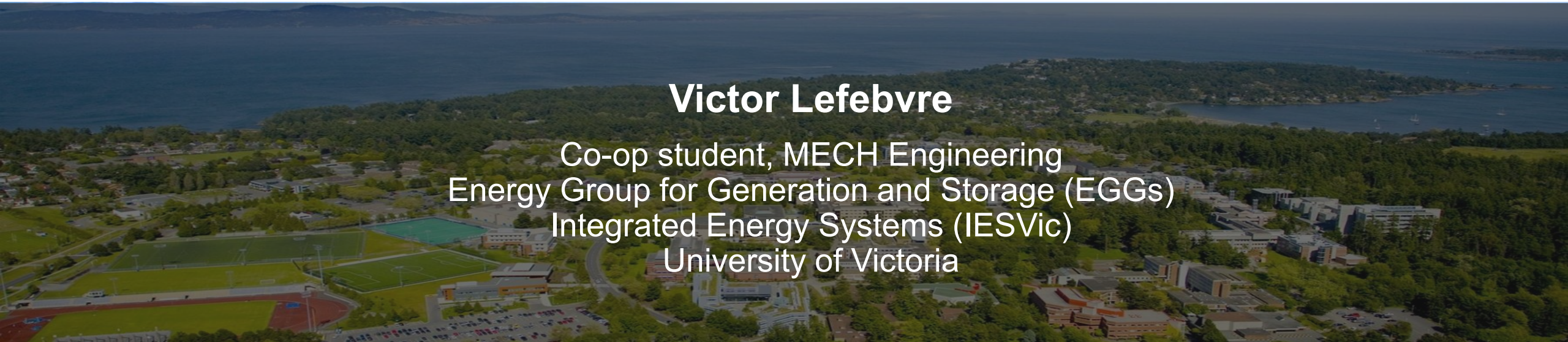
Investigating PTL Defects and MPLs for PEMWE using Stochastic Modelling

EGGs Research Update | August 19th, 2025 | ECS 128



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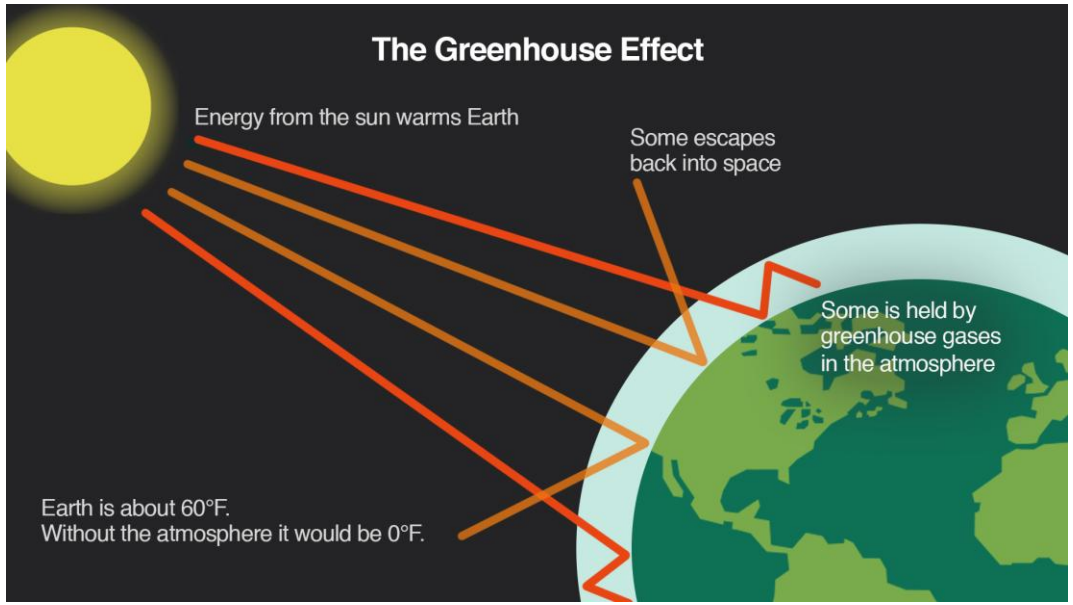
Integrated Energy Systems (IESVic)
University of Victoria

Problem needing a solution: climate change

- Fossil fuels : >75% Global GHG [1]



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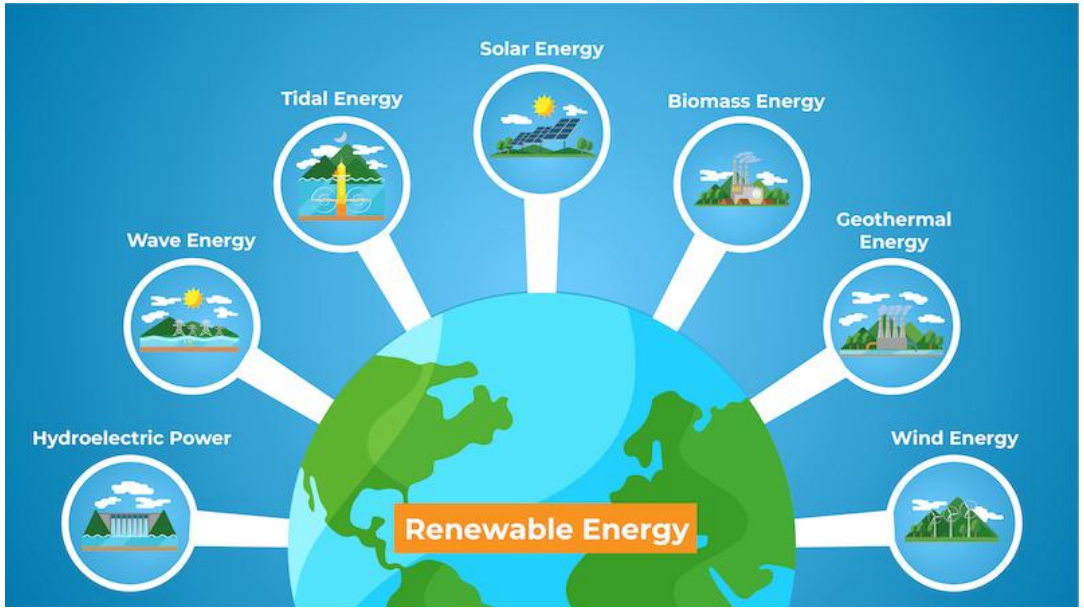
Clean H_2

Clean Energy Challenges: Hydrogen solution

- Multiple suitable replacements; all with their own challenges
  - Unreliability, rare materials, expensive set ups
- Clean hydrogen : manufacturing industry and transport sector [2]
- Proton exchange membrane water electrolyzers: Solution



