Verification and Model Sensitivity Analyses for Computational Fluid Dynamics Simulations of Wire-Wrapped Nuclear Fuel Assemblies

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ASME Verification and Validation Symposium

May 18-20

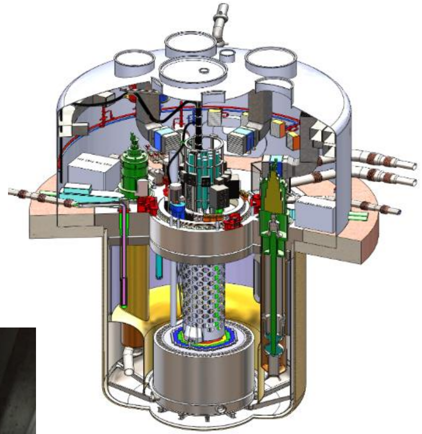
Las Vegas, NV

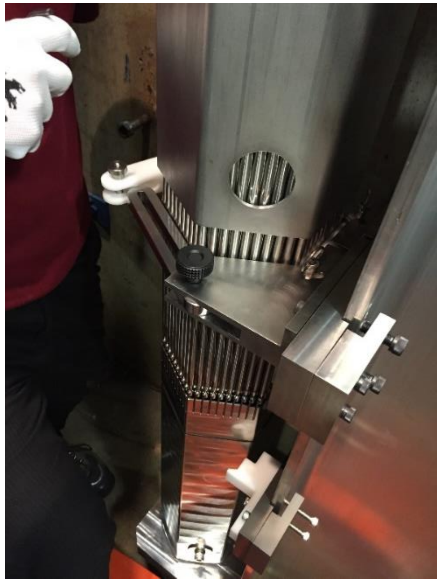
Outline

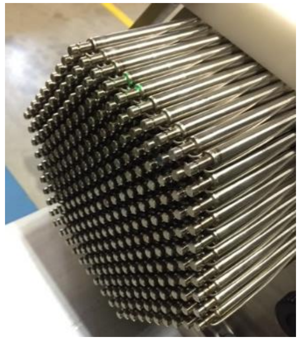
- TerraPower & Advanced Fuel Assembly Flow Characterization Project description
- Code verification
  - Approach (Method of Manufactured Solutions)
  - Order of accuracy results
- Solution verification
  - Geometry, approach, & meshes
  - Mesh refinement results
- Sensitivity studies
  - Turbulence models
  - Momentum source coefficient
- Summary & future work

TerraPower

- TerraPower was started by Bill Gates, Nathan Myhrvold, & others after invention session in 2006. Privately funded.
- Goal: Investigate advanced fission reactors for world-scale energy production
- Key requirements included high fuel utilization, low barriers to exportation, enhanced safety, and improved cost
- Traveling Wave Reactor was chosen
  - "Breed-and-burn" concept enables fast reactor without reprocessing
  - Has been discussed in literature since at least 1958
- Sodium Fast Reactors utilize ducted fuel assemblies with helically wire-wrapped fuel pins
  - Pressure difference, thermal creep, and irradiation cause ducts and pins to deform over time
  - Prediction of thermal and flow performance vital to overall reactor performance and safety







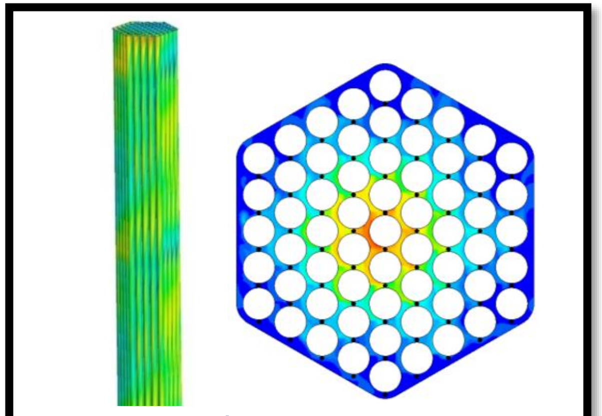
Mock-up of simulated wire-wrapped fuel pin

