Reproducible determination of 3D model and porosity of fuel cell cathode layers from pFIB-SEM data

MCDS Capstone Project Final Report

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Abstract

This project presents a reproducible pipeline for 3D reconstruction and porosity analysis of fuel cell cathode layers using pFIB-SEM image data. Existing approaches rely heavily on manual parameter tuning, which introduces inconsistencies across datasets and limits reproducibility (Ferner et al., 2024a). To overcome the scarcity of labeled data, we also generate synthetic 3D porous structures using Porous Microstructure Analysis (PuMA) (Ferguson et al., 2018) and Blender (Blender Foundation, 2023), allowing us to create diverse training datasets with known ground truth. Our approach improves reproducibility and sets the foundation for future integration with scalable machine learning models and automated analysis of real and synthetic materials.

1 Introduction

Fuel cells are used to convert the chemical energy from a fuel (such as hydrogen) and an oxidant (such as oxygen) into electricity (Appleby, 1990). They are made up of different layers: the Cathode and Anode where the chemical reactions happen, a Gas Diffusion Layer to transport gases, water and electrons and a Polymer Electrolyte Membrane to allow protons to cross while keeping both reactions separate. Throughout this project we will focus on the cathode layer where the oxygen and protons, coming from the anode, come together to form water and electrons. To facilitate the reaction, the material has high surface area. This is done by having a large number of empty areas or pores. In order to improve the efficiency of fuel cells, researchers are interested in studying the microstructure of the layers (Park et al., 2012). This can be done via imaging methods such as pFIB-SEM (Plasma-Focused Ion Beam Scanning Electron Microscopy) as described in the paper by Ferner et al. (2024b).

This capstone project aims to improve on the shortcomings of previous image processing methods by training a machine learning model that infers key volume characteristics from the 2D images of the volume. Since real-world data do not contain ground-truth labels, we will generate our own synthetic data set for training. Therefore, our project contains three main steps: generating a synthetic dataset, training an image processing model, and validating the model pipeline.

2 Hypothesis/Project Goal

Project Goal: The goal of our project is to obtain the porosity and 3D structure of the fuel-cell cathode layer in a reproducible and accurate way.

Constructive: It is possible to generate a synthetic 3D model with known porosity and pore size distribution.
Evaluation Method: We will compare the metrics of the 3D model with desired metrics. Specifically, porosity can be measured by calculating the ratio of pore voxels to the total voxels.

Formative: Compared to traditional methods, which can change the porosity result by up to 10% with small adjustments, our proposed pipeline should be much more stable.
Evaluation Method: We will vary the parameters during processing and compare the amount of fluctuation of the porosity measurements. We aim to keep the variation in measurements below a certain threshold (e.g. 5%), showing that our approach is less sensitive to parameter changes.

Empirical: The proposed solution will significantly outperform the SOA baseline in both accuracy and efficiency.
Evaluation Method: We will compare our system with existing methods looking at both the accuracy of the porosity predictions and the time it takes to process each image. Our goal is to

achieve a noticeable reduction in prediction errors (around 15–20% improvement) and faster processing times without sacrificing accuracy.

3 Relationship to Prior Work

Our project builds directly on the imaging and segmentation techniques introduced by Ferner et al. (2024a). They developed a method that used high-resolution pFIB-SEM to create 3D images of fuel cell catalyst layers and performed porosity analysis through grayscale thresholding. Specifically, after the streak artifacts were removed and the image data were pre-processed, they used intensity thresholding to separate the pore space from the solid material. After processing and cleaning all slices, the binary results were combined into a full 3D volume. Although their method is powerful, the results are highly sensitive to input parameters that were selected manually, which can lead to inconsistencies when applied across different datasets.

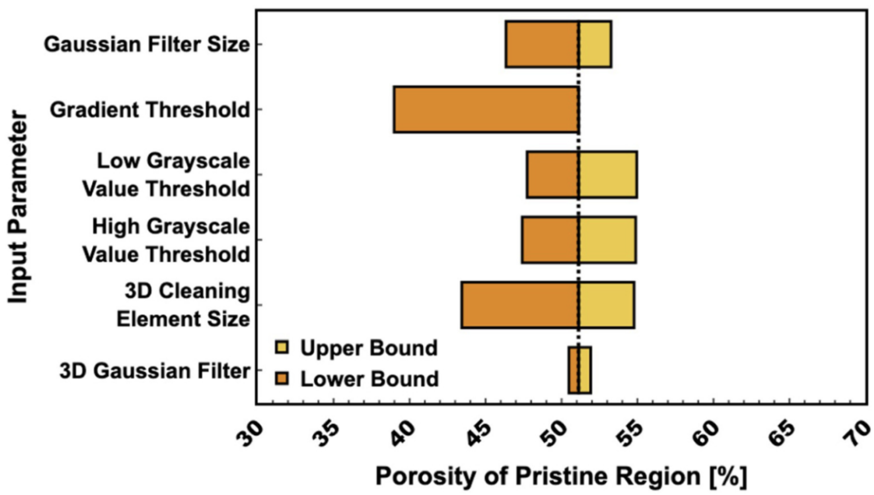

Figure 1: Small changes in processing parameters can significantly affect porosity results (Ferner et al., 2024a)

Therefore, to develop a more reproducible method for analyzing the porosity and pore size distribution in the material, we propose a new hybrid approach that combines synthetic data generation using customizable porosity and pore geometry, with machine learning models trained for accurate 3D reconstruction and porosity estimation. By introducing a fully modular and extensible pipeline, our system advances reproducible image-based material characterization and addresses key limitations of previous methods, including parameter sensitivity, lack of scalability, and limited reproducibility.