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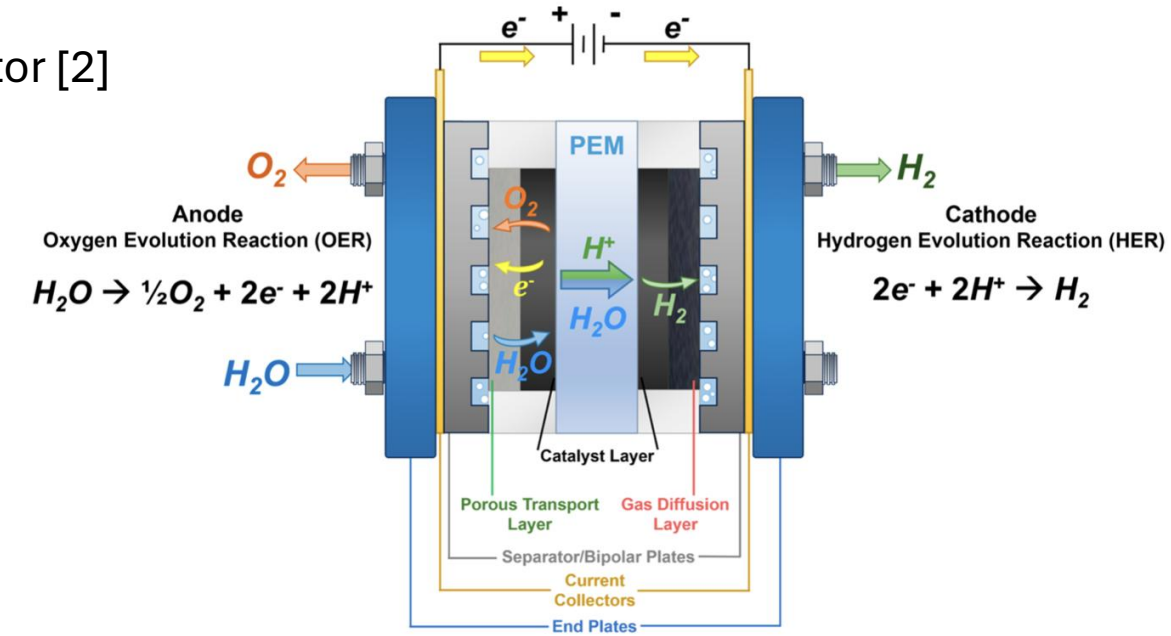


https://pubs.acs.org/doi/pdf/10.1021/acs.chemrev.3c00904?ref=article_openPDF

"In 2023, global hydrogen production emitted 920 Mt CO_2.[...] Between 75% and 95% of these emissions occur directly at the point of production [...] Hydrogen from electrolysers is emissions-free at the point of production"

[https://www.iea.org/reports/global-hydrogen-review-2024/ghg-emissions-of-hydrogen-and-its-derivatives#abstract]

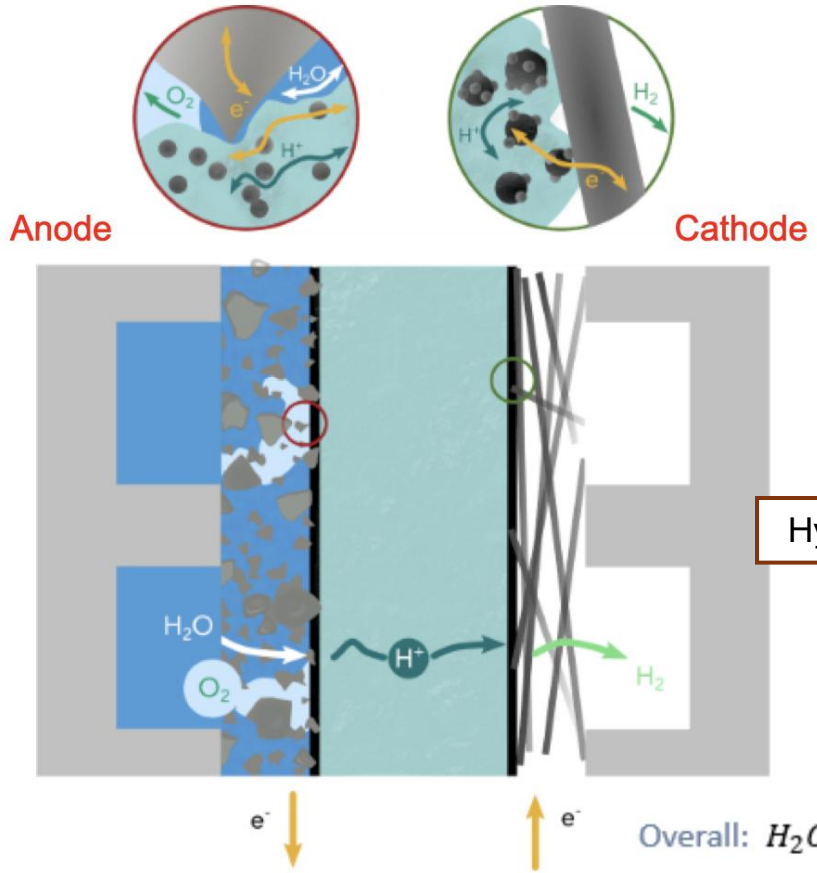
The solution: Proton Exchange Membrane Water Electrolyzers

- Functioning of the cell
- Using renewable energy source results in zero carbon emissions!
- Main issues:
  - Cost of clean hydrogen VS Reforming natural gas
  - Durability of the system under pressure

Research focus for 2 co-ops:

- PTL defects

- MPL



Anode: $H_2O \rightarrow 2H^+ + \frac{1}{2}O_2 + 2e^-$
(OER - Iridium catalyst)

Oxygen Evolution Reaction

Cathode: $2H^+ + 2e^- \rightarrow H_2$
(HER - Platinum catalyst)

Hydrogen Evolution Reaction

Overall: $H_2O \rightarrow H_2 + \frac{1}{2}O_2$

J. K. Lee, Development of Ionomer-free Porous Transport Electrodes or PEM Water Electrolyzers, Canada's Rising Stars in Electrochemical Systems Symposium, April 25, 2024

Porous Transport Layer: function

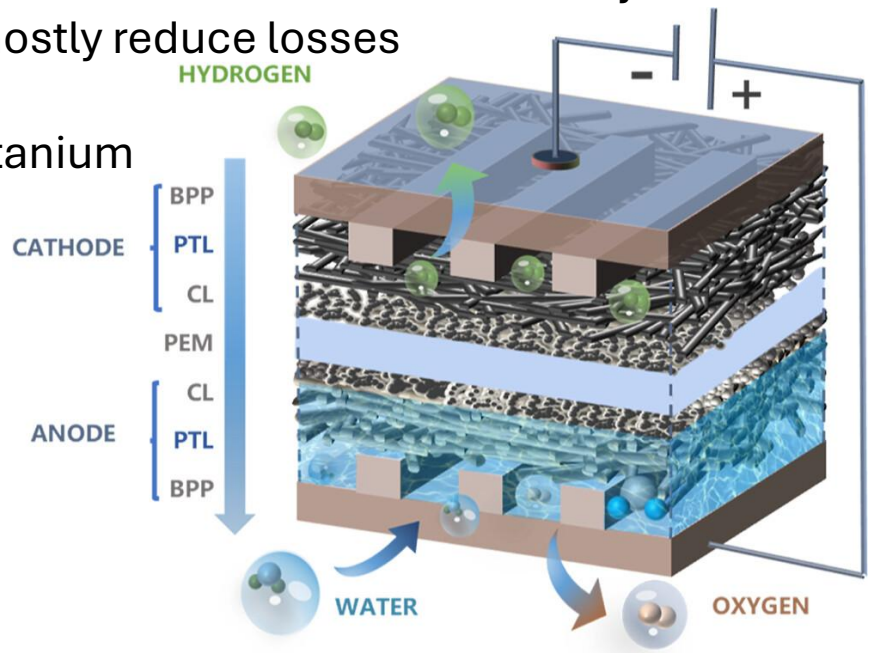
- PTL and GDL

- Role of PTL:
  - Uniformly distribute the reactant (H_2O)
  - Conduct electrons
  - Physically support the CL

Result: Preserve the PEM and better efficiency
but mostly reduce losses

- Material : Titanium

22 47.867
Ti
Titanium



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Presence of defects in PTL…?