Advanced Fuel Assembly Flow Characterization

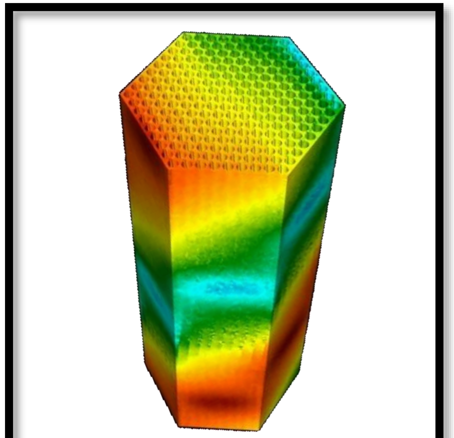
- DOE grant project consisting of experiments and numerical simulations of wire-wrapped bundles (non-deformed & deformed) for verification and validation of CFD tools

TerraPower

- Technical Lead
- Experiment Design
- **Industrial-Level (RANS) Verification & Validation Simulations**



TP Designed 61 Pin Experiment



Wire Wrap Bundle Simulation Expertise

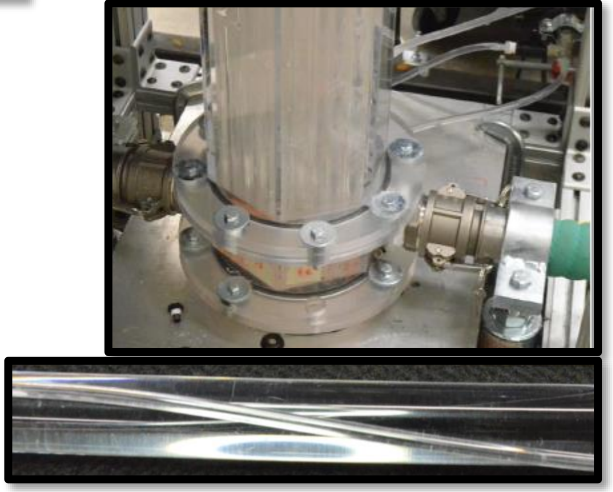
Argonne NATIONAL LABORATORY

- High Resolution (LES) Validation Simulations

AREVA

- Programmatic Lead
- Heated Bundle Experiments in Water
- Pressure & Temperature Measurements

Heated Bundle Test Expertise



Flow Visualization Expertise

TEXAS A&M UNIVERSITY®

- Isothermal Bundle Experiments in P-Cymene
- Pressure & Laser Based Velocity Measurements

Industry-Level V&V Simulations of Wire-Wrapped Bundles

- Previous wire-wrapped experiments were not designed with CFD V&V in mind & none take later-in-life geometric deformations into account
- Code Verification (Method of Manufactured Solutions)
- Pre-Test medium-fidelity RANS simulations
  - Simulations with designed geometries (momentum source used in place of wire-wrapping)
  - Solution verification simulations
  - Model sensitivity simulations
  - Compare blind simulations with experimental results when they become available
- Post-Test RANS simulations
  - Simulations with as-built geometry and measurement locations
  - Validation with experiments
  - Choice of optimal approach/models

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Code Verification

1. Verify Star-CCM+ commercial code for TerraPower's core design efforts
2. Start with simple equations & build physics & models until consistent with core design CFD modeling
3. Use Method of Manufactured Solutions (MMS) to obtain exact solutions

Establish math model	$\mathcal{L}(u) = 0$
Choose the solution *a priori*	$\hat{u}$
Operate PDE onto solution to obtain analytical source term	$s = \mathcal{L}(\hat{u})$
Insert source term into PDE (the new PDE now has the chosen exact solution)	$\mathcal{L}(u) = s$