4 Fall Semester Development Goals

At the beginning of the semester, our primary milestones focused on creating a reliable synthetic dataset and developing a full reconstruction pipeline. Specifically, we aimed to:

- Generate synthetic 3D structures in PuMA software (Ferguson et al., 2018) with known porosity and pore size distributions
- Convert these structures into 2D slices with realistic illumination using Blender (Blender Foundation, 2023)
- Develop and train a segmentation model (Step 1) capable of producing accurate 2D masks from the slices with perspective and lighting.
- Develop and train a reconstruction model (Step 2) to transform the 3D mask volume into a mesh representation and calculate the 3D porosity.

Most of these goals were met. We successfully produced synthetic image data, implemented multiple cropping strategies, and completed both Step 1 (2D segmentation using cross-entropy loss) and Step 2 (3D volume reconstruction with cross-entropy and smoothness constraints). The only partially unmet goal was further refining the realism and variability of the synthetic lighting pipeline, which required additional iteration and is discussed in later sections. Overall, the major technical components of the pipeline were developed as planned and validated against the initial expectations.

5 Project Requirements

5.1 Intended Users

Our project targets multiple user groups who will benefit from the proposed pFIB-SEM-based computer vision pipeline for analyzing fuel cell cathode layers. Each group interacts with the system in distinct ways:

Fuel Cell Researchers and Scientists These users aim to study the microstructure of cathode layers to understand performance drivers like porosity and pore distribution. Currently, they rely on manual or parameter-sensitive methods that often yield inconsistent results. Our system will provide a robust and reproducible method for generating 3D reconstructions from pFIB-SEM data, enabling researchers to compare samples or studies with minimal tuning.

Machine Learning Researchers and Developers This group focuses on developing computational tools for analyzing pFIB-SEM data. Our synthetic dataset generator and model pipeline offer a modular machine learning pipeline for benchmarking segmentation and 3D reconstruction algorithms. It also serves as a reference framework for future improvements and experimentation.

Fuel Cell Manufacturers This group benefits from downstream information enabled by better material characterization. Over time, they can indirectly use the system for quality control in manufacturing through standardized porosity analysis.

5.2 Functional Requirements

The system delivers a robust pipeline that transforms raw pFIB-SEM image data into a reliable 3D model of fuel cell cathode layers with accurate porosity estimation. The primary functionalities include:

Image Correction The pipeline starts when users upload raw 2D/3D images or a stack of slices. The system detects tilt and uneven background illumination, then applies cropping and alignment to isolate the Region of Interest (ROI). The corrected image is saved and passed to the preprocessing module.

Data Preprocessing Corrected images undergo noise filtering (e.g., Gaussian or median filters) followed by intensity normalization to ensure consistent pixel value ranges. These steps prepare the data for classification.

Void and Solid Classification Each slice is analyzed using intensity-based thresholding, with Otsu's method (Otsu, 1979) as the default. Pixels are classified as "void" (pore) or "solid." The resulting binary images are used for 3D reconstruction.

Synthetic Data Generation Users provide parameters such as desired porosity and size distribution. A 3D synthetic structure with labeled regions is generated and added to the training dataset to improve model robustness.

Deep Learning-Based Computer Vision Pipeline This pipeline trains or loads a model to analyze real or synthetic data. It handles feature extraction, porosity estimation, and visual output generation (e.g., porosity maps, pore size histograms).

5.3 Non-Functional Requirements

Tolerance to Parameter Variations Porosity estimation should remain within $\pm 5\%$ when preprocessing parameters are varied.

Data Handling Capacity The system must support high-resolution, large datasets without memory overflow or crashes.

Reliability and Reproducibility The same input configuration must yield consistent outputs.

Extensibility and Modularity Components such as the synthetic data generator, thresholding classifier, and model trainer should be replaceable or upgradable independently.

Transparency All operations, parameters, and intermediate outputs should be timestamped and logged for traceability.

5.4 Resource Requirements

Data Requirements

- **pFIB-SEM Image Data:** High-resolution images from real fuel cell cathode samples for testing and validation.
- **Synthetic Data:** Generated 3D datasets with known porosity and structure, used for training and benchmarking.
- **Ground Truth Annotations:** Porosity labels from manual or computer vision-based methods.

Software Requirements

- **Fiji (ImageJ):** For visualization, preprocessing, and reslicing of pFIB-SEM images.

Human Resources

- **Data Annotator:** Personnel may be needed for manual validation of segmentation outputs.

6 Experiment/System Design Overview

The system is built on two main elements:

- **Image Processing Module** The image processing module is able to process incoming images from pFIB-SEM data and reconstruct the porous material in 3D. It consists of two main steps: image segmentation and 3D reconstruction.

