EVALUATION OF PORE GEOMETRY ON POROUS CELL THERMAL BEHAVIOR

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• Investigate how heterogeneities in system composition affect thermal response of system

• “Heterogeneity” is subjective
  o Depends on aspects of interest
  o Can be found at large scale (e.g., system level) or fine scale (e.g., material level)
• Response to heterogeneity crucial in variety of thermal applications
  o E.g., gas turbine power, electronics, flame retardants, hypersonics, energy storage, geosciences, advanced materials

• Especially of interest in nuclear fuel assemblies
  o UO₂ is common nuclear material
    ▪ Satisfactory chemical & irradiation tolerance
    ▪ Porous material
    ▪ 5%-10% porosity to prevent swelling
  o Affected by mfg. processes & environmental conditions
    ▪ Pressed powder sintering at high temperatures

INTRODUCTION

APPLICATION

Example Fuel Assembly³

UO₂ Sintered Pellets²
Many different works looking at response
  - Theoretical analytical responses
    - Since late 1800s
  - Computational analyses
    - FEA, level set, resistor network, 2D, 3D

Works in literature generally not supported by verification & validation (V&V)

In the past looked at circular pores & fillers

Now looking at non-circular pore geometries
• Porous unit cell as fundamental building block of a material
• Ordered structure
• 3 basic geometries
  o Triangle, Square, and Ellipse ($R_a/R_p=2$)
• Vary size & clocking angle of pore with respect to cell & temperature gradient
  o Porosity: $\alpha$
  o Clocking angle: $\theta_a$
• Enforced domain temperature gradient
  \( T_H - T_C \)

• Varied porosity
  \( \alpha = \frac{A_\alpha}{(WL)} \)

• Varied clocking angle
  \( \theta_\alpha \)

• Induced heat flow
  \( q' \)

• Quantity of Interest (QoI)
  \( k^* = \frac{(q'L)}{(k_1W(T_H-T_C))} \)
• Unstructured triangular meshes

• Generated using Gmsh$^5$
• Characteristic mesh size
  \[ h_H = \sqrt{\left( \frac{1}{N_{h,t}} \right) \sum_{t=1}^{N_{H,t}} A_t} \]

• Systematic mesh refinement
  - 5 meshes per system geometry (H=5,4,3,2,1)
  - \( h_{H+1}/h_H \approx 2 \)

Example Systematic Mesh Refinement of Square Pore System

Notional Linear Triangle Element
• Solving governing heat equation
  \[ k \left( \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) + S = 0 \]
  - 2D, isotropic, steady-state

• Galerkin finite element method
  - Linear interpolation shape function, \( N \)
  \[ \int_{\Omega} (\nabla N)^T K \nabla N d\Omega T = \int_{\Omega} N^T S d\Omega - \int_{\Gamma} N^T q_n d\Gamma \]
• Solution
  o Implemented in Fortran
  o Conjugate gradient update
  o Exit criteria
    ▪ Heat equation Euclidean norm residual $\leq 10^{-8}$

• Post-Processing & Visualization
  o MATLAB
• **Method of Manufactured Solutions (MMS)**
  
  - Verify order of accuracy of implemented method
  - Signal existence of bugs in code

• **Formal order of accuracy for FEM: 2**

• **MMS QoI: Temperature**

• **Governing equation:**
  
  \[ k \left( \frac{\partial^2 T_{MMS}(x,y)}{\partial x^2} + \frac{\partial^2 T_{MMS}(x,y)}{\partial y^2} \right) + S_{MMS}(x, y) = 0 \]

• **Solution:**
  
  \[ T_{MMS}(x, y) = \cos(2\pi x) \sin(\pi y + 0.75) \]

• **Source Term:**
  
  \[ S_{MMS}(x, y) = 5\pi^2 k \cos(2\pi x) \sin(\pi y + 0.75) \]

• **Error (Euclidean norm and \( L_\infty \) norm metrics):**
  
  \[ \epsilon_{L_2,h} = \sqrt{\sum_{i=1}^{N_v} [T_i - T_{MMS}(x_i, y_i)]^2 / N_v} \quad \epsilon_{L_\infty,h} = \max_i |T_i - T_{MMS}(x_i, y_i)| \]
• Grid Convergence Index (GCI)
  - Used to estimate numerical uncertainty in QoI
    - QoI: $k^*$
  - Global deviation uncertainty estimator approach

\[
\hat{p} = \ln \left[ (r_{1,2}^{\hat{p}} - 1) \left( \frac{|u_{h,3} - u_{h,2}|}{u_{h,2} - u_{h,1}} \right) + r_{1,2}^{\hat{p}} \right] / \ln(r_{1,2} r_{2,3})
\]

\[
\Delta p = \min \left[ \frac{1}{N_v} \sum_{i=1}^{N_v} \min(|p_f - \hat{p}_i|, 4p_f), 0.95p_f \right]
\]

\[
p^* = p_f - \Delta p
\]

\[
FS(p^*) = F_0 - (F_0 - F_1) \left( \frac{p^*}{p_f} \right)^8
\]

\[
U_{num} = FS(p^*) \left| \frac{u_{h,2} - u_{h,1}}{r_{1,2} p^* - 1} \right|
\]
• Observed order of accuracy
  \[ p_{O,H} = \ln(\varepsilon_H/\varepsilon_{H+1}) / \ln(h_H/h_{H+1}) \]
• All geometries converge to approximately second order accurate
RESULTS
SOLUTION VERIFICATION [1]

Temperature Contours with Mesh Refinement

Temperature Contours with Varying Porosity
RESULTS

SOLUTION VERIFICATION [2]

- $k^*$ for variable geometry
  - Triangle: [5,35]%, [0,30]$^\circ$
  - Square: [5,45]%, [0,45]$^\circ$
  - Ellipse: [5,35]%, [0,90]$^\circ$

- Rotational symmetry
RESULTS
SOLUTION VERIFICATION [3]

- GCI method for $U_{num}$
- Variable geometry
  - Triangle: [5,35]%, [0,30]°
  - Square: [5,45]%, [0,45]°
  - Ellipse: [5,35]%, [0,90]°

Approximate Numerical Uncertainty for Square Pore Systems
Approximate Numerical Uncertainty for Triangular Pore Systems
Approximate Numerical Uncertainty for Elliptical Pore Systems
• Non-physical correlation

\[ f_{\text{corr}} = a_0 + a_1 \alpha + a_2 \alpha^2 + \ldots + (a_3 \alpha + a_4 \alpha^2) \theta \alpha + (a_5 \alpha + a_6 \alpha^2) \theta^2 \alpha \]

<table>
<thead>
<tr>
<th></th>
<th>Triangle</th>
<th>Square</th>
<th>Ellipse</th>
</tr>
</thead>
<tbody>
<tr>
<td>( a_0 )</td>
<td>1.0000\times10^0</td>
<td>1.0000\times10^0</td>
<td>1.0000\times10^0</td>
</tr>
<tr>
<td>( a_1 )</td>
<td>-2.3917\times10^0</td>
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<td>1.0336\times10^0</td>
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<td>( a_6 )</td>
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<td>-1.3531\times10^{-5}</td>
<td>-4.3940\times10^{-7}</td>
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</tbody>
</table>
• Conclusions
  o Covered range of 2D structures
  o 2nd order accurate numerical method
  o Numerical error estimation using GCI method
  o Low (<6%) error correlations for $k^*$

• Future Work
  o Propagate numerical uncertainty into correlations
  o Variation in polygonal pore internal angle ratios
  o Variation in elliptical pore aspect ratios
ACKNOWLEDGMENTS

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