- Occur during production

- No research found

- Other industries : common defects

Goal:
Help quantify the effect of those defects on the general efficiency of the fuel cell, but also specific impacts on structural and flow properties and on ohmic and transport losses.

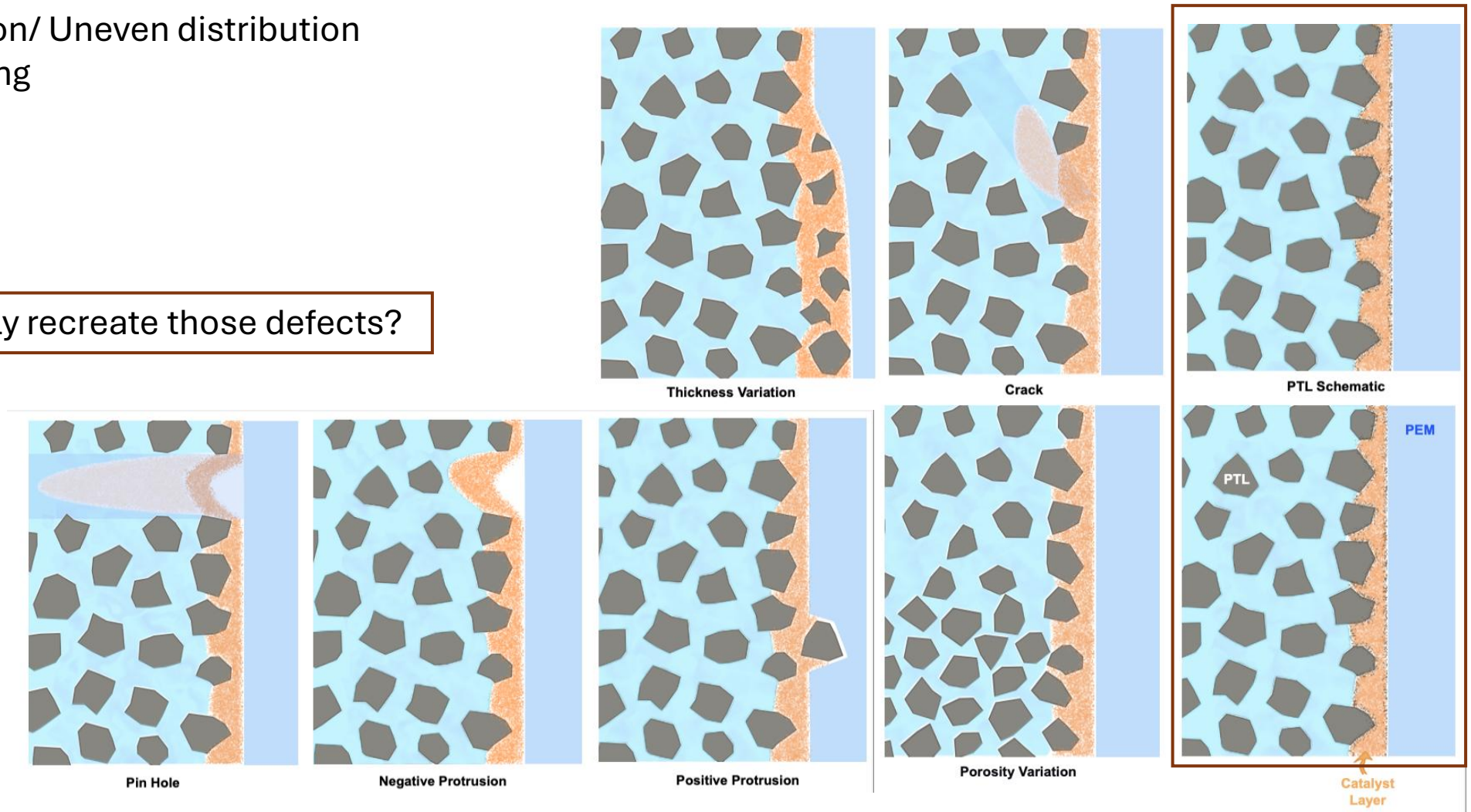
Porous Transport Layer: defects

Potential impacts:

- Delamination of the CL
- Pressure variation/ Uneven distribution
- Water channelling
- Low efficiency
- Low durability

How to purposefully recreate those defects?

Most common defects in other industries
ex. Filtering . [3] [4] [5] [6] [7]



Stochastic method: the first step

Inexpensive!

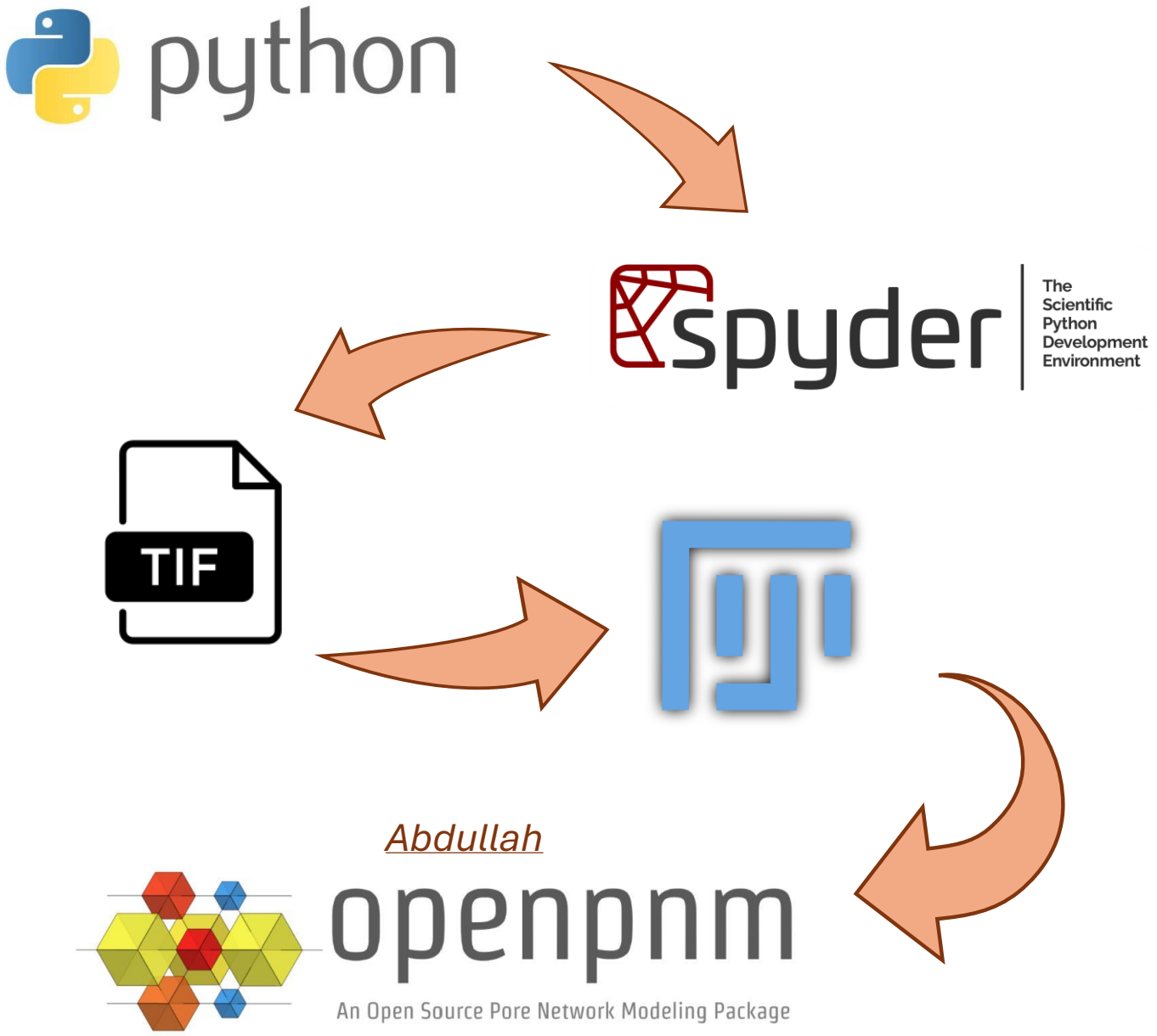
Stochastic modelling:

- Python coding
- Fiji (ImageJ) add/remove defects

Research strategy:

- Generate base PTLs (3)
- All defects onto same base
- Porosity variation
- Thickness variation

Compared to mean values of the bases



Stochastic method: model generation

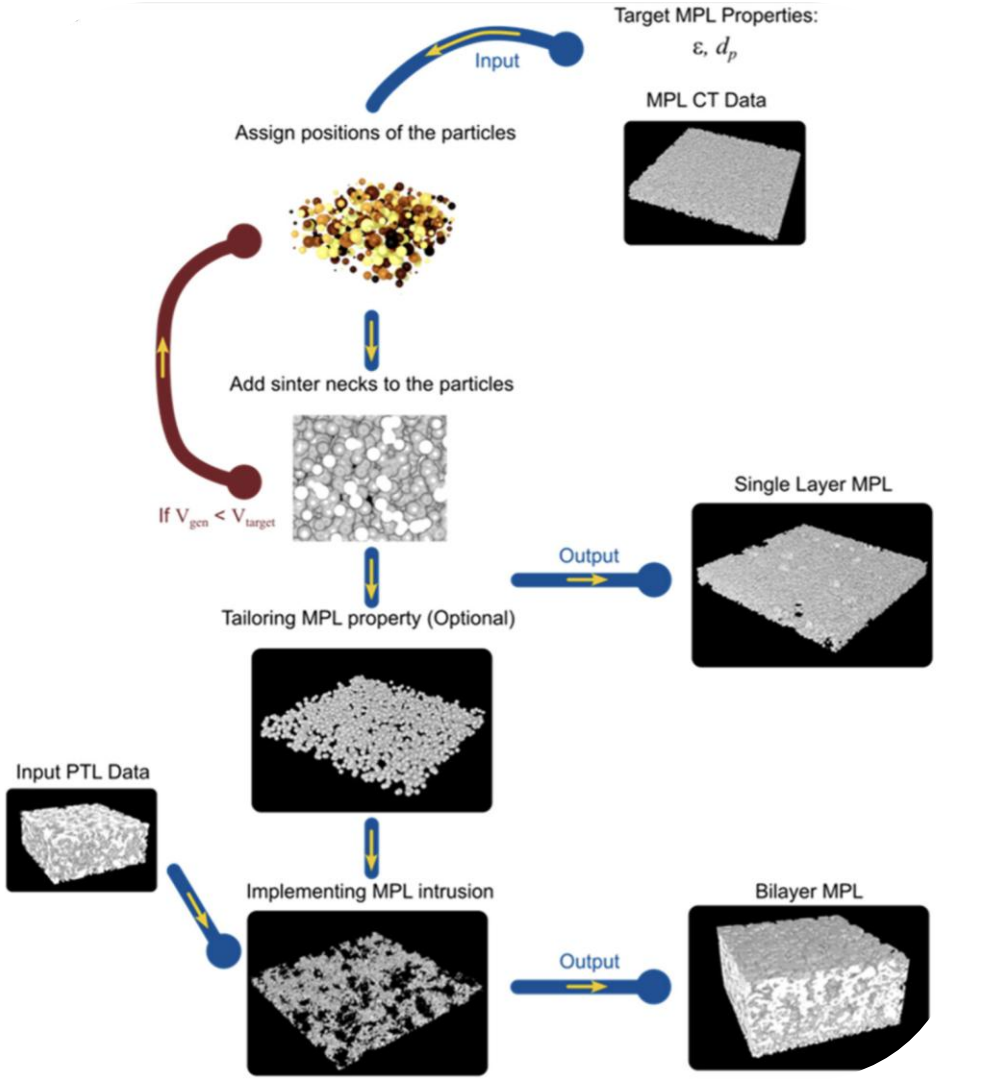
Constant parameters:

- Volume: 1000 x1000 x 250
- Set resolution: 1 voxel/micron
- Powder radius of 12.5 microns with 10% variation

Size : 100MB

Code process:

- Dr. Lee's powder generation code



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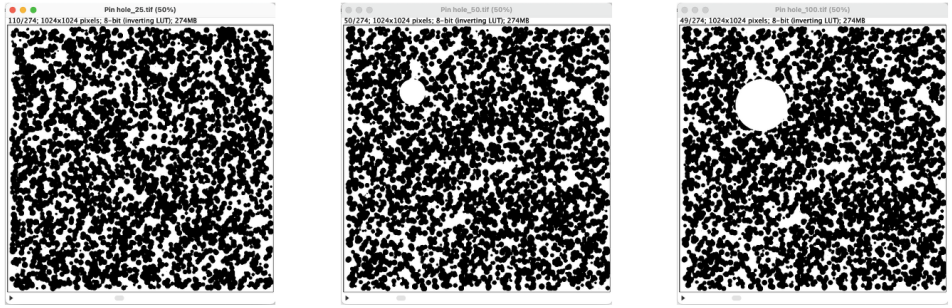
Stochastic method: defects generated

Models	Powder radius (µm)	Radius Variation (%)	Porosity	Thickness (µm)	Width (µm)	Length (µm)
Base 1, 2, 3	12.5	10	0.38	250	1000	1000

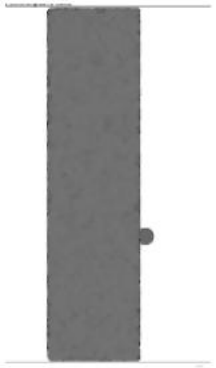
Models	Defect radius (µm)
Protrusion 1	25
Protrusion 2	50
Protrusion 3	100
Negative Protrusion 1	25
Negative Protrusion 2	50
Negative Protrusion 3	100

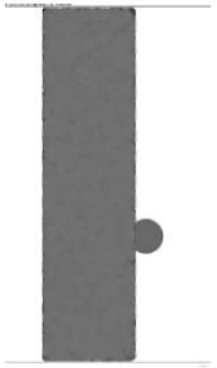
Models	Defect radius (µm)
Crack 1	5
Crack 2	10
Crack 3	25
Pin hole 1	25
Pin hole 2	50
Pin hole 3	100