- **Synthetic Data Generator** In order to train the Image Processing Module, it was necessary to generate our own synthetic data due to limited real data and the absence of ground truth. The Synthetic Data Generator made it possible to generate our own synthetic dataset.

6.1 Image Processing Module

The Image Processing Module is able to process raw pFIB-SEM data and reconstruct the 3D material. It is split up into two main models: image segmentation and 3D reconstruction.

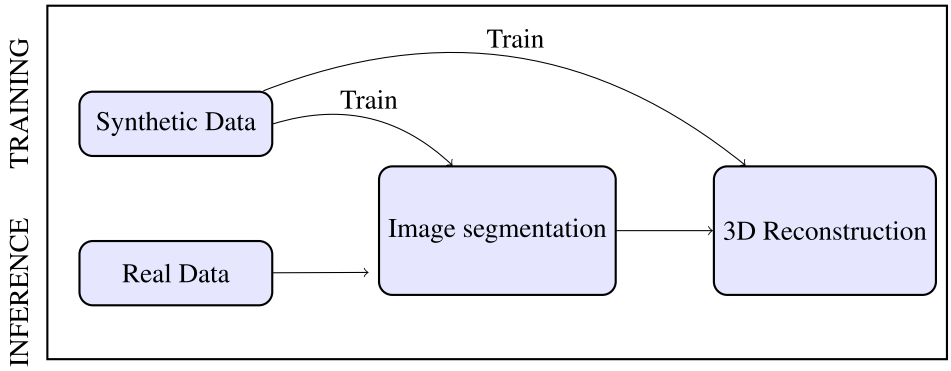

Figure 2: Dataflow diagram of the system

- **Image segmentation:** Image segmentation takes a raw image and outputs a binary mask that indicates pores from the material.

  Indeed, the pFIB-SEM technology works by carving away material and taking snapshots at regular intervals. Thus, due to the high porosity of the material studies, the images have areas of shadows, extra material can be seen through the pores and the perspective matters. This steps creates a mask to analyze the slice and determine what is pore/material.

  The Image Segmentation model is built using a 2D Unet. The input is a raw image and the output is a binary mask. It is trained using our own Synthetic Dataset.

- **3D Reconstruction:** After each individual slice from the input data has been processed by the Image Segmentation step, we rely on 3D Reconstruction to output a 3D structure.

6.2 Synthetic Data Generation Module

Since we are lacking ground truth 3D reconstruction on existing datasets, we have generated our custom synthetic data. We created 3D porous structures using the Porous Microstructure Analysis software (PuMA) (Ferguson et al., 2018). It made it possible to generate quickly a large amount of realistic porous materials. The parameters were adjusted to mimic real materials. The rendering of the images was done using the 3D software Blender (Blender Foundation, 2023). Blender is open-source software that allows us to realistically render 3D volumes. This made it possible to add lighting and creating realistic shadows. It was also possible to adjust the camera to obtain a similar angle to real data. Additionally, we are leveraging Blender API (Blender Foundation, 2023) with a Python script to slice these 3D models and take an image of each slice similar to how real SEM images are made. This allows us to quickly generate a large amount of synthetic data.

7 Experimental Design

7.1 Dataset

- **Real-World pFIB-SEM Data:** We have 3 small but high-value datasets from costly real-world material experiments. However, we do not have the exact ground truth values for porosity or pore size distribution. We only have an approximate estimate based on the paper described by Ferner et al. (2024a). Specifically, these files include:
  - **Pristine** Layer coated on plastic. So this is the catalyst layer exactly as it is, with no mechanical or chemical stress.
  - **Un-compressed Full** Layer coated on Nafion. It doesn't have any pressing.
  - **Compressed Full** Layer coated on and pressed onto Nafion. This version has been mechanically squeezed to improve contact and density. So its similar to the conditions inside an actual fuel-cell stack. This is close to what industry uses.

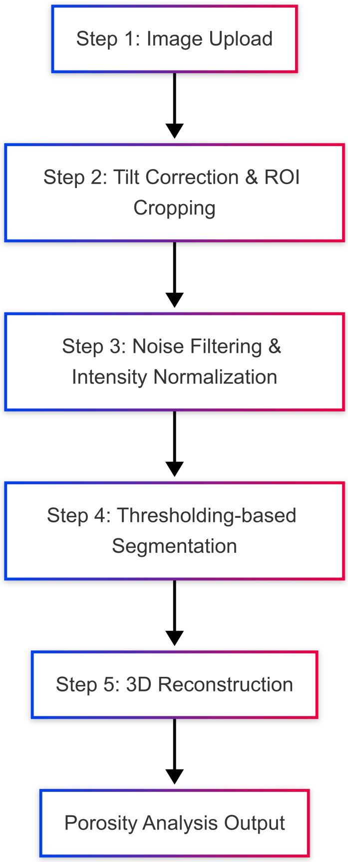

Figure 3: This flowchart shows the full pipeline we used to create our synthetic dataset, designed to match the target porosity and pore size distribution. Specifically, the Image Processing Pipeline Model section covers Steps 1–4, while the Synthetic Data Generation Module includes Steps 5–6. With these steps completed, we can train our model on a more varied and representative dataset.

