

Thank you again for meeting with me earlier this week. I am looking forward to meeting with you again on Monday. Would you be able to send me a Zoom link for the meeting?

I was hoping that during our meeting on Monday, we would be able to finalize my research question and determine some short—and long-term goals for my project. Would it also be possible for you to send me PDF copies of the literature we went over together at the last meeting? I would like to take another look at them.

Thanks, Antara Krishnamurthy

**Monday Meeting** Sep 23, 2024, 4:00pm - Sep 23, 2024, 5:00pm (GMT-07:00) Pacific Time - Los Angeles

> Dr. Karan sent me an email back, telling me that he would send me notes and articles for me to look over. He also said that he would send me a Zoom link for our Monday meeting.

Hi Antara.

I will send you my notes (handwritten) on the research background/rationale. I will also send you the articles.

Hopefully, I can send by tomorrow evening.

I'll send you zoom link for 4 pm meeting on Monday.

Kunal

I sent an email back thanking him.

Thank you so much!

Dr. Karan sent me the first paper he wanted me to look at along with some thoughts/notes.

Hi Antara.

Read the first 3 pages of this paper (pages 475-477). I have highlighted the text that will be critical in developing the narrative for the research.

The narrative is: high activity catalyst development is not sufficient to ensure high performance in an actual fuel cell device.

The actual performance depends on – (a) catalyst utilization or accessibility in the electrode (b) ease of transport of gaseous reactant, i.e. oxygen (c) ease of transport of protons participating in the electrochemical reaction, and (d) to less extent, electron transport to the catalyst.

For reaction to take place on Platinum catalyst at the cathode, all three reacting species must arrive or be transported.

Cathode reaction:  $O_2(gas) + 4H^+ + 4e^- \rightarrow 2H_2O$ 

if we cut off supply of any of the three reactants (O2, H+ or e-), the catalyst cannot be effective or will end up being unutilized. Hence, the microscopic structure of the catalyst layer is very important.

I'll share the other papers. I share my notes on the link between the building blocks (catalyst, ionomer), the ink (solvent, catalyst, ionomer) and the final microscopic structure of the catalyst layer.

Stay tuned.

Dr. Karan

I emailed back, saying that I would have it read by Monday.

Thank you so much for sending me this paper. I will have it read by Monday!

Dr. Karan sent me some notes on why it is important to study catalyst ink effects.

Here are some of my thoughts/notes on why we need to study catalyst ink effects.

Dr. Karan

#### See Mentor Written Notes for September 20th.

Dr. Karan sent me another article with specific sections to read.

Read section 1, section 2; section 2.1 (no need to go in depth), section 2.4; section 4.6; section 6 (all of it).

You do not have to read all of it before Monday meeting.

Dr. Karan

## September 24, 2024:

I sent a summary of the things we discussed during our meeting yesterday.

#### Hi Dr. Karan

Thank you so much for taking the time to meet with me yesterday. I wanted to review the things we discussed during out meeting.

- We reviewed some diagrams, and you explained the complicated process of designing fuel cells.

- You sketched a fuel cell structure and will email it to me.

- We discussed the structure of fuel cells and how to optimize performance

- We went over some of the variables that the experiment conducted at the lab has.

Before our meeting next Monday, I will have the rest of the papers you sent me read. I will also have an outline of the introduction section of my research proposal completed with possible research questions.

I hope I haven't forgotten to include anything important we have discussed. Please let me know if I missed anything.

I am looking forward to seeing you again next week!

Sincerely, Antara Krishnamurthy

## September 25, 2024:

Dr. Karan sent me the notes from our meeting on September 23rd.

#### Hi Antara.

Attached are the review notes. Read the Sep 20<sup>th</sup> notes again to assimilate how catalyst layer structure affects the performance. And, how catalyst layer structure depends on the catalyst ink formulation used to make catalyst layer.

You have captured most of the important points of our 23<sup>rd</sup> September meeting.

