Geometry modeling of open-cell foams for efficient fluid flow and heat transfer computations using modified Kelvin cells

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Outline

(1) Introduction
   CFD modeling of heat transfer and fluid flow in open-cell foams

(2) Geometry modeling
   Analysis of the reference foam
   Generation of modified Kelvin cells

(3) Determination of effective properties
   Finite volume method for effective thermal conductivity
   Lattice-Boltzmann method for permeability

(4) Results
   Representative volume element (RVE)
   Effective thermal conductivity
   Permeability

(5) Conclusions & outlook
CFD modeling of open-cell foams

Two major classes of approaches

1. macroscopic modeling: volume-averaged equations using eff. properties
2. microscopic modeling: taking into account the intricate geometry
   → computationally expensive for the entire physical domain

Alternative method

- approximation of geometry using idealized structure with same geometric properties, e.g. array of cylinders, Weaire-Phelan structures, Kelvin cells, ...
- periodicity reduces the size of the computational domain
- allows extended parametric studies or complete resolution of small-scale structures

**DNS inside idealized porous medium**

\( \text{Re}_D = 400 \) [Werzner et al., 2013]
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Reference foam

- manufactured using the replica technique on the basis of a polyurethane sponge [Schwartzwalder and Somers, 1963]
- material: \( \text{Al}_2\text{O}_3 \) (\( k = 18.66 \text{ W/mK} \))
- dimensions: 121 x 121 x 58 mm\(^3\)
- pore density: 10 ppi
- voxel representation available from 3D computed-tomography scan (resolution \( \Delta x = 70 \mu\text{m} \))

selection considered for the simulations (\( 718^3 \approx 370 \text{ million voxels} \))
Morphology of the reference foam

CT geometry analysis using 3D image analysis software MAVI

Results

- porosity: 85.56 %*
- number of pores: 11,693
- pore diameter: 4.77* ± 1.13 mm
- facets per pore: 15.08 ± 2.07
- av. strut width: 6.80 mm

(*parameters used for generation of Kelvin cells)

[Rößger and Jorschick, 2014]
Generation of modified Kelvin cells

The Kelvin cell [Thomson, 1887]

- polyhedron consisting of 14 faces: 8 hexagons and 6 squares
- space-filling unit-cell with lowest surface area
- resembles the polyhedra encountered in reticulate foams

Model generation

- three types are considered:
  - open square windows (o)
  - closed square windows (c)
  - half-closed square windows (hc)
- ligaments and closed faces are modeled by cylinders using implicit functions
- connections are rounded using the Blinn transformation [Storm et al., 2013]
### Overview of considered Kelvin cells

<table>
<thead>
<tr>
<th>nr. of closed windows</th>
<th>0 [o]</th>
<th>6 [c]</th>
<th>3 [hc]</th>
</tr>
</thead>
<tbody>
<tr>
<td>pore diameter</td>
<td></td>
<td>4.77 mm</td>
<td></td>
</tr>
<tr>
<td>porosity</td>
<td>85.98 %</td>
<td>85.05 %</td>
<td>85.51 %</td>
</tr>
</tbody>
</table>

**iso-surface representation**

**voxel mesh used for the simulations**

(69 x 69 x 69)
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Modeling of fluid flow

Lattice-Boltzmann method (LBM)

- LBM is used to obtain solutions of the mass and momentum conservation equations
- Physical domain is discretized into a uniform voxel mesh
- Fluid flow is treated as movement of particle populations, which undergo consecutive streaming and collision processes over a discrete lattice
- Macroscopic properties are obtained as moments of particle distributions

Boundary conditions

- Periodicity on all domain boundaries
- No-slip on all solid voxels

Possible velocities in D3Q19 phase space around a single lattice node

Scaling of LBM code

- Intel Xeon E5-2630 V2
- Lattice updates/sec vs. # CPUs
- Data points for different numbers of CPUs (e.g., 1, 10, 100, 1000) showing a linear scaling trend.
Evaluation of permeability tensor and extreme values

**Determination of permeability tensor**

- evaluated at Darcy flow condition: \( \text{Re}_k = u_D \sqrt{\kappa/\nu} \leq 1 \ (\approx 0.2) \)
- Darcy’s law:

\[
\begin{bmatrix}
K_{xx} & K_{xy} & K_{xz} \\
K_{yx} & K_{yy} & K_{yz} \\
K_{zx} & K_{zy} & K_{zz}
\end{bmatrix}
\begin{bmatrix}
\frac{\partial p}{\partial x} \\
\frac{\partial p}{\partial y} \\
\frac{\partial p}{\partial z}
\end{bmatrix}
= -\mu
\begin{bmatrix}
\bar{u}_x \\
\bar{u}_y \\
\bar{u}_z
\end{bmatrix}
\]

**Eigenvalues and eigenvectors**

- eigenvalues are defined by a homogenous linear system:

\[
(K - \lambda I) \cdot \vec{v} = 0
\]
- solution consists of three eigenvalues \( \lambda \) and corresponding eigenvectors \( \nu \), which form an orthogonal system
- min., max. and average permeability are obtained as:

\[
\kappa_{\text{min}} = \min(\lambda) \quad \kappa_{\text{max}} = \max(\lambda) \quad \kappa_{\text{avg}} = \frac{1}{3} \sum \lambda
\]
# Modeling of heat transfer and determination of ETC