Note: Since data collection method is destructive, each stack came from a separate batch and shows different structures.

- **Synthetic Blender Data:** These data are generated by slicing 3D porous objects in Blender (Blender Foundation, 2023), where pore structures and distributions are parameterized. We expect that the true pore-size distribution follows a log-normal fit as described by Ferner et al. (2024a). Since these synthetic data sets will have a known 'ground truth' (or at least a close approximation), they are crucial to measuring accuracy and validating porosity calculations.

7.2 Machine Learning Models/Algorithms/Pipeline

Our system uses a two-stage machine learning pipeline to reliably estimate porosity and reconstruct the 3D structure of fuel-cell cathode layers from pFIB-SEM imagery. We designed the pipeline to be modular on purpose—each stage can be refined or swapped out as we collect more real data, making the entire workflow flexible, extensible, and easy to improve over time.

Step 1: 2D Slice Segmentation Model The first stage uses a U-Net–based convolutional neural network (Ronneberger et al., 2015) to segment individual 2D slices into pore and solid regions. We selected U-Net (Ronneberger et al., 2015) due to its strong performance on biomedical and materials imaging tasks where fine-grained spatial localization is required. The model takes our lightened synthetic slices as input and learns to segment them using a cross-entropy loss, with an optional Dice term to help balance the uneven distribution between pore and solid regions.

Step 2: 3D Reconstruction Model In the second stage, we stack the 2D segmentation outputs into a 3D voxel grid and let the model refine this volume into a clean, consistent binary structure. The reconstruction network is a 3D U-Net (Özgün Çiçek et al., 2016) that learns how pores and solids should connect across slices, smoothing out noise and enforcing realistic continuity in the material.

Machine Learning Pipeline We first segment each slice in 2D and then reconstruct the full volume in 3D. The 2D model is lightweight and easy to train on large amounts of synthetic data, while the 3D model enforces the global structure that single slices cannot capture. This workflow mirrors how pFIB-SEM data are collected and remains easy to interpret. Because real data lack full ground truth, we rely primarily on PuMA (Ferguson et al., 2018) and Blender-generated (Blender Foundation, 2023) synthetic data to run controlled experiments on porosity and pore-size distributions.

7.3 Evaluation Metrics

We evaluate our system using metrics that capture both segmentation quality and 3D reconstruction accuracy. Because real pFIB-SEM data lack exact ground truth, quantitative benchmarking relies on synthetic datasets, while real data are used for qualitative checks.

Pixel-Level Metrics

- **Cross-Entropy Loss:** Measures pixel-wise classification error.
- **IoU:** Computed for both pore and solid classes to evaluate segmentation quality under class imbalance.

- **Dice Score:** Captures structural overlap between prediction and ground truth and also acts as an optional regularizer during training.

Volumetric Metrics

- **3D IoU:** Overlap between predicted and ground-truth voxel volumes.
- **Smoothness:** A Laplacian-based measure of slice-to-slice consistency.

8 Test Design

Our testing strategy evaluates the system at three levels: slice-level segmentation, 3D reconstruction quality, and material-property estimation. To ensure reproducibility and isolate failure modes, we designed controlled experiments on synthetic data and qualitative comparisons on real data.

Step 1 Testing: 2D Segmentation We evaluate the 2D U-Net (Ronneberger et al., 2015) using a standard train/validation/test split of synthetic slices generated from PuMA structures (Ferguson et al., 2018). After training, we measure performance on held-out slices using IoU, Dice score, and pixel accuracy.

Step 2 Testing: 3D Reconstruction For the 3D U-Net model (Özgün Çiçek et al., 2016), we first generate synthetic ground-truth volumes with known porosity and pore-size distributions. We then compare the reconstructed predictions against these volumes using 3D IoU and smoothness metrics. Testing includes ablation evaluation—e.g., removing the smoothness term—to understand the contribution of each architectural component.

End-to-End Pipeline Testing We also evaluate the full system by taking synthetic 3D volumes, slicing and lightening them in Blender (Blender Foundation, 2023), running segmentation with Step 1, and reconstructing them with Step 2. This lets us check how well the pipeline handles error accumulation across stages. For real pFIB-SEM data, we compare the predicted porosity with literature estimates (Ferner et al., 2024a) and verify that the results stay stable when we slightly vary preprocessing parameters.

9 Deployment Model

- **Code Repository:** We will host all source code in a version-controlled GitHub repository. This repository includes scripts for data preprocessing, image segmentation, 3D reconstruction, and porosity calculation.
- **Environment Configuration:** To ensure consistency between different systems, we provide a `requirements.txt` file listing all versions of the Python library.
- **Containerization:** When we are in the stage of developing a machine learning model, we will try to containerize the entire pipeline using Docker. This approach packages dependencies, libraries, and tools together to prevent version conflicts.
- **Documentation and Examples:** We will also include detailed usage instructions and example datasets to be provided in the repository. The step-by-step documentation guides users through installing dependencies, running basic tests, and processing input data from the sample.

In general, we believe that this deployment strategy will make our pipeline easy to adapt and reproduce.