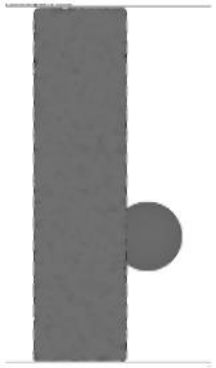
Pin Hole defect



Radius 25 Radius 50 Radius 100





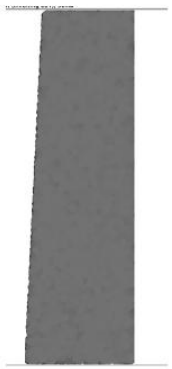


Defects added using Fiji (ImageJ)

Stochastic method: defects generated pt.2

Models	Powder radius (µm)	Radius Variation (%)	Porosity 1	Porosity 2
Porosity Variation 1	12.5	10	0.38	0.60
Porosity Variation 2	12.5	10	0.38	0.19

Models	Powder radius (µm)	Radius Variation (%)	Porosity	Thickness Variation (%)
Thickness Variation 1	12.5	10	0.38	20
Thickness Variation 2	12.5	10	0.38	40
Thickness Variation 3	12.5	10	0.38	60



20%

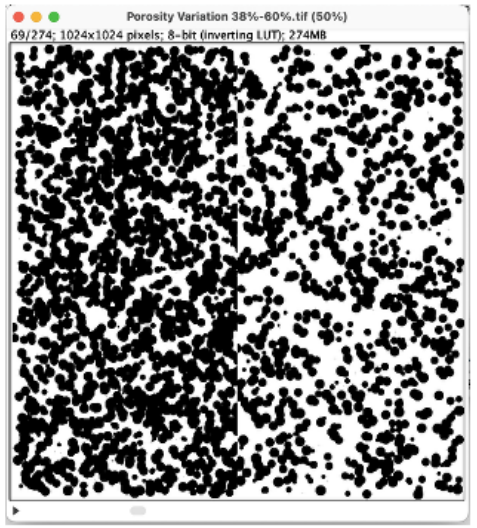
40%

60%

Change in volume ex.:
(powder coordinates)
Y=[0,1000]
X = [0,1000 + Y/20]
Z=[0,250]

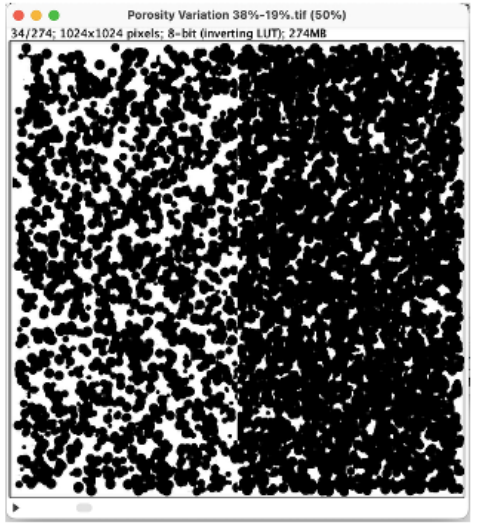
Added together using Fiji (ImageJ)

38%



60%

38%



19%

Models recuperated by Abdullah for PNM

Expanded research: Micro Porous Layers modelling

This semester:
Research

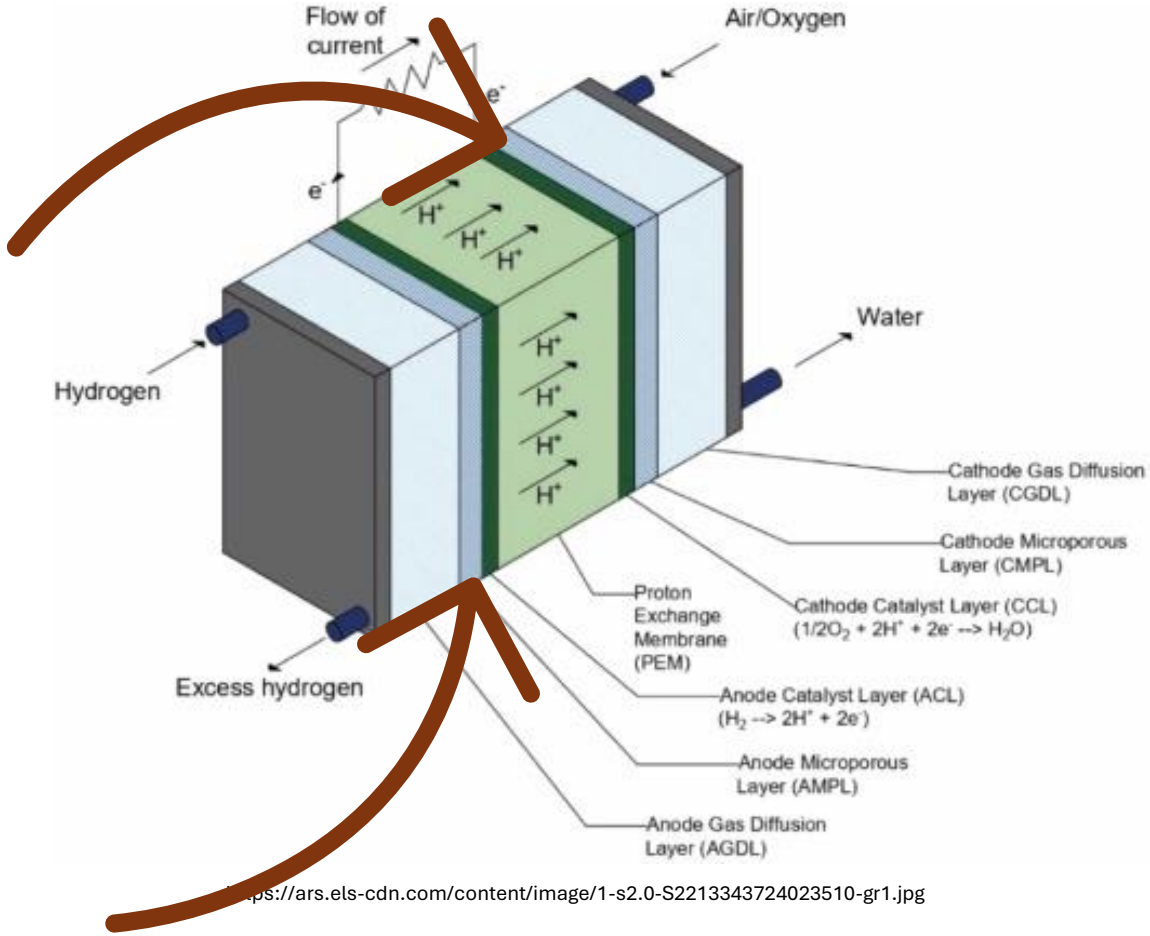
- Function of MPL
  - Improve contact with CL
  - Lower stress on membrane
  - Better pressure distribution

Result:

- Longer lifetime for PEM
- Closer CL particles
- Better electron conductivity

[8] [9] [10] [11] [12]