Dr. Karan

#### See Mentor Written Notes for September 23rd.

## September 27, 2024:

I wrote an email to Dr. Karan reminding him of our upcoming meeting on Monday.

Hi Dr. Karan,

I hope you are doing well. I just wanted to send a quick reminder about our scheduled meeting on Monday at 4:00 p.m. I am looking forward to talking with you again then.

Sincerely, Antara Krishnamurthy

## September 30, 2024:

Dr. Karan emailed me to reschedule our meeting.

Hi Antara.

It may be difficult to have a meeting today. Can we meet 4 pm on Thursday?

Dr. Karan

I confirmed that the time worked for me.

Yes, Thursday works for me.

## **October '24 Email Communication**

## October 04, 2024:

I emailed Dr. Karan a summary of the things we discussed during our meeting.

Hi Dr. Karan,

Thank you so much for taking the time to meet with me yesterday. I wanted to review the things we discussed during our meeting.

We reviewed the research question I formulated based on the papers you gave me, looked at each of their pros and cons, and considered the feasibility of researching them in the lab. We also decided which question to use. I will reword the question to better fit the experiments run in the lab.

We went over the rough outline I created for the introduction section of my research proposal and discussed any modifications to be made to better suit the research.

Before our next meeting on Monday, I will have the background information part of the introduction written and the research question rewritten.

Could you send me papers on the catalyst ink so that I can collect more information for my research proposal?

I hope I haven't forgotten to include anything important we have discussed. Please let me know if I missed anything.

I am looking forward to seeing you again next Monday!

Sincerely, Antara Krishnamurthy

## October 08, 2024:

I emailed Dr. Karan a summary of the things we discussed during our meeting.

Thank you so much for taking the time to meet with me yesterday. I wanted to review the things we discussed during our meeting.

- We reviewed the background information in the introduction section of my research proposal. You suggested some changes to make it flow better and connect to the research question better.

- We reviewed my outline for the research proposal and discussed specific things to include to create a better flow in the background information section.

- You walked me through the best way to read a lengthy research/review paper.

Before our next meeting on Thursday, October 17th, I will have the background information section of the research proposal done. I will try to read some of the papers you sent me about the catalyst ink before our next meeting as well.

I reformatted the research question to better fit something I will actually be able to see happen in the lab. I have written the question below for you to review. Could you please send me any modifications you would make to the question so I can reword it?

How do coating parameters impact the structure of the catalyst layer and thereby affect the structure and properties of a proton exchange membrane fuel cell (PEMFC)?

I hope I haven't forgotten to include anything important we have discussed. Please let me know if I missed anything.

I am looking forward to seeing you again on the 17th!

Sincerely, Antara Krishnamurthy

## October 16, 2024:

I scheduled an email to Dr. Karan as a reminder for our upcoming meeting tomorrow.

Hi Dr. Karan,

I hope you are doing well and had a happy Thanksgiving. I just wanted to send a quick reminder about our scheduled meeting today at 4:00 p.m. I am looking forward to talking with you again.

Sincerely, Antara Krishnamurthy

## October 17, 2024:

Dr. Karan confirmed our meeting and asked me to send him a copy of my research proposal.

See you then. Send me your proposal before the meeting.

Kunal

I wrote back with a copy of the email.

Here is a copy of what I have written so far.

## October 19, 2024:

I sent Dr. Karan a summary of our meeting on October 17th.

Thank you so much for taking the time to meet with me on Thursday. I wanted to review the things we discussed during our meeting.

- We decided that my project would be an experimental-based project.
- For the science fair portal, I have no ethics to declare about the project.
- There are no significant risks to the project.
- All materials are handled according to the material safety data sheet
- Create an eye-catching title to get people interested.
- For methodology, I will find out from Dr. Garcia how to get permission to be allowed into the lab and you will be showing me the methods when I visit the lab.

Before our next meeting on Monday, I will have the introduction to the RP done.

