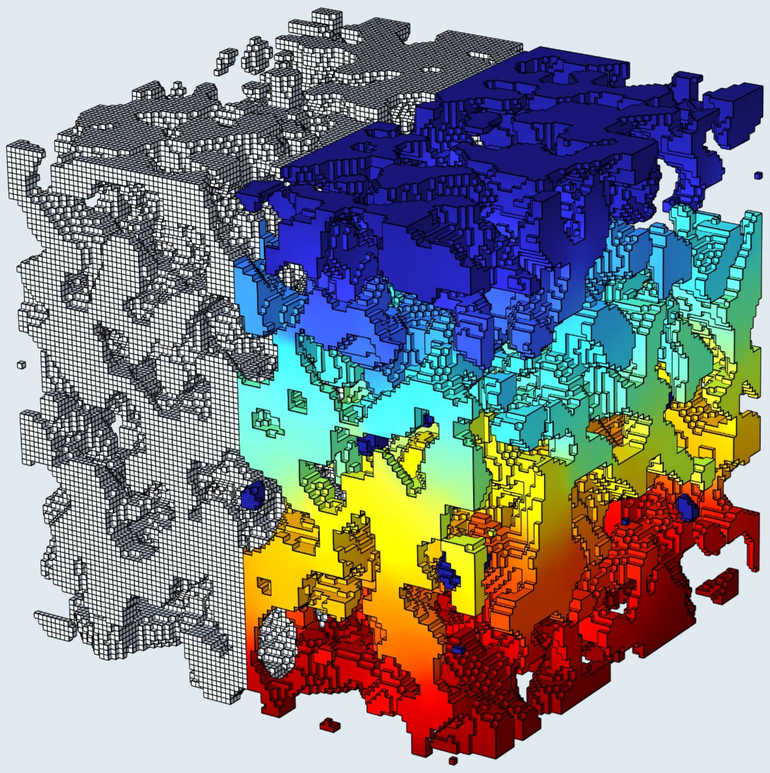

A Workflow to Facilitate Multiphysics Simulations on Explicitly Resolved Microstructures

Seamlessly import ready to use microstructures into COMSOL Multiphysics® software to perform multiphysics simulations at the voxel level.

A. Abena
Johnson Matthey Technology Centre, Sonning Common, Reading, United Kingdom.

Introduction

Capturing microstructure details is essential to investigate transport of species and reactions taking place at the micro-scale level in a cathode catalyst layer of a PEM fuel cell. To this end, a three-dimensional geometry of the microstructure is generally created/reconstructed using dedicated software and then imported into COMSOL Multiphysics® software. Due to the complexity of the geometry, the size of the file to be imported can be quite large, and it usually requires time consuming extra steps to make the microstructure ready to be used in the model under development. By contrast, this work presents a workflow to seamlessly import ready to use microstructures into COMSOL Multiphysics software, which also allows the user to perform simulations at the voxel level.

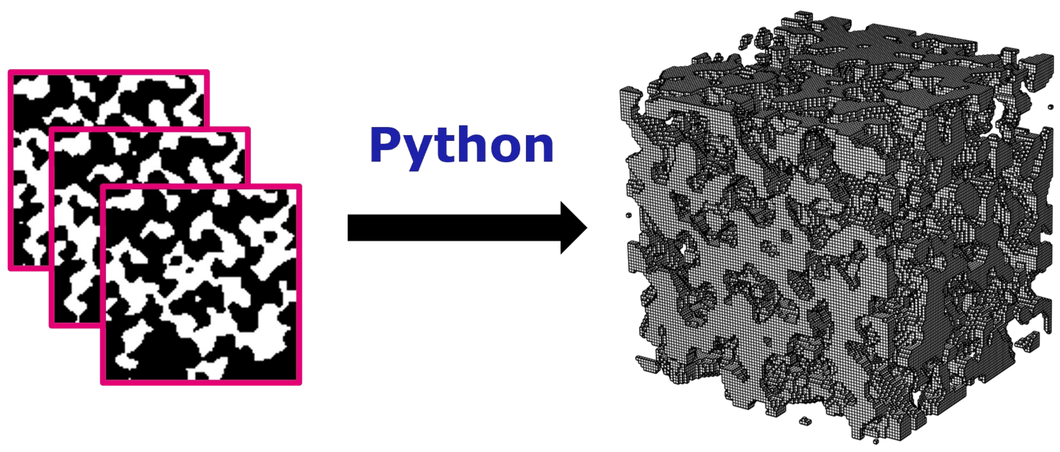

FIGURE 1. From a stack of two-dimensional images to a three-dimensional mesh.

Methodology

A bespoke Python code (Ref. 1) was created to read the microstructure from a stack of two-dimensional images and output a mesh file with a mphtxt extension (Figure 1). Each element in the mesh file corresponds to a voxel in the original three-dimensional microstructure. The Python code was optimised to minimise the computation time for large microstructures. The mesh file was then easily imported in COMSOL Multiphysics software thanks to the import mesh capability.

To test the proposed workflow, a simulation of oxygen transport in the void phase of the catalyst layer was simulated using the Transport of Diluted Species interface available in COMSOL Multiphysics software.

Results

The model outputs the oxygen concentration field (Figure 2), and it was numerically validated against GeoDict™ software calculating the values for relative diffusivity (Ref. 2) along the three axes (Table 1).

TABLE 1. Relative diffusivity (%) for numerical validation.

Software	x-axis	y-axis	z-axis
COMSOL Multiphysics®	8.34	8.14	8.54
GeoDict™	7.12	6.99	7.25

The model lays a solid foundation to implement additional physics taking place in the cathode catalyst layer of a PEM fuel cell.

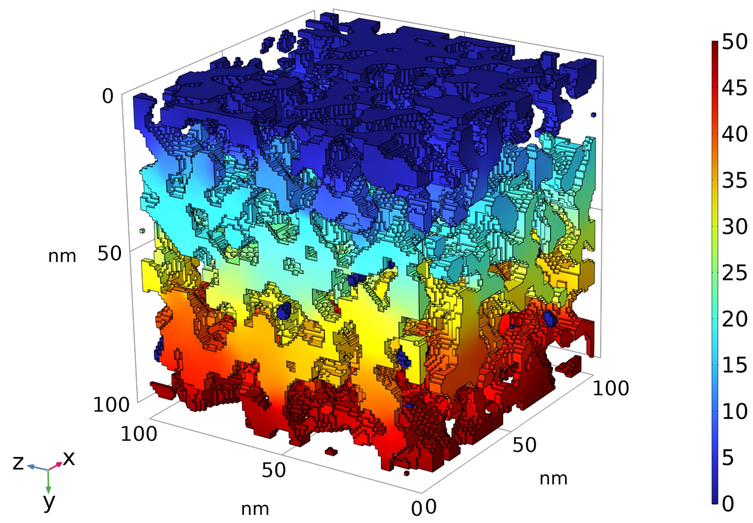

FIGURE 2. Oxygen concentration field (mol/m^3) in the void phase of an explicitly resolved microstructure.

REFERENCES

1. *Anaconda Software Distribution.* Computer software. Vers. 23.1.0. Web. <https://anaconda.com>.
2. J. Becker, A. Wiegmann, L. Cheng, B. Planas. GeoDict 2024 User Guide. DiffuDict handbook. Math2Market GmbH, Germany, doi.org/10.30423/userguide.geodict.

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