10 Risks/Challenges

- **Synthetic–Real Gap** Our synthetic Blender (Blender Foundation, 2023) datasets may not perfectly mimic real cathode layers. Even if they approximate a log-normal distribution of pore sizes, variations in actual samples (e.g., unexpected artifacts) can affect the accuracy of the pipeline.
- **Lack of Exact Ground Truth** We do not have definitive pore size or porosity values for the real pFIB-SEM data. Hence, verifying the performance of the pipeline is based on approximations or indirect comparisons from the literature, which can introduce uncertainty.
- **High Computational Costs** Handling large 3D volumes with iterative segmentation, reconstruction, and machine learning can be resource intensive. This could limit the number of experiments or hyperparameter searches we can run.

11 Tools and Dependencies

We rely on a focused set of Python libraries to manage and process our data: `os` for basic file operations, `numpy` for array handling and `tifffile` for reading image stacks. We use `scipy.ndimage` and `skimage.morphology` to filter images and perform various morphological operations, while `matplotlib` helps us visualize results clearly. Furthermore, we generate synthetic pore structures with Blender (Blender Foundation, 2023), and Git serves as our version control platform, keeping the work of our team organized and consistent. Together, these tools provide a straightforward yet powerful environment for data manipulation, image analysis, and collaborative development.

12 Results

We evaluate our system across four experimental conditions: (1) the realism and statistical correctness of the synthetic data; (2) the segmentation model's performance using CE loss, Dice score, IoU, and pixel accuracy; (3) the reconstruction model's ability to recover consistent 3D structure; (4) how closely the predicted porosity and pore-size distribution match the synthetic ground truth; and (5) how stable the entire pipeline is when synthetic or real data pass through both stages end-to-end. In the subsections below, we summarize the key experimental results obtained at the current stage of the project.

12.1 Synthetic Pore-Size Distribution

To validate the realism of our PuMA-generated (Ferguson et al., 2018) structures, we compare their pore-size histogram against a log-normal fit. Figure 4 shows the resulting distribution.

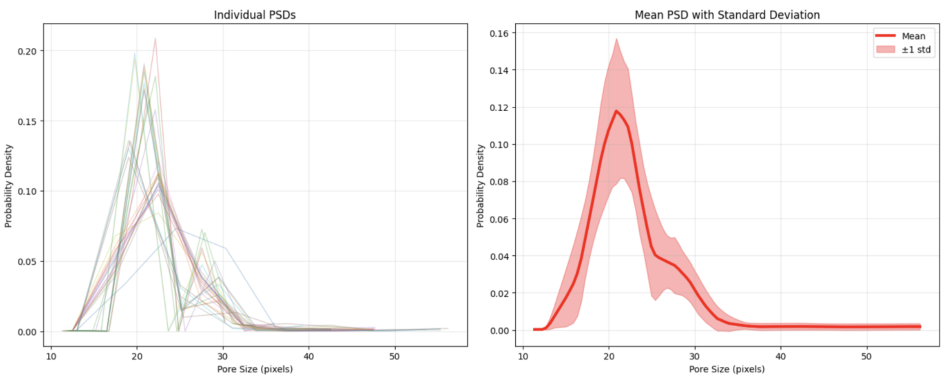

Figure 4: Synthetic pore-size distribution. X-axis: pore diameter (nm). Y-axis: normalized frequency. The distribution closely follows a log-normal curve, consistent with reported fuel-cell cathode measurements.

The strong alignment with a log-normal trend indicates that our synthetic samples capture realistic pore statistics and are appropriate for training and evaluation.

12.2 Synthetic and Lightened Slices

Figures 5 and 6 illustrate how we transform clean 2D mask slices into visually realistic inputs using Blender (Blender Foundation, 2023).

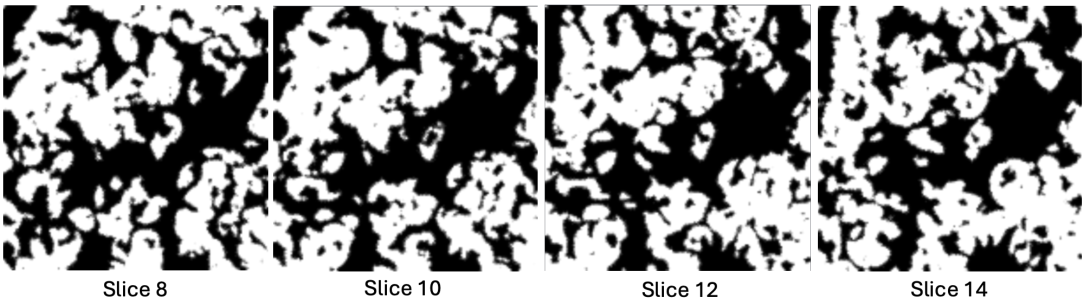

Figure 5: Raw synthetic mask slices extracted along the Z-axis of the PuMA volume(Ferguson et al., 2018). Each slice is a clean binary representation of pores (black) and solid material (white). These masks act as the ground-truth labels during training and are not used as input images.