Sincerely, Antara Krishnamurthy

#### He replied, saying he is looking forward to reading my RP.

Thanks for the summary of our meeting, Antara. I am looking forward to reviewing your research proposal document.

Dr. Karan

## October 23, 2024:

#### I sent Dr. Karan a summary of our meeting on October 23rd.

#### Hi Dr. Karan,

Thank you so much for taking the time to meet with me on Monday. I wanted to review the things we discussed during our meeting.

- I shared my research proposal with you for your review and feedback.

- You will be specifically looking to see if the proposal flows and tells a story.

- I will add a bit more about the catalyst ink specifically to the introduction, as that is the main focus of the research.

- You suggested that I should add some figures to the introduction so people who may not have as much knowledge of the subject can still make connections.
- You will be adding some information about the methodology so I can begin working on the section.

I will have the rest of the research proposal done by the end of this week, maybe without the methodology section. We will meet again on Thursday, October 31st, at 4:00 p.m. I am looking forward to speaking with you again then.

Sincerely, Antara Krishnamurthy

# **November '24 Email Communication**

## November 03, 2024:

I sent Dr. Karan an email with the final draft of my written project proposal.

Hi Dr. Karan,

I hope you are having a great weekend! I have finalized my research proposal with all the edits you have given me and have attached the final copy to this email.

- I took the information you gave me about the methodology and just formatted it into paragraphs, as that is what Dr. Garcia is looking for when marking the RP.

- I have added a figure that shows the transports within a fuel cell. The diagram is from <u>Performance assessment and economic perspectives of integrated PEM fuel cell and PEM electrolyzer for electric power</u> <u>generation.</u> I have also attached an image of the figure to this email for your review.

Please let me know if there are any more final changes you would like me to make before I submit the proposal tomorrow.

I am looking forward to meeting with you tomorrow.

Sincerely, Antara Krishnamurthy

https://1drv.ms/w/c/493a57a833be4c80/EZXIfqSzCr1Es\_ syVAL3Ze0BohBcwJK36m4uPOVeV3M3nQ

November 11, 2024:

I sent Dr. Karan an email with my oral presentation.

Hi Dr. Karan,

This is a copy of my oral presentation. I haven't added citations for the images yet, but I will be finishing those tonight.

Sincerely, Antara Krishnamurthy

https://1drv.ms/p/c/493a57a833be4c80/EV7brqG3E9NImFTbi0huHgYB\_ GgUxzJD2gyvmEHkdhwhNg

## November 13, 2024:

I sent Dr. Karan an email asking about our meeting today.

Hi Dr. Karan,

I hope you had a good weeked. Are we still meeting today?

Antara

Were we meeting today? I thought it was tomorrow.

We can meet today. Give me 10 mins.

Kunal

Okay, sounds good!

## November 19, 2024:

I sent Dr. Karan an email thanking him for letting me come into the lab.

Antara Kri... Tue, Nov 19, 11:17 AM (9 days ago) ☆ ⓒ ∽ : to Kunal マ

Hi Dr. Karan,

Thank you so much for letting me come into the lab yesterday and meet Vahid. I learned a lot and it was great to see the different processes that I've been reading about.

I also wanted to let you know that I got my marks back for the written research proposal and oral presentation. I got a 99 on the written proposal and a 97 on the oral presentation.

I was just wondering whether there was anything for me to read or look over before our next meeting on Monday, November 25th? During our next meeting I was also hoping we could talk about a long-range plan so I can have a rough idea of what I will be acomplishing in the next few months.

I look forward to speaking with you again soon.

Sincerely, Antara Krishnamurthy

## November 28, 2024:

I sent Dr. Karan an email with a list of all the papers I have read and asked if there are any more I should read.

Here is a list of all the papers I have read thus far.

- Bridging the gap between highly active oxygen reduction reaction catalysts and effective catalyst layers from proton exchange membrane fuel cells.

- Structure, property, and performance of catalyst layer in proton exchange membrane fuel cells.

