Computer Based Design of Porous Transport Layers of PEM Fuel Cells

Dr. Jürgen Becker

EVS30 / f-cell
Stuttgart
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We help our clients to profitably engineer better materials and processes through digital solutions.

We believe that to understand is to improve.
<table>
<thead>
<tr>
<th>GeoDict The Digital Material Laboratory</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Filtration</strong></td>
</tr>
<tr>
<td>Mostly automotive, filter media &amp; filters for water, sludge, oil, air and fuel</td>
</tr>
<tr>
<td><strong>Electrochemistry</strong></td>
</tr>
<tr>
<td>Fuel cell media &amp; battery materials, catalyst materials</td>
</tr>
<tr>
<td><strong>Composites</strong></td>
</tr>
<tr>
<td>CFRP, GFRP, mostly automotive, lightweight materials</td>
</tr>
<tr>
<td><strong>Oil and Gas</strong></td>
</tr>
<tr>
<td>Digital rock physics, digital sand control</td>
</tr>
</tbody>
</table>
Development of Materials by Digital Material Design
GeoDict
Development of Materials by Digital Material Design

- Import CT scans
- Import FIB-SEM data

Image Acquisition

Development of Materials
GeoDict
Development of Materials by Digital Material Design

Image Acquisition

Development of Materials
GeoDict
Development of Materials by Digital Material Design

Determine:
- Pore size distribution
- Fiber size and orientation
- Grain size and shape
Development of Materials by Digital Material Design

Image Acquisition

Image Analysis

Development of Materials
GeoDict
Development of Materials by Digital Material Design

Gas diffusion layer

Catalyst layer

Modelling Microstructures

Development of Materials
GeoDict
Development of Materials by Digital Material Design

Image Acquisition → Image Analysis → Modelling Microstructures → Development of Materials
GeoDict

Development of Materials by Digital Material Design

Permeability tensor \((m^2)\):

<table>
<thead>
<tr>
<th></th>
<th>2.007e-11</th>
<th>-2.87729e-13</th>
<th>-4.85037e-13</th>
</tr>
</thead>
<tbody>
<tr>
<td>-2.43395e-13</td>
<td>2.10784e-11</td>
<td>-5.02884e-14</td>
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<tr>
<td>-5.9795e-13</td>
<td>1.09459e-13</td>
<td>1.56916e-11</td>
<td></td>
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</table>

Effective diffusivity in %:

<table>
<thead>
<tr>
<th></th>
<th>63.2608</th>
<th>-0.395186</th>
<th>-0.643377</th>
</tr>
</thead>
<tbody>
<tr>
<td>-0.364076</td>
<td>64.7705</td>
<td>-0.18344</td>
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</tr>
<tr>
<td>-0.962924</td>
<td>0.22963</td>
<td>58.9095</td>
<td></td>
</tr>
</tbody>
</table>

Tortuosity factors and Tortuosity:

<table>
<thead>
<tr>
<th>Direction</th>
<th>Tortuosity Factor (\kappa)</th>
<th>Tortuosity (\tau)</th>
</tr>
</thead>
<tbody>
<tr>
<td>X Direction</td>
<td>1.27950494</td>
<td>1.13115</td>
</tr>
<tr>
<td>Y Direction</td>
<td>1.249680381</td>
<td>1.11789</td>
</tr>
<tr>
<td>Z Direction</td>
<td>1.37401316</td>
<td>1.17218</td>
</tr>
</tbody>
</table>

Macroscopic Material Parameters

Permeability vs. Water Saturation
## Development of Materials by Digital Material Design

### Macroscopic Material Parameters

<table>
<thead>
<tr>
<th>Geometric parameters</th>
<th>Conduction parameters</th>
<th>Diffusion &amp; flow parameters</th>
<th>Saturation parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>Porosity</td>
<td>Thermal conductivity</td>
<td>Permeability</td>
<td>Cap. pressure curve for Drainage and Imbibition</td>
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<tr>
<td>Pore size distribution</td>
<td>Thermal Flux</td>
<td>Diffusivity</td>
<td>Saturation dependent permeability, diffusivity, conductivity</td>
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<tr>
<td>Surface area</td>
<td>Temperature distribution</td>
<td>Particle concentration</td>
<td></td>
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<tr>
<td>Length of contact lines</td>
<td>Electrical conductivity</td>
<td>Path of single particle</td>
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<td>Tortuosity/Gurley value</td>
<td>Electrical Flux</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Electrostatic potential distribution</td>
<td></td>
<td></td>
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</tbody>
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- Porosity
- Pore size distribution
- Surface area
- Length of contact lines
- Tortuosity/Gurley value
- Thermal conductivity
- Thermal Flux
- Temperature distribution
- Electrical conductivity
- Electrical Flux
- Electrostatic potential distribution
- Permeability
- Diffusivity
- Particle concentration
- Path of single particle
- Cap. pressure curve for Drainage and Imbibition
- Saturation dependent permeability, diffusivity, conductivity
GeoDict
Development of Materials by Digital Material Design

Image Acquisition → Modelling Microstructures → Microstructure Simulation → Macroscopic Material Parameters

Development of Materials
1. Made CT scans of Toray TGP H 060 at different compression levels
2. Measured diffusivity at different compression levels experimentally
3. Computed diffusivity on the CT scans
GeoDict
Development of Materials by Digital Material Design

Image Analysis ➔ Modelling Microstructures ➔ Microstructure Simulation ➔ Macroscopic Material Parameters

Image Acquisition ➔ Change Geometry ➔ Material Property ➔ Experimental Verification

Development of Materials
Case Study:
Determine relative permeability for a gas diffusion layer

... considering variable wettability

... and compression.
Gas Diffusion Layer Model

GDL:
- Carbon fibers, 7 µm diameter
- 20 wt% binder
- 200 µm thickness

Model
- 1 µm resolution
- Voxel grid
- 600x600x200 = 72 Mio. cells
- Stochastic process
Modelling of Clamping Pressure

Fibers: linear elastic, transverse isotropic
Binder: linear elastic, isotropic

Solver:

FeelMath
Fraunhofer ITWM

Runtime: 1h 17 min (8x)
Introducing Variable Wettability

- Marked a cylinder as area with higher wettability

Other options:
- distinguish between binder and fibers
- mark individual fibers
- ...
Gas Diffusion Layer Models with Different Wettability

Constant Wettability

Variable Wettability
Water Entering into an Uncompressed GDL with Constant Wettability
Water Entering into an Uncompressed GDL with Variable Wettability
Comparison:
Saturation at Fixed Capillary Pressure

Constant Wettability

Variable Wettability
Water Entering into a Compressed GDL with Constant Wettability
Water Entering into a Compressed GDL with Variable Wettability
Comparison: Saturation at Fixed Capillary Pressure

Constant Wettability
Variable Wettability
Simulated Relative Permeability (Uncompressed GDL)

Both air and water perm. increase for patterned wettability!
The basic idea:

Microstructures define macroscopic properties!

- Model porous microstructure of transport layers and electrodes
- Simulate transport processes
- Simulate mechanical behavior
- Analyze geometry

**GeoDict** predicts macroscopic material properties based on the 3D microstructure and enables you to improve the materials.
Thank You!

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