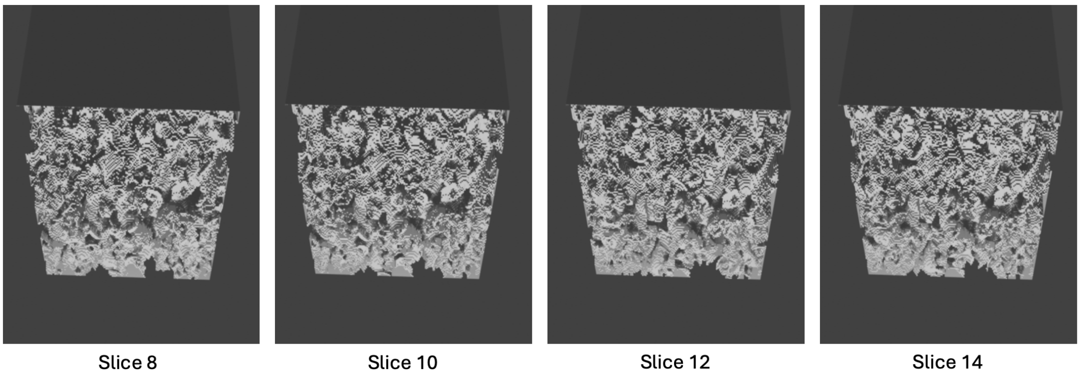

Figure 6: Blender-rendered slices (Blender Foundation, 2023). Instead of 2D masks, Blender renders the full 3D porous structure using a camera tilted at approximately 52°, matching the acquisition angle reported in the original pFIB-SEM workflow. This produces realistic SEM-style shading, depth cues, and surface noise. Although these images correspond to the same Z-locations as the masks above, the 3D lighting and viewing geometry make them appear volumetric rather than flat. These lightened renders are used as model inputs.

System behavior: The Blender (Blender Foundation, 2023) rendering step intentionally introduces shadows, gradients, and textural noise that mimic pFIB-SEM artifacts. Because these images come from a 3D render rather than a flat mask, they appear volumetric and textured, improving model robustness by forcing the network to handle non-uniform illumination and realistic surface variation.

12.3 Segmentation Results

Our 2D U-Net (Ronneberger et al., 2015) achieves strong segmentation quality, reaching a validation pixel accuracy of **93.14 %** and a foreground IoU of **90.49 %** by Epoch 180. The model converges smoothly, with the training loss decreasing to **0.0368**. The corresponding training and validation curves are shown in Figure 7.

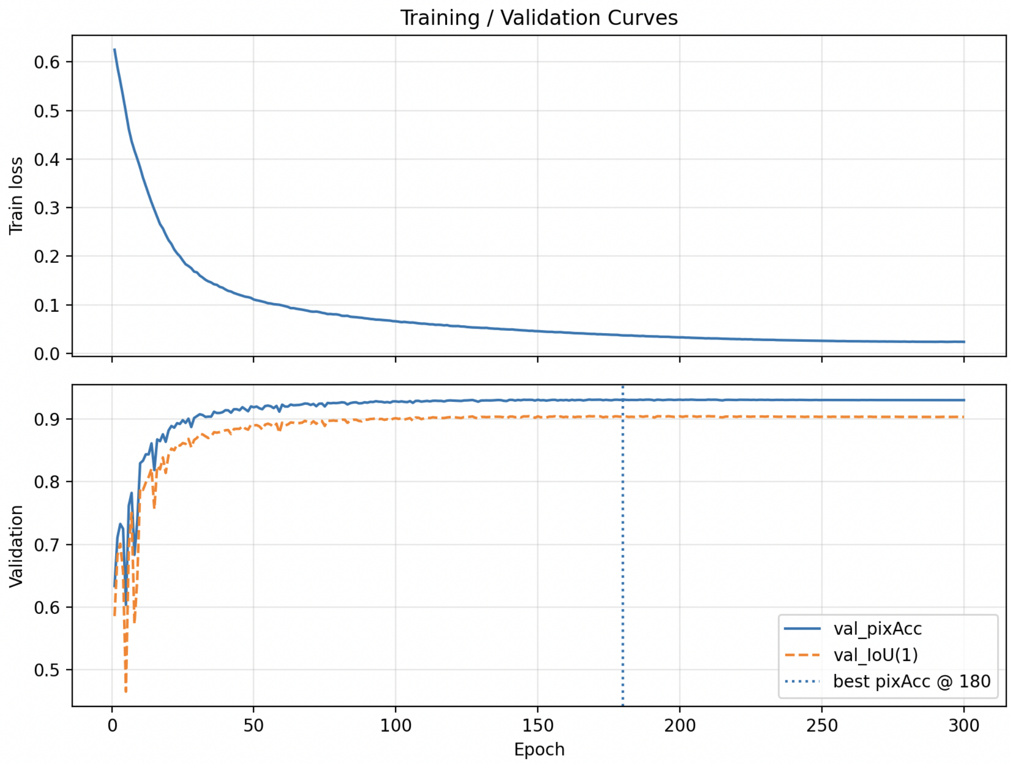

Figure 7: Training and validation loss curves.

These results suggest that the model can reliably separate pore and solid regions, even when the input slices include challenging lighting variations. Figure 8 shows a representative comparison between the model prediction and the ground-truth mask.