- Dictating Pt-based electrocatalyst performance in polymer electron fuel cells, from formulation to application.

- Tailoring electrode microstructure via ink content to enable improved rated power performance for platinum cobalt/high surface area carbonbased polymer electrolyte fuel cells.

- The controllable design of catalyst inks to enhance PEMFC performance: a review

- Recent progress in understanding the dispersion of stability of catalyst ink for proton exchange membrane fuel cell and water electrolyzer.

- effect of catalyst ink properties on the performance of proton exchange membrane fuel cell and water electrolyzer: a mini-review.

Please let me know if there are any other papers you think it would be beneficial for me to read.

Thanks, Antara Krishnamurthy

## November 29, 2024:

I sent an email to Dr. Karan reminding him of our upcoming meeting on Monday.

I hope this email finds you well. I just wanted to send a quick reminder about our scheduled meeting on Monday at 4:00 p.m. I am looking forward to speaking with you again then.

Sincerely, Antara Krishnamurthy

# **December '24 Email Communication**

## December 04, 2024:

Hi Dr. Karan,

I hope this email finds you well! I just wanted to reach out to ask how I should get in touch with Vahid in order to schedule times for me to come into the lab. Is there an email I should use or some other means of communication?

Also, would it be possible to get more papers or resources that you think would be beneficial for me to read?

I look forward to hearing from you and speaking with you again soon.

Sincerely, Antara Krishnamurthy

## December 05, 2024:

Hi Antara.

I am trying to get hold of Vahid. He was not in the lab yesterday. I'll get back to you soon.

### Dr. Karan

I sent him an email back asking for papers.

Okay, thank you! Are there any more papers I can read in the meantime?

## December 11, 2024:

I sent an email to Dr. Karan about the next steps of my project.

Hi Dr. Karan,

I was just wondering whether you have been able to get in contact with Vahid so we can schedule times to meet in the lab before I leave for winter break.

I was also wondering if it would be possible to get more papers or resources that you think would be beneficial for me to read.

I look forward to hearing from you and speaking with you again on Monday.

### Sincerely, Antara Krishnamurthy

## December 16, 2024:

I sent another email to Dr. Karan asking about scheduling a meeting with Vahid, a graduate student.

Good Morning, Dr. Karan,

I was wondering if you have been able to contact Vahid so we can schedule a time to meet in the lab before my school ends for winter break next Friday, December 20th. I can also come into the lab in early January before my midterms begin on Jan 10th if that is more convenient with the lab's schedule. Midterms run from January 10th to January 21st, so I will not be able to come to the lab during those days.

Would it also be possible to get more papers or resources that you think would be beneficial for me to read so I can do some reading over winter break?

I look forward to speaking with you later today.

Sincerely, Antara Krishnamurthy

Dr. Karan sent me an email saying that he is unable to meet today.

Hi Antara.

I wouldn't be able to meet today. Vahid is available for meeting everyday of this week. You can respond to his email and keep me copied.

Kunal

Dr. Karan,

Okay, sounds good! Would you just be able to send me some papers whenever you get the chance. I know that it is a busy time right now, but I would really appreciate having papers to read over my break.

#### Sincerely,

Antara

Dr. Karan sent me an email copying Vahid so we could schedule a meeting in-person at the lab.

Hi Vahid.

As discussed last week, Antara would like to visit the lab to gain further understanding of the experiments. Can you please coordinate the visit times with her? Keep me copied on the emails.

I will be busy grading the final exams and finishing other commitments this week.

Dr. Karan

Vahid sent me an email with times that he is available to meet.

### Dear Anantara,

We can meet on following days between 2PM to 3 PM. Let me know which day works? Or if you need to be here later times like 4 PM ?

Thanks,

Vahid

-- . ...., ....

I meant to say following days of this week. So let me know which day works best for you Anantara. Thanks, Vahid

I replied back with a time that works for me to meet

Hi Vahid,

Would Friday at 4:30 work for you? My school only lets out at 3:30, so I would need some time to get home and then drive to the university.