Using stochastic modelling…



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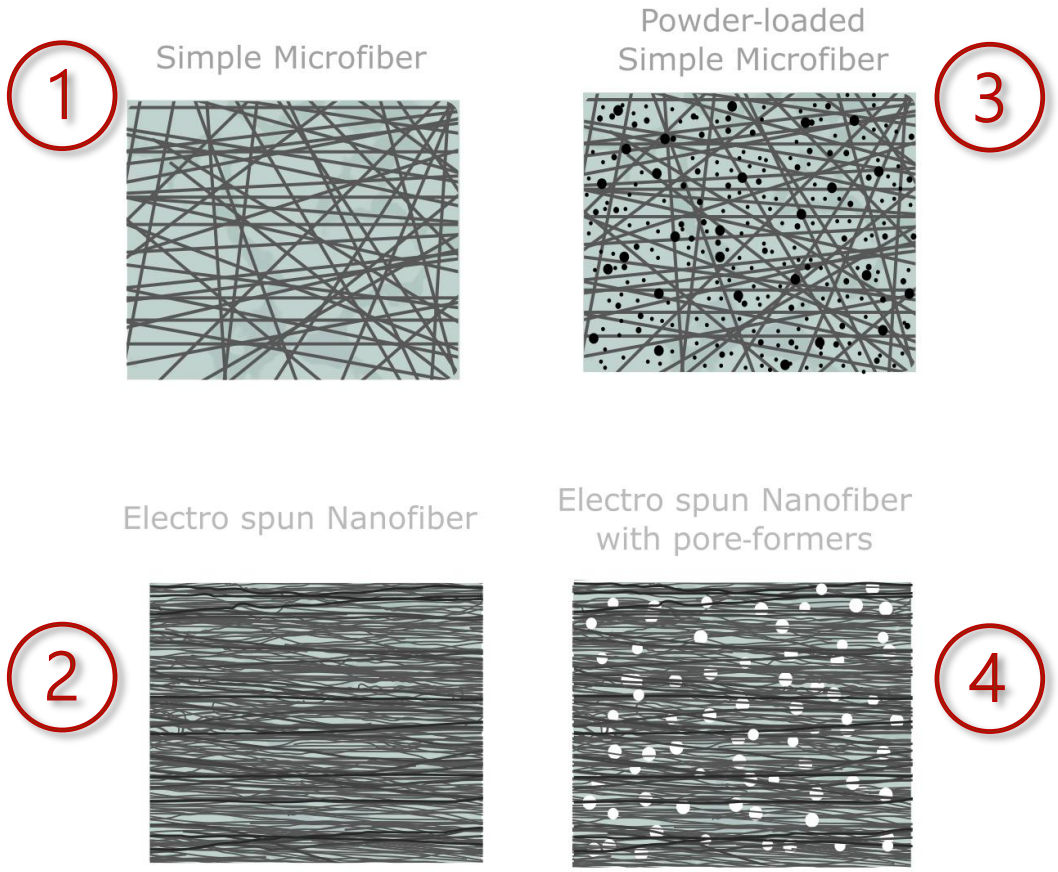
Research have shown that adding an MPL could in fact improve the contact by 50%! [8]

Micro porous Layers: modelling types

4 types of MPL to model:

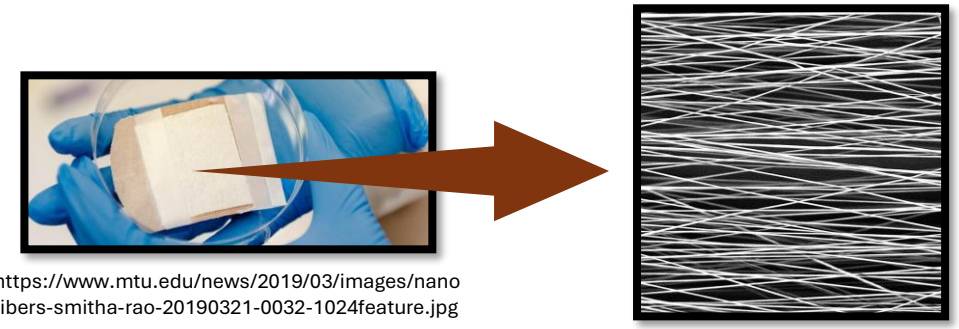
1. Simple microfiber
2. Electrospun nanofiber
3. Powder loaded microfiber
4. Electrospun nanofiber with pore formers



Electrospun VS Simple fiber

Nano size	Micro size
Aligned	All direction
Curvy	Straight

Electrospun fiber for medical use



https://www.mtu.edu/news/2019/03/images/nanofibers-smitha-rao-20190321-0032-1024feature.jpg

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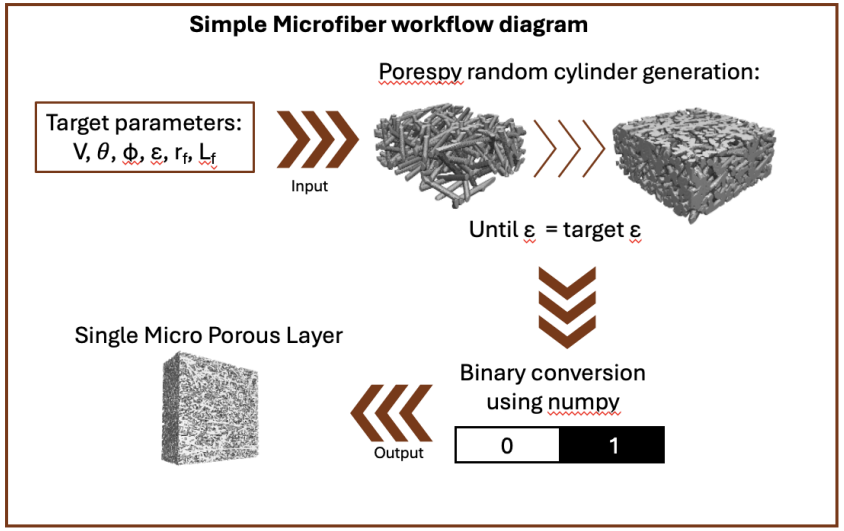
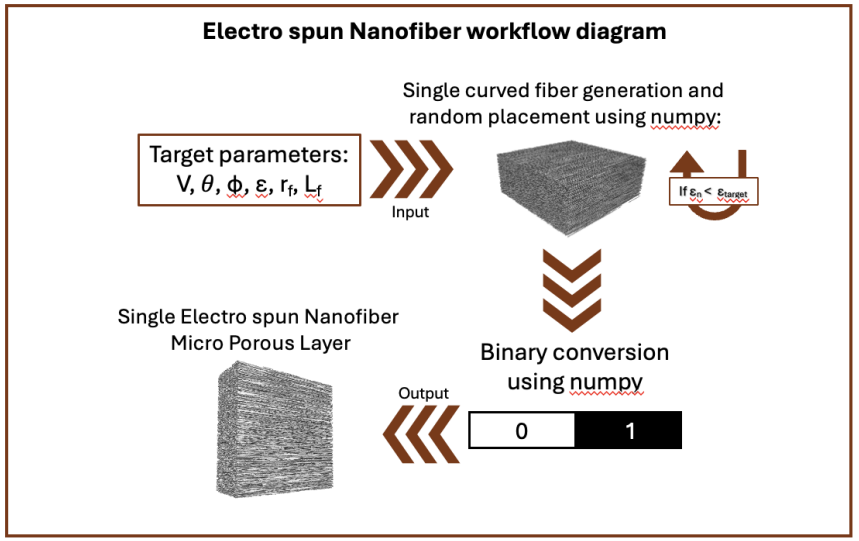
Electrostatic repulsion between surface charges from a viscoelastic fluid [13]

