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Large Scale 3D Flow Distribution Analysis in HTPEM Fuel Cells

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Outline of this talk

Introduction:
- ZBT Duisburg GmbH
- High temperature PEM (HTPEM) fuel cell
- Aim of this 3D study

Methodology:
- Computational subdomains
- Governing equations
- Solver settings, meshing and solution procedure

Experimental and theoretical results:
- PIV-measurements
- Experimental/simulation results
- Theoretical results

Summary:
- Conclusion
- Outlook

Large Scale 3D Flow Distribution Analysis in HTPEM Fuel Cells
ZBT Duisburg GmbH established in 2001
TAZ established in 2008
Hydrogen and fuel cell related activities in several divisions → LTPEM and HTPEM fuel cell R&D

**Focusing the HTPEM technology, e.g.:**
- Bipolar-plate and component development
- Fuel cell and fuel cell stack prototype design
- Operation (short and long-term)
- System integration
- Locally resolved measurements

**Theoretical analysis, e.g.:**
- Analytical calculations
- CFD/FEM modeling and simulation
- System simulation
→ coupled to experimental investigations
High temperature PEM (HTPEM) fuel cells

HTPEM fuel cells electrochemically convert energy stored in a fuel and oxidant into electricity

Benefits against the LTPEM fuel cell technology (e.g. no humidification needed)

Relatively new technology (e.g. $\text{H}_3\text{PO}_4$ behaviour during operation not fully understood yet)

Overall goal:

- Development a complete large scale 3D HTPEM fuel cell assembly model
- Coupled CFD/FEM analysis
- 2D and 3D-studies presented at the European COMSOL conferences (2007 and 2008)

Aim of this study:

- Modeling and simulating fluid-flow behaviour
- Evaluate flow-field performance (6 different types)
- Compare results to PIV-measurements
- Optimize flow-field layout (bipolar-plate production)?

Bipolar-plate mass production at the ZBT: e.g. injection moulding – LTPEM fuel cell applications
Computational subdomains (reference case)

50 [cm$^2$] 6 channel parallel serpentine flow-field

3D model → extended to the third dimension (here $z$) (gas channel volume)

Geometry import (standard neutral formal '*.iges'-file)

Dimensions:
Single gas channel 0.001 [m] by 0.001 ($y$, $z$)
Porous media thickness 400·10$^{-6}$ [m]
(uncompressed) ($z$)
→ woven cloth-type material properties
(E-tek (ELAT) products)

Bipolar-plate for HTPEM fuel cell applications

Reference case 3D model geometry
### Governing equations – subdomain settings

<table>
<thead>
<tr>
<th>Subdomain</th>
<th>Governing equation(s)</th>
<th>Variables</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gas channel</td>
<td>Navier-Stokes equations (momentum transport - laminar flow)</td>
<td>( u, v, w, P, )</td>
</tr>
<tr>
<td></td>
<td>( \nabla \cdot u = 0 )</td>
<td>( Pinl_{chns} )</td>
</tr>
<tr>
<td></td>
<td>( \rho \cdot u \cdot \nabla u = \nabla \left( -P \cdot I + \eta \cdot \left( \nabla u + (\nabla u)^T \right) \right) ) + ( F )</td>
<td>( \rightarrow \text{weak contribution added / additional DOF} )</td>
</tr>
<tr>
<td>Porous media (GDL)</td>
<td>Brinkman equations</td>
<td>same as above</td>
</tr>
<tr>
<td></td>
<td>( \nabla \cdot u = 0 )</td>
<td></td>
</tr>
<tr>
<td></td>
<td>( \frac{\eta}{k_p} \cdot u = \nabla \left( -P \cdot I + \frac{1}{\varepsilon} \cdot \left( \eta \cdot \left( \nabla u + (\nabla u)^T \right) - \frac{2}{3} \cdot \eta \cdot (\nabla u) \cdot I \right) \right) ) + ( F )</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Darcy’s law equation ( u = -\frac{k_p}{\eta} \cdot \nabla P )</td>
<td>( Pd )</td>
</tr>
</tbody>
</table>

- Physical properties of air @ 160°C used (typical HTPEM fuel cell operating temperature)
- GLS streamline diffusion (free flow) / crosswind diffusion \( C_k = 0.1 \)
### Governing equations – boundary conditions