Sincerely,

Antara

We both confirmed the time

.

Yes, that works. Let's meet on Friday at 4:30 PM.

Sounds good. See you then.

# **January '25 Email Communication**

## January 06, 2025:

I sent an email to Dr. Karan asking if we would be meeting because school has resumed.

Hi Dr. Karan,

I was wondering if you still wanted to meet via zoom at 4:00pm since school has resumed?

Sincerely, Antara

He emailed back, saying that he is busy and can't meet today.

## Hi Antara.

Let us skip the meeting today. I need to catch up with my group first. We can try later this week.

Dr. Karan

I sent him times in the week that I am available to meet.

# Okay, sounds good! Let me know when works best for you! I won't be able to meet on Tuesday or Thursday this week, but every other day works for me.

I sent Dr. Karan another email during class telling him that we are back in class and asking for more papers.

Happy New Year! I hope you had a wonderful holiday!

Regular classes resumed for me today, but we have a midterm study break from Friday, January 10th, until Monday, January 20th. During this time, I can meet via Zoom, but it may be difficult for me to make it to the lab for in-person meetings.

Would it be possible to get more papers or resources that you think would be beneficial for me to read? I would like to use some of my free time during this break to do some reading so I am staying caught up on research.

I know that today is not a good day for us to meet, so please let me know a time that works for you. I am able to meet any time this week except for Tuesdays and Thursdays.

Sincerely, Antara Krishnamurthy

## January 19, 2025:

I sent Dr. Karan an email asking if he is available to meet tomorrow.

Hi Dr. Karan,

I hope this email finds you well. I was wondering whether you are free to meet tomorrow via Zoom to discuss the next steps of my project.

Sincerely, Antara

## January 20, 2025:

He responded to my email saying that we can meet at our usual time.

See you at 4 pm. I will also meet with Vahid before our meeting. I finish my lecture/lab at 3pm.

Kunal

## January 22, 2025:

I sent Dr. Karan a summary of our meeting on Monday.

Hi Dr. Karan,

Thank you so much for taking the time to meet with me on Monday. I wanted to review the things we discussed during our meeting.

- We reviewed some of the important upcoming deadlines for my project.

- January 30: Introduction Section of Final Paper
- February 19: Procedures section
- March 11: In-School Science Fair
- March 21: Results Section
- April 25: Discussion and Conclusions
- May 28: Final Paper

- You mentioned that you will be asking Vahid to share some results of his experiments with me.

- You also mentioned that you will be sending me papers that are pertinent to my research and that are related to the results Vahid has collected.

- I will ask Dr. Garcia what section of the final paper should include the hypothesis and variables and send that information to you.

I hope I haven't forgotten to include anything important we have discussed. Please let me know if I missed anything.

I am looking forward to speaking with you again on Monday!

Sincerely, Antara Krishnamurthy

## January 24, 2025:

I sent another email to Dr. Karan and Vahid asking for data.

Hi Dr. Karan,

I hope you are doing well. I was wondering whether you have had a chance to talk to Vahid about sharing some data that I can have for my project. As I mentioned during our meeting on Monday, the in-school science fair is in six weeks. Our teacher has been insisting that we have to get started on analysis right away in order to be prepared for the science fair.

I am looking forward to meeting with you again on Monday.

Sincerely, Antara Krishnamurthy

## January 30, 2025:

Dear Antara,

Happy new year, Wish all the success with your project and future projects. Attached the data i presented before. Thanks, Vahid

One attachment • Scanned by Gmail (i)



Thank you so much for this data, Vahid! I was wondering whether it would be possible to get raw data points rather than graphs so I can go through the process of creating the graphs myself to do the analysis and better understand the data.