4. Conduct Order of Accuracy studies for most rigorous code verification

$$\varepsilon_h = u_h - \tilde{u}$$

Discretization Error (ε_h), **Discrete Solution** (u_h), **Exact Solution** ($\tilde{u}$)

$$\|\varepsilon_h\|_2 = \left(\frac{1}{\Omega}\int_\Omega |\varepsilon_h|^2 d\omega\right)^{1/2}$$

L_2 Norm (global error)

$$\hat{p} = \frac{\ln\left(\frac{\|\varepsilon_{rh}\|}{\|\varepsilon_h\|}\right)}{\ln(r)}$$

Observed Order of Accuracy

$$r \equiv \frac{h_{\text{coarse}}}{h_{\text{fine}}}$$

Grid Refinement Factor (**Cell Size Ratio**)

5. Troubleshoot if Observed Order of Accuracy (OOA) does not match Formal Order of Accuracy (FOA)

Governing Equations

Manufactured Solution

- Analytic functions w/ smooth derivatives
- No need to be physically realistic

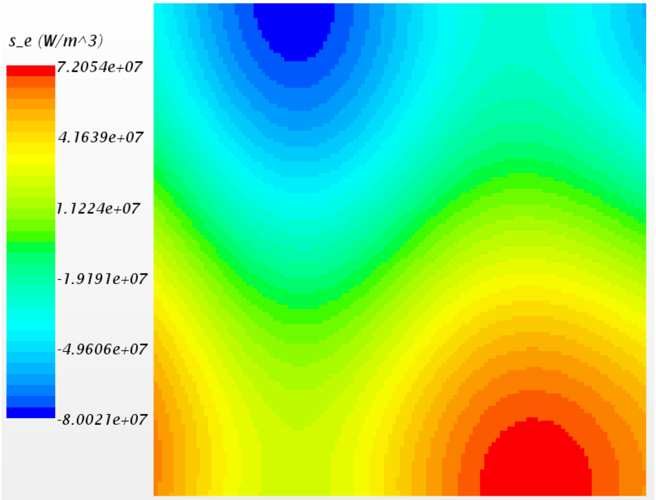
$$\rho(x,y) = \rho_0 + \rho_x \sin\left(\frac{a_{\rho x}\pi x}{L}\right) + \rho_y \cos\left(\frac{a_{\rho y}\pi y}{L}\right)$$

$$u(x,y) = u_0 + u_x \sin\left(\frac{a_{ux}\pi x}{L}\right) + u_y \cos\left(\frac{a_{uy}\pi y}{L}\right)$$

$$v(x,y) = v_0 + v_x \cos\left(\frac{a_{vx}\pi x}{L}\right) + v_y \sin\left(\frac{a_{vy}\pi y}{L}\right)$$

$$p(x,y) = p_0 + p_x \cos\left(\frac{a_{px}\pi x}{L}\right) + p_y \sin\left(\frac{a_{py}\pi y}{L}\right)$$

Analytical source term s_e for energy equation



2D Subsonic Steady Ideal-Gas Euler Equations

$$\frac{\partial(\rho u)}{\partial x} + \frac{\partial(\rho v)}{\partial y} = s_m(x,y)$$

$$\frac{\partial(\rho u^2 + p)}{\partial x} + \frac{\partial(\rho u v)}{\partial y} = s_x(x,y)$$

$$\frac{\partial(\rho v u)}{\partial x} + \frac{\partial(\rho v^2 + p)}{\partial y} = s_y(x,y)$$

$$\frac{\partial(\rho u e_t + p u)}{\partial x} + \frac{\partial(\rho v e_t + p v)}{\partial y} = s_e(x,y)$$

$$p = \rho R T$$

Equation, ϕ	ϕ_0	ϕ_x	ϕ_y	ϕ_z	$a_{\phi x}$	$a_{\phi y}$	$a_{\phi z}$
ρ (kg/m^3)	1.	0.15	-0.1	0.	1.	0.5	0.
u (m/s)	70.	5.	-7.	0.	1.5	0.6	0.
v (m/s)	90.	-15.	8.5	0.	0.5	2./3.	0.
w (m/s)	0.	0.	0.	0.	0.	0.	0.
p (N/m^2)	$1.\times10^5$	0.2×10^5	0.5×10^5	0.	2.	1.	0.

