Predicting Transport Properties of Porous Layers Based on Pore-Scale Models

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PEM Fuel Cell

ELECTRIC CIRCUIT (40% - 60% Efficiency)

Fuel H (Hydrogen)

O₂ (Oxygen) from Air

Heat (95°C)
Water or Air Cooled

Air + Water Vapor

Used Fuel Recirculates

Flow Field Plate

Gas Diffusion Electrode (Anode)

Gas Diffusion Electrode (Cathode)

Proton Exchange Membrane (Electrolyte)
PEM Fuel Cell

Gas Diffusion layer
PEM Fuel Cell

Aim: engineer a better GDL!

Better?
- higher conductivity
- higher diffusivity
- higher stability
- ??
Predicting Transport Properties of Porous Layers Based on Pore-Scale Models

1. General Approach

2. Application to PEM fuel cells
   - Gas Diffusion Layer
   - Catalyst Layer
Aim: Virtual Material Design
Aim: Virtual Material Design

Lab

Porous Medium

measure

Properties

Properties are:
- pore size distribution
- permeability
- diffusivity
- cap. pressure curve
- ...

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Computer

Model
Aim: Virtual Material Design

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Porous Medium

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Properties

Computer

Model
generate

Voxel Mesh

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**Lab**
- Porous Medium
- measure
- Properties

**Computer**
- Model
  - generate
  - Voxel Mesh
  - calculate
  - Properties

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Properties
Bridge the Gap - Step 1: Validate Calculations

Porous Medium

measure

Properties
Bridge the Gap - Step 1: Validate Calculations

Porous Medium → measure → Properties

Properties → image → CT Image
Bridge the Gap - Step 1: Validate Calculations

Porous Medium → image → CT Image

measure

CT Image ↘

filter & segment

Voxel Mesh

Properties
Bridge the Gap - Step 1: Validate Calculations

1. Measure properties of the Porous Medium.
2. Convert to CT Image.
3. Filter & segment the CT Image to create a Voxel Mesh.
4. Calculate properties of the Voxel Mesh.
5. Obtain properties from the Voxel Mesh.

This process bridges the gap between experimental data and computational models.
Bridge the Gap - Step 1: Validate Calculations
Bridge the Gap - Step 1: Validate Calculations

... and Measurements

... and Imaging

**Porous Medium**

- image
  - CT Image
    - filter & segment
      - Voxel Mesh
        - calculate
          - Properties
            - compare
            - Properties
Bridge the Gap - Step 2: Validate Modeling

CT Image

filter & segment

Voxel Mesh

calculate

Properties

Model
Bridge the Gap - Step 2: Validate Modeling

CT Image

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generate

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Bridge the Gap - Step 2: Validate Modeling

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Properties
Bridge the Gap - Step 2: Validate Modeling

CT Image

- filter & segment
- calculate

Voxel Mesh

Properties

Model

- generate
- calculate

Voxel Mesh

Properties

compare
The GeoDict Idea

- **Porous Medium**
  - image
- **CT Image**
  - filter & segment
  - generate
  - Voxel Mesh
  - calculate
  - Properties
- **Model**
  - Properties
- **Properties**

measure
The GeoDict Idea

Lab

- Porous Medium
  - measure
  - Properties
- CT Image
  - filter & segment
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    - calculate
    - Properties
- Model
  - generate
  - Properties
The GeoDict Idea

Lab → Porous Medium → measure → Properties → CT Image → filter & segment → Voxel Mesh → calculate → Properties → Model → generate → Lab

Tomograph → CT Image
The GeoDict Idea

Porous Medium → CT Image

CT Image → Voxel Mesh

Voxel Mesh → Model

Model → Properties

Properties → calculate

Porous Medium → measure

measure → Lab

Lab → Tomograph

Tomograph → image

image → CT Image

CT Image → filter & segment

filter & segment → Voxel Mesh

Voxel Mesh → generate

generate → Model

Model → Properties

Properties → calculate

GeoDict
The GeoDict Software

**Geometry**
- CT Image
- Nonwoven Model
- Sintered Structures Model
- ...

**Predictions**
- Permeability
- Diffusivity
- Capillary Pressure
- ...

- Voxel Mesh
Model: Nonwovens - Straight Fibres

Poisson line process using:
- fibre diameter
- fibre cross sectional shape
- anisotropy
- porosity
Model: Nonwovens - Some Variants

Straight fibres plus binder

Curved fibres
Model: Woven Fabric
Property: Permeability

Macroscopic description
(homogenized porous media model)

Darcy’s law:
\[ u = -\frac{1}{\mu} \kappa \nabla p \]