Sincerely, Antara Krishnamurthy

Here you are. Vahid From: Antara Krishnamurthy <<u>antarakris30@gmail.com</u>> Sent: Thursday, January 30, 2025 10:06 AM To: Vahid Mazinani <<u>vahid.mazinani@ucalgary.ca</u>> Subject: Re: Data [

Core attachment • Data

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...
<antara.xlsx>

# **February '25 Email Communication**

## February 03, 2024:

Vahid sent me an email with more raw data.

Thanke	w data for size-elect		and pore width for	different water con	lieni.
Vahid					
From: Antara Kris	hnamurthy < <u>antarakri</u>	s30@gmail.com>			
Sent: Thursday, .	anuary 30, 2025 6:42	PM			
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77 60					

### Reply:

Thank you very much!			
•••			

### To Vahid:

Hi Vahid,

What units the particle size and electrical conductivity are measured in?

Antara

## February 05, 2025:

#### To Vahid:

#### Hi Vahid,

I hope you are doing well. I have graphed the raw data you sent me earlier this week using Microsoft Excel and have attached the file to this email. I am still working on adding some stuff to the graphs, such as axis labels and changing the scale, but the link should update, and I change the graphs. I assume that the data you sent me is already averaged from the data you collected, but I was wondering whether you had the full, unaveraged data points. One of the standards for the science fair is having error/standard deviation bars on our graphs, and I cannot add those without the full data set.

Additionally, I was wondering whether there was a time next week that I would be able to come into the lab to learn more about the methodology of the experiment and how the data is collected and analyzed. I can come in any day next week except for Thursday and Friday.

Sincerely, Antara Krishnamurthy

tps://1drv.ms/x/c/493a57a833be4c80/EQvFJk-f2tZNhNIJx0gXWOwBR6ioFzff1eqobYJd3ZYggw

## February 09, 2025:

From Vahid:

I can actually show you how i measure electrical conductivity and DLS this week, i think tuesday can be good to set a time.

To Vahid:

Sounds good! I can be there Tuesday at 4:30 if that works for you.

•••

## February 10, 2025:

From Vahid:

Ok

Get Outlook for iOS

## February 11, 2025:

From Vahid:



## February 15, 2025:

To Vahid:

Hi Vahid,

Would you be able to send me information about how the preperation of the catalyst layer?

Antara

```
> On Feb 11, 2025, at 4:34 PM, Vahid Mazinani
<<u>vahid.mazinani@ucalgary.ca</u>> wrote:
>
>
> <ELECTRICAL W60 306B2 2 probe Copper vs 4 probe.xlsx><partilce
size vs water content -error bar.xlsx><W50 DLS PARTICLE SIZE .xlsx>
```

From Vahid:

Here you are,

Remember to read and rewrite your own version, Also reference me as this work will be published by me and Dr. Karan in a few months.

Thanks, Vahid					
From: Antara Krishnamurthy < <u>antarakris30@gmail.com</u> > Sent: Saturday, February 15, 2025 11:19 AM To: Vahid Mazinani < <u>vahid.mazinani@ucalgary.ca</u> > Subject: Re: remind me methodology in a few days					
[△EXTERNAL]					
<b>One attachment</b> • Scanned by Gmail ③	@₊				
Experimental Techniques					

To Vahid:

Antara Krishnamurt	Sat, Feb 15, 12:01 PM	☆	$\odot$	Ś	:
to Vahid 👻					

Thank you very much. I will make sure to include all the proper references!

•••

## **March '25 Email Communication**

## March 03, 2025:

To Vahid:

Hi Vahid,

I was wondering whether you have error bar calculations for 30wt% for the average particle size graph. The file you shared with me skips 30wt%.

Sincerely, Antara

Sorry, I meant for 60wt%. I had written down a number wrong.

From Vahid:

Sample W60 is updated recently.here you are.

Get Outlook for iOS

From: Antara Krishnamurthy <<u>antarakris30@gmail.com</u>> Sent: Monday, March 3, 2025 1:31:59 PM To: Vahid Mazinani <<u>vahid.mazinani@ucalgary.ca</u>> Subject: Re: Error Bars

[△EXTERNAL]

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4



To Vahid:

Thank you so much!