***Verification of a Compressible CFD Code using the Method of Manufactured Solutions*, Roy et al. AIAA 2002**
Table A.2 – Constants for 2D Euler Subsonic Manufactured Solution

Solver & Boundary Conditions

- Segregated Flow w/ default expert properties
- Segregated Fluid Temperature w/ default expert properties
- Gradients - Hybrid Gauss-LSQ, Venkatakrishnan limiters, default expert properties
- Two Dimensional, Steady, Inviscid, Ideal Gas
- Mass, energy, and momentum sources determined with manufactured solutions

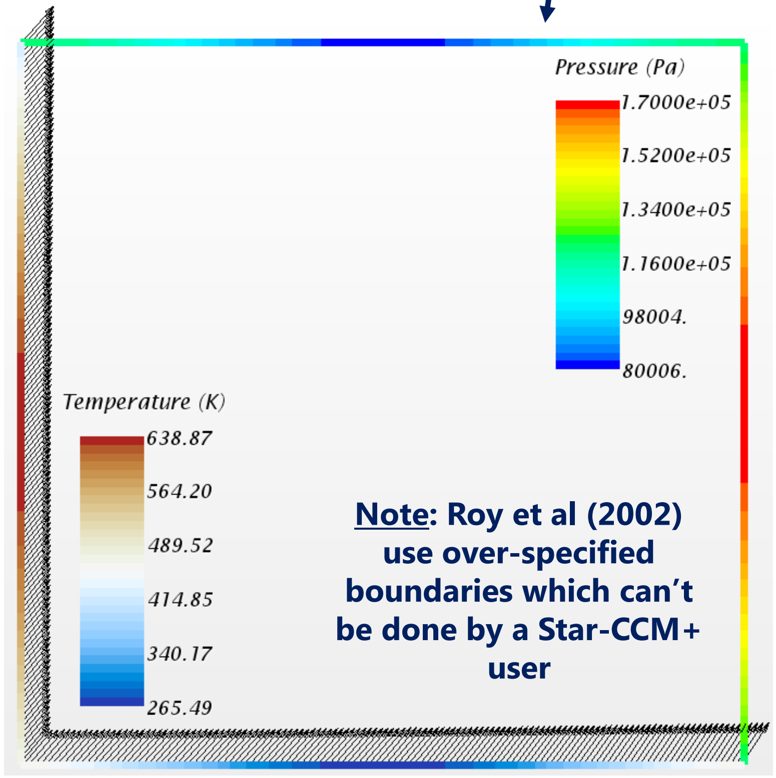
Mesh created with Star-CCM+ 2D mesher of LxL box (L = 1m)

Refinement levels:

h	16	8	4	2	1
Cells	8x8	16x16	32x32	64x64	128x128

Pressure Outlets

- *Specified Pressure with manufactured solution*
- *Velocity & Temperature extrapolated from interior using reconstruction gradients*
- *No inflow occurs!*