<table>
<thead>
<tr>
<th>Boundary</th>
<th>Governing equation(s)</th>
<th>Experimental data</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Inlet</strong></td>
<td>Constant laminar inflow</td>
<td>Volume per time unit 1000 [ml/min] (MFC)</td>
</tr>
<tr>
<td></td>
<td>( L_e \cdot \nabla_t \cdot \left( P \cdot I - \eta \cdot \left( \nabla_t u + \left( \nabla_t u \right)^T \right) \right) = -\vec{n} \cdot P_{0,e} )  ( \nabla_t u = 0 )</td>
<td></td>
</tr>
<tr>
<td><strong>Outlet</strong></td>
<td>Pressure (no viscous stress)</td>
<td>No back pressure (pressure loss measured)</td>
</tr>
<tr>
<td></td>
<td>( \eta \cdot \left( \nabla_t u + \left( \nabla_t u \right)^T \right) \cdot \vec{n} = 0 ) ( P = P_{0,\text{out}} )</td>
<td></td>
</tr>
<tr>
<td><strong>Walls</strong></td>
<td>No slip</td>
<td>n.a.</td>
</tr>
<tr>
<td></td>
<td>( u = 0 )</td>
<td></td>
</tr>
<tr>
<td><strong>Gas channel to porous media interface</strong></td>
<td>Continuity → Navier-Stokes/Brinkman ( n \cdot \left( \eta_1 \cdot \left( \nabla u_1 + \left( \nabla u_1 \right)^T \right) - p_1 \cdot I - \eta_2 \cdot \left( \nabla u_2 + \left( \nabla u_2 \right)^T \right) + p_2 \cdot I \right) = 0 )  ( \text{Navier-Stokes/Darcy} )</td>
<td>n.a.</td>
</tr>
<tr>
<td></td>
<td>Pressure and velocity constraints</td>
<td></td>
</tr>
<tr>
<td></td>
<td>( P, u_{\text{chdl}}, v_{\text{chdl}}, w_{\text{chdl}} )</td>
<td></td>
</tr>
</tbody>
</table>

**Large Scale 3D Flow Distribution Analysis in HTPEM Fuel Cells**
Solver settings/meshing/solution procedure

COMSOL MP 3.5a / 8 core HP workstation (Windows XP 64 bit – 64GB Ram)

1) Iterative solver or 2) Parametric iterative solver → fluid viscosity $\eta$
   - BiCGStab (linear system solver)
   - Preconditioner: Geometric multigrid solver (3 levels) V-cycle
   - Pre-/postsmoother: Vanka (pressure update) GMRES solver
   - PARDISO coarse direct solver
   → Convergence criteria $1 \cdot 10^{-6}$ [-]

- Maximum element size $0.8 \cdot 10^{-3}$ [-] (mesh case 0)
- Triangular elements on boundaries → Prism elements for subdomain meshing
- 3 elements layer (gas channel and porous media subdomain)

→ All simulations performed using the same
i) geometrical aspects
ii) HTPEM fuel cell operating conditions
   and material properties

Large Scale 3D Flow Distribution Analysis in HTPEM Fuel Cells
PIV-measurements (reference case)

Experimental set-up:

- Experimental fluid-flow data obtained by particle image velocimetry (PIV)
- 12-bit CCD camera
- Fluorescence filter
- Dual-pulse Nd:YAG laser
- Transparent HTPEM fuel cell
  → Water model conditions
  → Dimensional analysis using the Reynold’s number

Snapshots at different times scales
- PIV-measurements (x-y-plane)
Experimental/simulation results (reference case)

→ Quantitative comparison to CFD simulation results

Velocity vectors – PIV-measurements (x-y-plane)

Fluid bypassing between adjacent channels – PIV-measurements (x-y-plane)

Velocity vectors and gas bypassing between adjacent channels – simulation results (arrow plot @ x-y-plane, \( z = -170 \cdot 10^{-6} \) [m])

→ same shape of the bypassing flow observed in the simulations

Large Scale 3D Flow Distribution Analysis in HTPEM Fuel Cells
Experimental/simulation results (reference case)

→ e.g. Preliminary experimental PIV-investigations

- Fluid bypassing observed at the 180° bends (x-y-plane)
- Velocity vectors within a gas channel – typical shape observed (x-y-plane)
- Velocity vectors and streamline plot within the gas channel close to a 180° bend (arrow plot @ x-y-plane, z = -170·10⁻⁶ [m])