\( u \): average flow velocity
\( \kappa \): permeability tensor \textit{unknown}
\( \mu \): viscosity
\( p \): pressure

Microscopic description
(pore structure model)

Stokes equation:
\[ -\mu \Delta u + \nabla p = 0 \]

Boundary conditions: no-slip on fibre surface, pressure drop
\( \kappa \) can be determined from the solution!
Property: Relative Permeability

Two-step approach:
Property: Relative Permeability

Two-step approach:

1. Use pore morphology method (Hilpert, 2001) to determine distribution of air and water phase.

   Idea: a pore is filled with the non-wetting fluid (=water), if
   \[ p_c \geq \frac{2\sigma}{r} \cos \beta \]
Property: Relative Permeability

Two-step approach:

1. Use pore morphology method (Hilpert, 2001) to determine distribution of air and water phase.
   - Idea: a pore is filled with the non-wetting fluid (=water), if
     \[ p_c \geq \frac{2\sigma}{r} \cos \beta \]

2. Solve Stokes equation on the remaining pore space to determine wetting phase (=air) permeability
Property: Diffusivity

Macroscopic description  
(homogenized porous media model)  
Fick's first law:  \[ j = -D^* \nabla c \]

D* : effective diffusivity [m²/s]  \textit{unknown}
j : diffusion flux [mol/m²/s]  
c : concentration [mol/m³]
Property: Diffusivity

Macroscopic description (homogenized porous media model)
Fick's first law: \[ j = -D^* \nabla c \]

\( D^* \): effective diffusivity \([\text{m}^2/\text{s}]\) \textit{unknown}

\( j \): diffusion flux \([\text{mol/m}^2/\text{s}]\)

\( c \): concentration \([\text{mol/m}^3]\)

Microscopic description (pore structure model)
Laplace equation: \[ -\Delta c = 0 \]

Boundary conditions: no-flux on fibre surface, concentration drop

\( D^* \) can be determined from the solution!
Summary Part I

Models:
- CT Images
- Fibrous nonwovens
- Woven structures
- Sintered structures
- Sphere packings
- Layered structures

Properties:
- Pore size distribution
- Surface area
- (Knudsen) Diffusivity
- Permeability
- Electric conductivity
- Heat conductivity
- Capillary pressure curve
- Bubble point
- Relative (= saturation dependent) permeability
- Relative (= saturation dependent) diffusivity
- Filter efficiency and life time
Application: Gas Diffusion Layer of PEM Fuel Cell

Joint work
PSI:
- CT Images of Toray paper at different compression levels
- Diffusivity and permeability measurements at different compression levels
ITWM:
- Compute diffusivity and permeability

Diffusivity

Perfect in tp-direction

Small differences in ip-direction
- ip-measurements performed on a stack of GDLs
- tomography image shows single layer between sample holder
Permeability

Perfect in tp-direction

Small differences in ip-direction
- ip-measurements performed on a stack of GDLs
- tomography image shows single layer between sample holder
Application: Catalyst Layer of PEM Fuel Cell

Problem: pore sizes < 100 nm
Catalyst Layer Model

Carbon agglomerates plus electrolyte

Elect. between Carbon Partikels
## Conductivity

Compare models with varying carbon and electrolyte volume fractions

<table>
<thead>
<tr>
<th>Vol% Carbon</th>
<th>Vol% Electrolyte</th>
<th>Porosity</th>
<th>Electronic Conductivity</th>
<th>Protonic Conductivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>35.4</td>
<td>12.2</td>
<td>52.4</td>
<td>6.6 %</td>
<td>1.1 %</td>
</tr>
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<td>40.9</td>
<td>5.2</td>
<td>53.9</td>
<td>9.7 %</td>
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<td>13.8</td>
<td>45.3</td>
<td>9.7 %</td>
<td>1.6 %</td>
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<td>20.7</td>
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<td>4.9 %</td>
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<tr>
<td>40.9</td>
<td>26.3</td>
<td>32.8</td>
<td>9.7 %</td>
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<tr>
<td>45.1</td>
<td>15.2</td>
<td>39.8</td>
<td>13.4 %</td>
<td>1.9 %</td>
</tr>
<tr>
<td>50.1</td>
<td>16.6</td>
<td>33.3</td>
<td>17.6 %</td>
<td>2.2 %</td>
</tr>
</tbody>
</table>
Summary Part II

Gas diffusion layer:
- validated method to determine diffusivity and permeability

Catalyst layer:
- no validation possible until 3D images are available
Thank You!

BMBF project PemCaD

Geometry generator, property predictor and virtual material designer

www.geodict.com