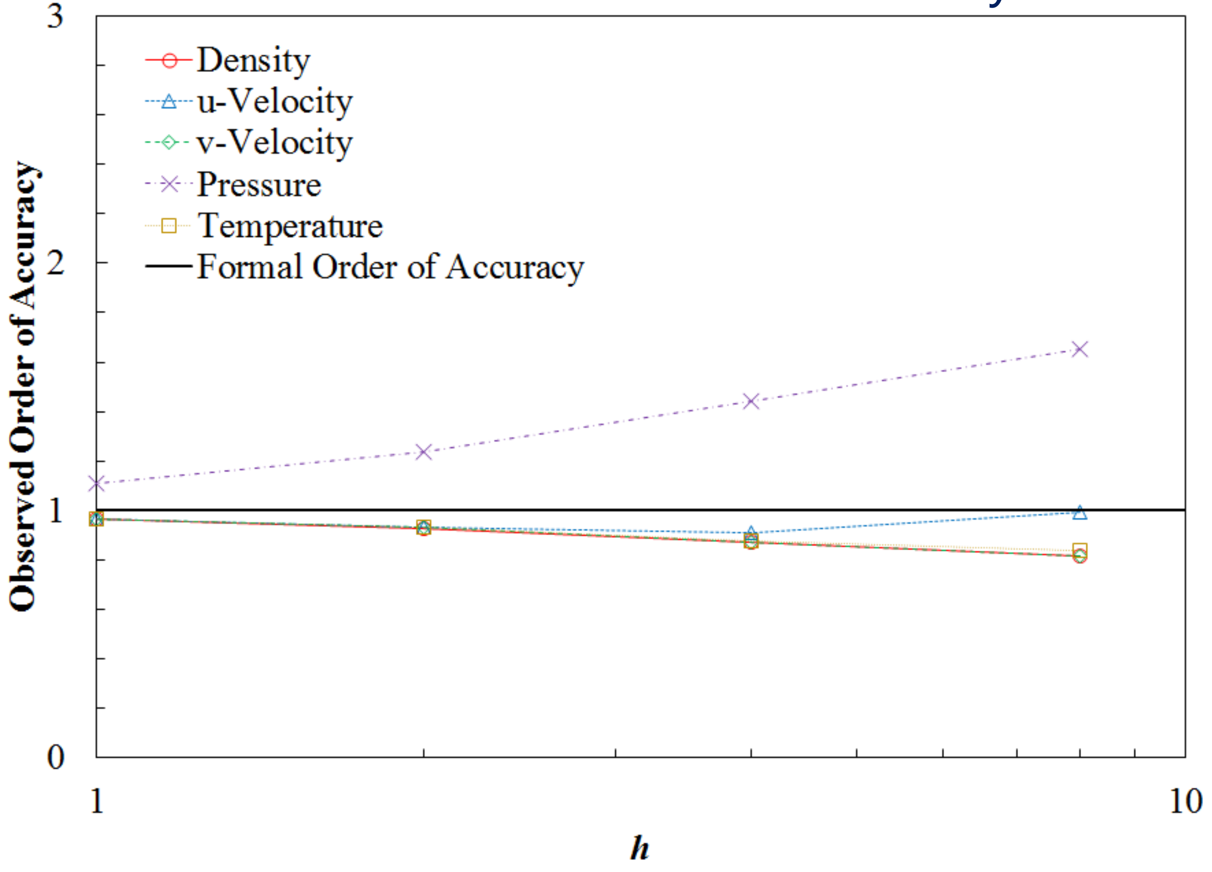


Velocity Inlets

- *Specified Velocity & Temperature with manufactured solution*
- *Pressure extrapolated from interior using reconstruction gradients*
- *No outflow occurs!*