→ quantitatively similar fluid-flow behaviour observed
### Simulation results

<table>
<thead>
<tr>
<th>Type</th>
<th>Channel/land [mm/mm]</th>
<th>Contact area [%/%]</th>
<th>Mesh elements [-]</th>
<th>DOF [-]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Serpentine # 1 (reference case)</td>
<td>1/1</td>
<td>52.3/47.7</td>
<td>137,898</td>
<td>2,075,382</td>
</tr>
<tr>
<td>Serpentine # 2</td>
<td>1/0.9</td>
<td>52.6/47.4</td>
<td>126,972</td>
<td>1,914,108</td>
</tr>
<tr>
<td>Mixed # 1</td>
<td>1/1</td>
<td>50.6/49.4</td>
<td>121,233</td>
<td>1,829,532</td>
</tr>
<tr>
<td>Mixed # 2</td>
<td>1/1</td>
<td>54.1/45.9</td>
<td>121,257</td>
<td>1,828,349</td>
</tr>
<tr>
<td>Straight</td>
<td>1/1</td>
<td>50.7/49.3</td>
<td>113,187</td>
<td>1,705,113</td>
</tr>
<tr>
<td>Criss-cross (pin type)</td>
<td>n.a.</td>
<td>73.5/26.5</td>
<td>58,988</td>
<td>1,055,744</td>
</tr>
</tbody>
</table>

**Large Scale 3D Flow Distribution Analysis in HTPEM Fuel Cells**
Simulation results

Gas channel velocity

- Uniform gas channel velocity observed for both serpentine type flow-fields
- Straight flow-field shows inherent maldistribution
- Criss-cross type flow-field shows low overall velocity

Gas channel velocity (slice plot @ $x$-$y$-plane, $z = 500 \cdot 10^{-6}$ [m]) (note: same color bar for flow-field 1-4)

Gas channel velocity (slice plot @ $z$-$y$-plane, $x/x_{max} = \frac{1}{2}$)

Gas channel velocity (cross-sectional plot @ $x/x_{max} = \frac{1}{2}, y = [0-y_{max}], z = 500 \cdot 10^{-6}$ [m])
Simulation results

Porous media velocity → maximum located close to the 180° bends

Porous media velocity (slice plot @ x-y-plane, z = -170·10^{-6} [m]) (note: same color bar for flow-field 1-5)

Porous media velocity vectors (arrow plot @ x-z-pane, y = -170·10^{-6} [m] – left, arrow plot @ x-z-pane, y/y_{max} = \frac{1}{2} - right)

Porous media velocity vectors (arrow plot @ x, y, z = -170·10^{-6} [m])

Large Scale 3D Flow Distribution Analysis in HTPEM Fuel Cells
Experimental/simulation results

Pressure loss measured using differential pressure transmitters

\[ \Delta P = f \cdot \frac{l_{ch}}{D_H} \cdot \rho \cdot \frac{\overline{u}^2}{2} + \sum K_i \cdot \rho \cdot \frac{\overline{u}^2}{2} \]

Pressure loss for different flow rates – including peripheral losses) (taken from C. Agrawal – ZBT internship report)

HTEPM fuel cell operated using a LabView controlled teststand

Pressure loss (slice plot @ x-y-plane, \( z = 500 \cdot 10^{-6} \) [m]) (note: same color bar for flow-field 1-6)
Summary

Conclusion:

→ PIV-measurements / CFD modeling and simulation / analytical calculations
→ to be used for flow-field layout and optimization (quantitative comparison is possible)
→ Free flow, porous media flow and pressure loss compared for 6 types of flow-fields
→ Gas channel bypassing highlighted

<table>
<thead>
<tr>
<th>Type</th>
<th>$u_{ch}$ [m/s]</th>
<th>$u_{GDL}$ [m/s]</th>
<th>$\Delta P$ [mbar]</th>
<th>Re [-]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Serpentine # 1</td>
<td>2.667</td>
<td>4.66·10^{-4}</td>
<td>9.36</td>
<td>72.3</td>
</tr>
<tr>
<td>Serpentine # 2</td>
<td>1.778</td>
<td>2.88·10^{-4}</td>
<td>4.5</td>
<td>46.8</td>
</tr>
<tr>
<td>Mixed # 1</td>
<td>0.866</td>
<td>8.79·10^{-5}</td>
<td>1.48</td>
<td>21.1</td>
</tr>
<tr>
<td>Mixed # 2</td>
<td>0.799</td>
<td>9.67·10^{-5}</td>
<td>1.88</td>
<td>23.9</td>
</tr>
<tr>
<td>Straight</td>
<td>0.849</td>
<td>2.75·10^{-4}</td>
<td>3.58</td>
<td>23.7</td>
</tr>
<tr>
<td>Criss-cross (pin type)</td>
<td>0.232</td>
<td>n.a.</td>
<td>0.4</td>
<td>15.4</td>
</tr>
</tbody>
</table>

Outlook:

- Include multiphysics into the model (flow-field layout is more than just momentum transport!)
- Investigate for current density and temperature distribution (both theoretical/experimental)
- Analyze porous media flow and gas channel bypassing for HTPEM fuel cells
- In-, outlet positioning
Thank you very much!

Questions?