## Governing equation

- steady-state heat conduction equation for heterogeneous materials, without heat source:

\[
\nabla \cdot (k \nabla T) = 0
\]

## Boundary conditions

- different temperatures on two opposite walls
- remaining walls adiabatic

## Determination of effective thermal conductivity

- after convergence of the temperature field, the average steady-state heat flux is evaluated over a plane of the computational domain:

\[
q_{av}'' = \frac{\int q'' \, dA}{\int dA}
\]

- ETC is obtained using averaged Fourier’s law of heat conduction:

\[
q_{av}'' = k_{eff} \frac{T_h - T_c}{L}
\]
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Results: representative volume element (RVE)

- **Porosity**
- **Permeability**
- **ETC**

**Length of the cubic partition** $L / d_{pore}$

**Relative error with respect to results of complete foam**

- $0\%$
- $10\%$
- $20\%$
- $30\%$
- $40\%$
- $50\%$

**Complete foam**

**Cubic partition**

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foam sample – velocity magnitude (1,0,0)

- inhomogenous distribution of velocity magnitude
- preferential paths with high velocities

Contour plot of velocity magnitude at a plane \( y = 25 \text{ mm} \)

Direction of pressure gradient \((1,0,0)\)
### Kelvin cells – velocity magnitude and temperature (1,0,0)

<table>
<thead>
<tr>
<th>open (o)</th>
<th>closed (c)</th>
<th>half-closed (hc)</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image1.png" alt="Image" /></td>
<td><img src="image2.png" alt="Image" /></td>
<td><img src="image3.png" alt="Image" /></td>
</tr>
<tr>
<td><img src="image4.png" alt="Image" /></td>
<td><img src="image5.png" alt="Image" /></td>
<td><img src="image6.png" alt="Image" /></td>
</tr>
</tbody>
</table>

#### Velocity Magnitude
- 2.2
- 2
- 1.8
- 1.6
- 1.4
- 1.2
- 1
- 0.8
- 0.6
- 0.4
- 0.2
- 0

#### Temp
- 1.0
- 0.9
- 0.8
- 0.7
- 0.6
- 0.5
- 0.4
- 0.3
- 0.2
- 0.1
- 0.0

TU Bergakademie Freiberg | GWA / IWTT | E. Werzner et al. | NM2PorousMedia 2014

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Comparison for permeability

<table>
<thead>
<tr>
<th>structure</th>
<th>permeability (10^{-7} m²)</th>
<th>minimum</th>
<th>maximum</th>
<th>average</th>
<th>av. error</th>
</tr>
</thead>
<tbody>
<tr>
<td>foam sample</td>
<td></td>
<td>1.37</td>
<td>2.25</td>
<td>1.77</td>
<td>-</td>
</tr>
<tr>
<td>Kelvin cell</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>open (o)</td>
<td></td>
<td>1.88</td>
<td></td>
<td></td>
<td>+6 %</td>
</tr>
<tr>
<td>closed (c)</td>
<td></td>
<td>1.73</td>
<td></td>
<td></td>
<td>+2 %</td>
</tr>
<tr>
<td>half-closed (hc)</td>
<td></td>
<td>1.81</td>
<td></td>
<td></td>
<td>-2 %</td>
</tr>
</tbody>
</table>

- foam exhibits anisotropy (Kelvin cells are isotropic)
- Kelvin cells with half-closed and closed windows give good prediction of average permeability
- effect of closed square windows is small
Comparison for effective thermal conductivity

<table>
<thead>
<tr>
<th>structure</th>
<th>effective thermal conductivity (W/mK)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>x</td>
</tr>
<tr>
<td>foam sample</td>
<td>0.91</td>
</tr>
<tr>
<td>Kelvin cell</td>
<td></td>
</tr>
<tr>
<td>open (o)</td>
<td>1.08</td>
</tr>
<tr>
<td>closed (c)</td>
<td>1.28</td>
</tr>
<tr>
<td>half-closed (hc)</td>
<td>1.18</td>
</tr>
</tbody>
</table>

- anisotropy of permeability and ETC correlate
- Kelvin cell with open windows gives best prediction of average ETC
- position of closed windows causes slight anisotropy for the half-closed Kelvin cells
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Conclusions

- accurate prediction of permeability and eff. thermal conductivity of open-cell foams require large computational domain: RVE ≈ (10 D_p)³
- optimal model structure depends on the property of interest:
  - eff. thermal conductivity: Kelvin cell with open windows (+2 %)
  - permeability: Kelvin cell w. half-closed windows (-2 %)
- idealized foam structures can reduce the computational effort by O(10³) or allow high-res simulations, e.g. for the DNS of turbulent flows

Outlook

- inclusion of additional geometric parameters to consider anisotropy:
  - anisotropy of pores by elongated Kelvin cells
  - statistics on number and orientation of closed windows
- DNS of higher Re flows: inertial coefficient and turbulence spectra
- applicability of turbulence models for turbulence inside porous media
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