System behavior: Models trained with combined CE+Dice loss consistently outperform CE-only, particularly on thin, high-curvature pore boundaries where pixel imbalance makes CE unstable. Dice regularization improves region cohesion, reduces boundary fragmentation, and yields higher IoU scores.

13 Error Analysis

Across experiments, we observed three consistent patterns of errors.

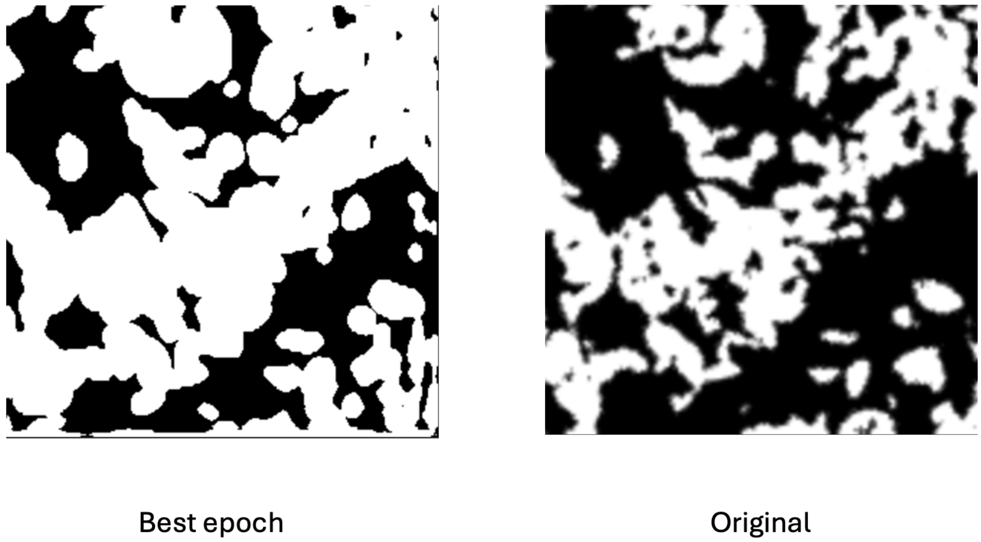

Figure 8: Segmentation quality comparison. Left: U-Net prediction. Right: ground truth mask.

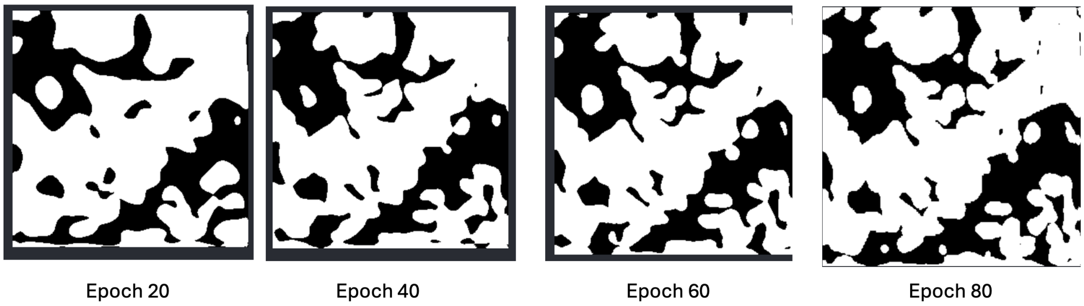

Figure 9: Segmentation result across different training epochs. Early predictions are noisy and overly smoothed; later epochs capture sharper pore shapes and more accurate boundaries.

Boundary Misalignment. Predicted pore boundaries were sometimes slightly offset or smoothed compared to the ground truth. This occurred because strong illumination gradients reduce edge contrast, and convolutional layers naturally smooth fine details. Future work should incorporate boundary-aware losses or sharper contrast augmentations.

Thin-Pore Under-Segmentation. Very narrow pore channels were occasionally missed. These structures contribute a small fraction of total pixels, so CE and Dice loss assign them low weight. Training with focal-Dice combinations or pore-size–aware sampling could alleviate this issue.

Synthetic–Real Gap. While synthetic data produced strong segmentation performance, real pFIB-SEM slices contain harsher noise and irregular artifacts not fully captured by Blender (Blender Foundation, 2023) lighting. This gap explains minor generalization drops on real samples. Adding domain-randomized noise models and artifact simulations (e.g., drift, charging) is a promising next step.

14 Discussion

During this Capstone project, we have successfully implemented a machine learning pipeline to reconstruct the 3D structure from sliced 2D images.The model was trained using synthetic data, since the data we obtained did not have ground truth.
Our innovative approach was able to train a model to 93% validation accuracy. However, it is difficult to assess the validity of the model output for real images. Indeed, while we have taken considerable steps to replicate the slicing and lighting conditions, there are still key differences between our synthetic images and the real images.

Slicing The 3D porous material are cut by a perfect plane in the synthetic dataset. However, we observe the slicing is more imperfect in real life.

Material shape The 3D porous material generated by PuMA are all cubic. This is not the shape distribution we observe in the real data. Adding variation in shape size might garantee a better generalization to more diverse shapes.

Image resolution All images were rendered using the same resolution. This aspect might not generalize well to images with different resolution.