Micro Porous Layers: modelling

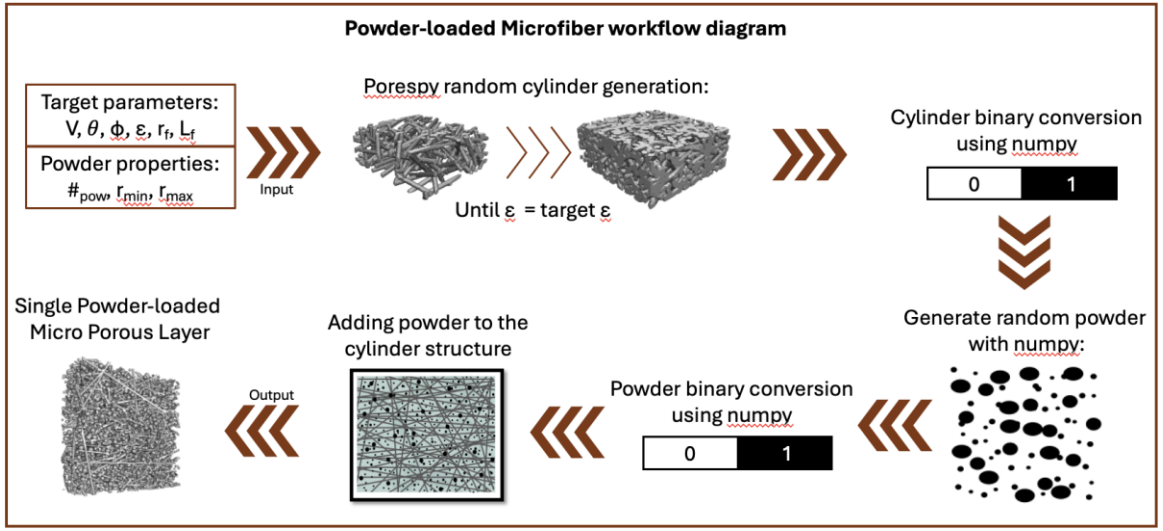
New modelling process:

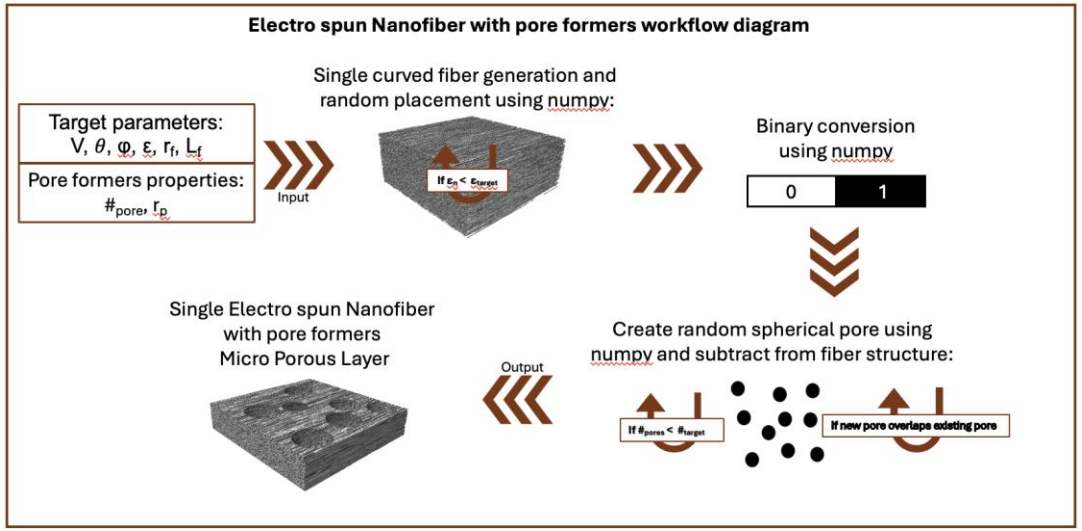
Dr. Lee
PTL work
No more Fiji (ImageJ)





Result: Increase quality and efficiency





Micro Porous Layers: parameters

Models	Fiber radius (μm)	Porosity	In-plan angle (°)	Out-of-plane angle (°)	Fiber length (μm)	Thickness (μm)	Width (μm)	Length (μm)	Pore former radius (μm)	Number of pore formers	Powder radius (μm)	Number of powder
Simple Fiber	2	0.400	89	89	NONE	100	250	250	N/A	N/A	N/A	N/A
Simple Fiber	2	0.800	89	89	NONE	100	250	250	N/A	N/A	N/A	N/A
Simple Fiber	5	0.400	89	89	NONE	100	250	250	N/A	N/A	N/A	N/A
Simple Fiber	5	0.799	89	89	NONE	100	250	250	N/A	N/A	N/A	N/A
Nanofiber	0.500	0.400	15	5	50-150	100	250	250	N/A	N/A	N/A	N/A
Nanofiber	0.500	0.800	15	5	50-150	100	250	250	N/A	N/A	N/A	N/A
Nanofiber	0.750	0.400	15	5	50-150	100	250	250	N/A	N/A	N/A	N/A
Nanofiber	0.750	0.800	15	5	50-150	100	250	250	N/A	N/A	N/A	N/A
Powder-loaded fiber	2	0.400	89	89	NONE	100	250	250	N/A	N/A	2-5	6600
Powder-loaded fiber	2	0.798	89	89	NONE	100	250	250	N/A	N/A	2-5	3500
Powder-loaded fiber	5	0.402	89	89	NONE	100	250	250	N/A	N/A	2-5	6600
Powder-loaded fiber	5	0.797	89	89	NONE	100	250	250	N/A	N/A	2-5	3500

Micro Porous Layers: parameters

Models	Fiber radius (μm)	Porosity	In-plan angle (°)	Out-of-plane angle (°)	Fiber length (μm)	Thickness (μm)	Width (μm)	Length (μm)	Pore former radius (μm)	Number of pore formers	Powder radius (μm)	Number of powder
Nanofiber with Pore-formers	0.500	0.408	15	5	50-150	100	250	250	10	20	N/A	N/A
Nanofiber with Pore-formers	0.500	0.432	15	5	50-150	100	250	250	20	10	N/A	N/A
Nanofiber with Pore-formers	0.500	0.519	15	5	50-150	100	250	250	30	11	N/A	N/A
Nanofiber with Pore-formers	0.750	0.408	15	5	50-150	100	250	250	10	20	N/A	N/A
Nanofiber with Pore-formers	0.750	0.432	15	5	50-150	100	250	250	20	10	N/A	N/A
Nanofiber with Pore-formers	0.750	0.476	15	5	50-150	100	250	250	30	7	N/A	N/A