## March 05, 2025:

To Dr. Garcia

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7	60	896.00	35.19785	
	80	749.00	21.19399	
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17 10 100	Content (set %) Electrical Conductivity (Sin	and the second second		
X	ASP Data G	araphs		

From Dr. Garcia

I did it! I can show you at lunch or after school today. Here is the file with the added bars.

Cheers,

Dr. Garcia

To Dr. Garcia

Hi Dr. Garcia,

I was wondering whether it would be possible to meet with you during my spare tomorrow. It's right before lunch.

Sincerely, Antara Krishnamurthy

## March 06, 2025:

### From Dr. Garcia

Antara, I've got a last minute meeting. We may need to delay until the second part of your spare block. I'll come look for you in the cafeteria or green chairs.--Beatriz Garcia-Diaz, PhD Science Lab Coordinator Webber Academy 1515 - 93rd Street, S.W. Calgary, Alberta T3H 4A8 Phone: (403) 277-4700 ext. 342

To Dr. Garcia

No worries, thanks for the heads up! I will be in the cafeteria.

## March 10, 2025:

To Dr. Karan

I hope you're doing well. I wanted to let you know that I no longer need weekly meetings since there won't be any major changes to my project in the coming weeks. The school science fair is tomorrow, and I'll find out on Wednesday whether I've qualified for the city science fair.

The deadlines for my next two papers have been shifted: the results section is now due on April 14, and the discussions and conclusions section is due on May 1. Would is be alright if I reach out via email if I have any questions and need to set up a meeting?

Sincerely, Antara

#### From Dr. Garcia

Dear ASP students:

I wanted to send a note to wish you the very best for tomorrow:

YOU GOT THIS!!! You have worked hard and are well prepared, you put thought and effort into making great posters and practice your oral presentation. You checked in with your mentors and with me. Now, go to bed early, have a good rest and you will shine tomorrow. Whatever the scores, or the medals, this is a huge milestone and you should be proud of your effort. When you look back on your ASP experience, this will be a highlight, so enjoy your day tomorrow, learn from your fellow science fair participants and be gracious and appreciative of the amount of work it took to get here.

See you all tomorrow (in full dress uniforms and well rested)

Cheers, Dr. Garcia

## March 12, 2025:

Beatriz ... Wed, Mar 12, 1:26 PM (23 hours ago) ☆ 🙂 ← : to Kunal, me ▾

Hello,

I just wanted to inform you that Antara's project won a gold medal and she was highly ranked in the Senior High Science Fair. Antara will be among the top 15 projects representing Webber Academy in the Calgary Youth Science Fair from April 10-12th. This is an incredible achievement considering the caliber of the projects. If you have time, you can go see her in action at the Olympic Oval on Saturday, April 12th from 9-11:30 am.

A huge thank you again for all you have done. Please extend this thank you note to your graduate student who helped Antara so much.

Cheers,

Beatriz

Thanks for informing, Beatriz. Congratulations to you, too!

Antara!! WOW. So proud of you. Heartiest Congratulations!

I am beaming.

I will certainly try to stop by on April 12<sup>th</sup> at the Olympic Oval.

Best, Dr. Karan

## March 19, 2025:

Hi Dr. Karan,

I hope this email finds you well.

I just wanted to send you an email updating you on everything I have been doing during ASP these past couple of weeks.

I know that Dr. Garcia sent you an email letting you know that I made it to the Calgary Youth Science Fair, so I have recently been working on finishing my portal for that. Thank you for all your help with my project. I wouldn't have made it this far without all your guidance.

This Friday will be the first day of my school's spring break. I will not be in Calgary between March 21 and April 5. My first day of school after spring break is April 7. During spring break, I will be writing the results section of my paper. Would it be possible for me to reach out via email if I have any questions?

Once again, thank you so much for all your help and guidance. I really appreciate it.

Sincerely, Antara