All in all, there are several key aspects from the synthetic dataset that might explain why generalizing to real data is more difficult than anticipated. It may be necessary to find additional arguments to strengthen the validity of the model on other datasets. This can be resolved by analyzing the output on real data, evaluating key attributes like global porosity, pore-size distribution and material characteristics.
It is also possible to increase the robustness of the model by adding variability and noice in the training data to ensure the model does not overfit to specific parameters.

15 Lessons Learned and Reflections

The Capstone project was an excellent opportunity to apply our Machine Learning skills to a real-life, practical problem. It was very interesting to work with another university department, and learn how to communicate about the current issues and resolutions given different people's expertise.

- Deciding which models should be used was the source of the biggest debates. It wasn't evident what path would work best, and we all had different ideas.
- We made several tradeoff due to time constraints. Given more time, we would have love to further fine-tune our models, by updating the loss functions and optimizing hyperparameters. However, we preferred to continue moving forward since the model was already performing well.
- The planning document proved to be the most significant. It was very useful to take the time to divide the work into smaller tasks and have an idea when things might be done. Most of the planning went according to plan. It would have been helpful to implement models faster and iterate instead of spending too much time brainstorming.
- The biggest hurdle was figuring out how to work in parallel. A lot of the work had to wait until previous parts of the pipeline were finished which led to a lot of small roadblocks.
- There were no significant changes from the initial plan. However, the initial design did not specify how each step would be implemented. A lot of the decisions later on were on implementation, model selection, and data engineering.

16 Future Work

The work done during this Capstone project has shown how synthetic data can be used to train an image processing pipeline for real-world data.

Future work could focus on further validating how models trained on synthetic data are able to accurately generalize to the real-world data. Indeed, it would be useful to increase the robustness of the models and avoid overfitting to the synthetic data. This can be done by generating noisier images, greater variance of rendering parameters (light, angle, ...), more natural slicing or example.

Furthermore, the model accuracy can be increased by parameter and hyperparameter tuning in order to increase learning.

17 Conclusion

Our Capstone Project focuses on using pFIB-SEM images of cathode layers to generate a 3D reconstruction of the layer in fuel cells. Due to the absence of ground truth for our data, we developed an innovative approach that relies on synthetic data to train our machine learning pipeline.

The work we have done is two-fold. First, we have crafted and generated a synthetic dataset using PuMA software (Ferguson et al., 2018) to generate porous material and Blender (Blender Foundation, 2023) to add light and perspective, slice the volume and render images. Secondly, we used our synthetic dataset to train a machine learning pipeline. We implemented a 2D U-Net (Ronneberger et al., 2015) to extract information from the raw slices and identify pores, achieving 93% accuracy. Then, we relied on a 3D U-Net to reconstruct the final 3D volume.

The results show great promise in using synthetic datasets to replicate and train machine learning pipelines when data is sparse and incomplete. Future work is needed to ensure that the model does not overfit to the synthetic data and can generalize to produce a reliable results on real data.

18 Acknowledgments

We would like to thank our mentor Roby Gautier for providing guidance, support, and expertise during the entirety of the Capstone Project. The project was well thought out and offered a novel and interesting approach to an existing problem. We appreciate the trust that we were given in coming up with solutions and ideas.

We appreciate the bi-weekly follow up we had with Professor Kemal Oflazer. The discussions, reflections, and insights provided helped us navigate challenges and incoming blockers better.

We would like to thank our Capstone Course Developer Annette Han for scheduling, managing, and organizing the course.

We also thank our team Teaching Assistant Gokulapriyan Balaji for providing support and guidance during this project.

19 Terminology, Definitions, Acronyms, and Abbreviations

Terminology	Definition
Fuel Cell	A device that converts chemical energy into electrical energy through an electrochemical reaction, typically using hydrogen as the fuel.
Porosity	The measure of void spaces within a material, usually expressed as a percentage of the total volume.
Cathode Layers	Sponge-like, catalyst-rich parts of a fuel cell where oxygen reacts to help turn chemical energy into electricity.
Plasma Focused Ion Beam Scanning Electron Microscope (pFIB-SEM)	Combines a plasma focused ion beam that precisely removes material with high-resolution scanning electron microscopy to quickly capture detailed 3D images at the nanometer scale. (Thermo Fisher Scientific, 2023).
Pore Distribution	Refers to how the pores, the tiny holes within a material, are spread out (e.g., evenly distributed or clustered in certain areas). This can affect how fluids move through the material.
Pore Size	Refers to the diameter or width of the tiny openings or voids within a material. This can directly influence how fluids can move through the material.
ROI	Region of Interest, the specific area within an image that contains relevant information for analysis.
Otsu's Method	An automatic image thresholding algorithm that determines the optimal threshold by minimizing intra-class variance (Otsu, 1979).
Reproducibility	The ability of a system to produce the same results when given the same inputs under identical conditions.
Modularity	A design approach that separates a system into distinct, independent components.
Decarbonization	The reduction of carbon dioxide emissions through the use of low-carbon power sources.

Terminology	Definition
Microstructure	The fine-scale structure of a material, including features not visible to the naked eye.

20 Citations and References

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