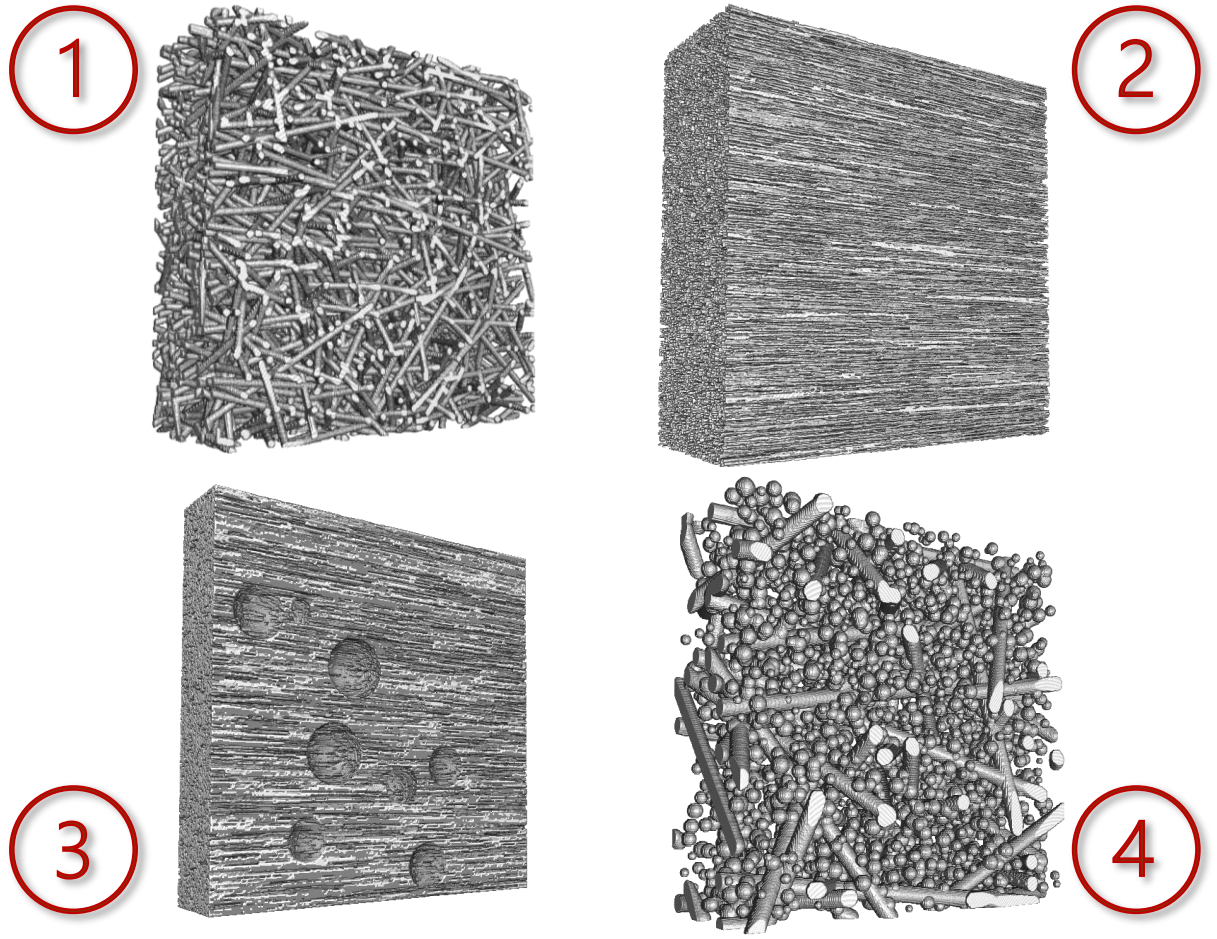
Size issue

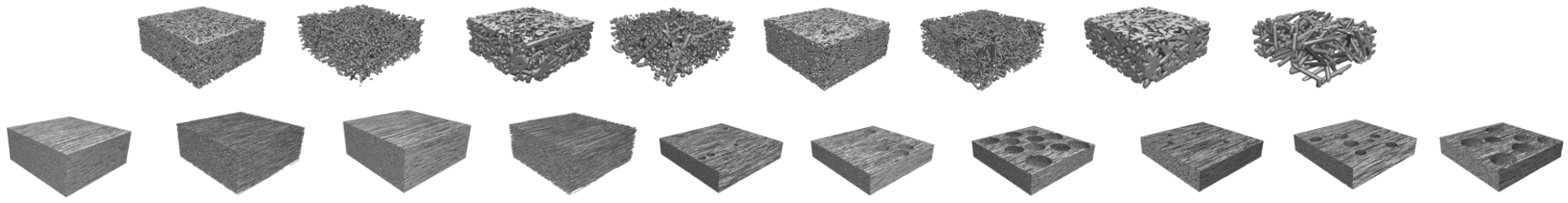
- Resolution of 0.25 :
  - Volume: 1000x1000x400 voxels
  - Actual domain: 250x250x100 microns

Micro Porous Layers: product

4 types:

1. Simple microfiber
2. Electrospun nanofiber
3. Electrospun nanofiber with pore formers
4. Powder loaded microfiber

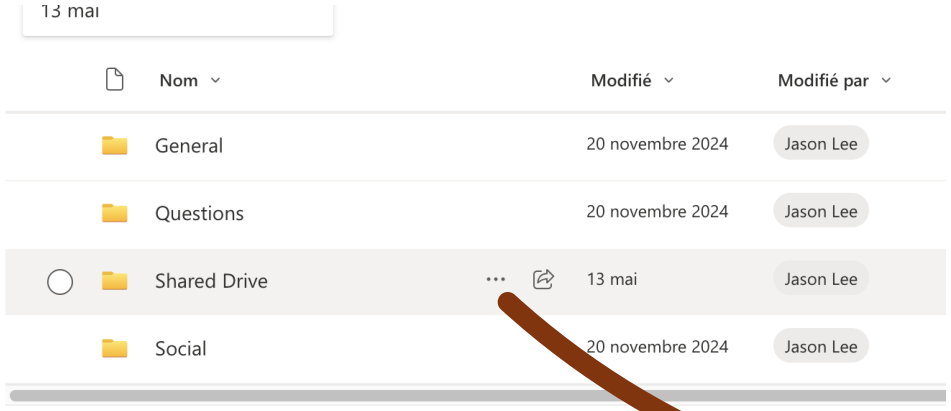


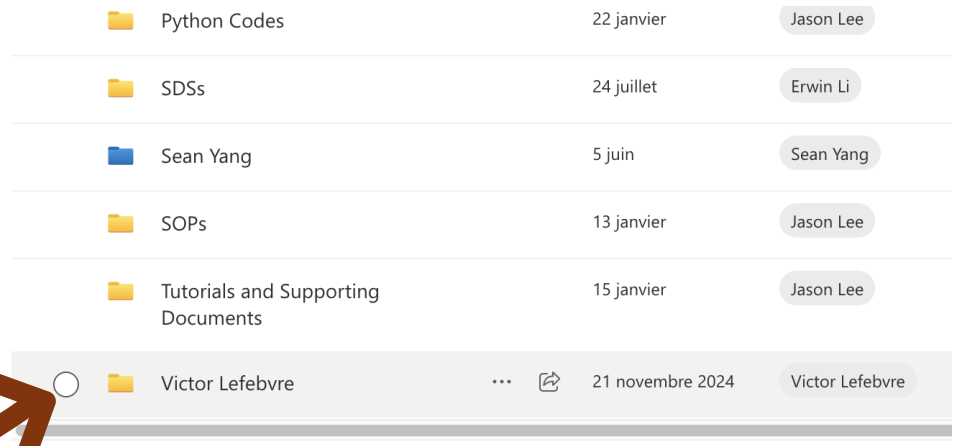


Trail of crumbs: documentation

- Safe operating procedure equivalent
- Individual documentation per code
- Uploaded onto Teams
- Reduce risk/errors and improve efficiency
- Examples: Random generation function; MJ

Table of Content





Summary

- Research porous layers
- Stochastic model
- Process documentation

Thank you!

References

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