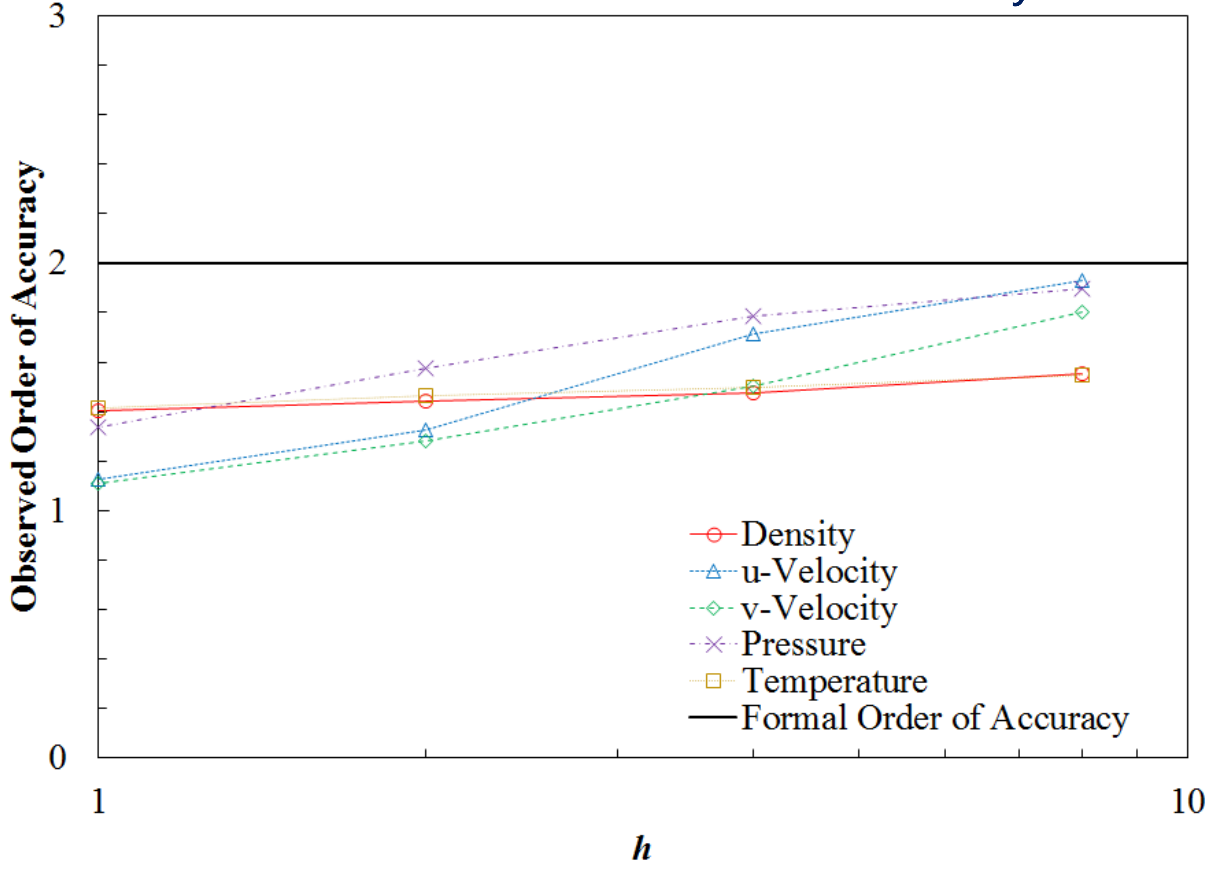
Results

1st-Order Formal Order of Accuracy



Observed Order of Accuracy approaches Formal Order of Accuracy with refinement

2nd-Order Formal Order of Accuracy



Observed Order of Accuracy drops well below Formal Order of Accuracy with refinement

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Current & Future Code Verification Work

- Working with CD-Adapco to resolve issue with 2nd-Order
  - Development team is checking simulation with over-specified BCs
- Have expanded MMS to Navier-Stokes equations
- Currently working on implementing RANS with two-equation turbulence models
- Future Work
  - Apply to 3D
  - Expand method to include all models required for core validation simulations

Solution Verification

- Round-Off Error investigated by testing simulation with both mixed and double precision
  - Results show no appreciable variation
- Iterative Error minimized by converging residuals to machine zero for all simulations
- Statistical Sampling Error not an issue
  - Variables of interest show no appreciable variation with iterations after solution is converged
- Conduct systematic mesh refinement and analyze variables of interest to determine if asymptotic range has been reached
- Perform Richardson Extrapolation to estimate discretization error

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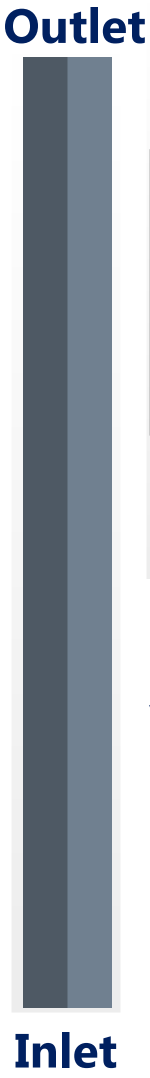
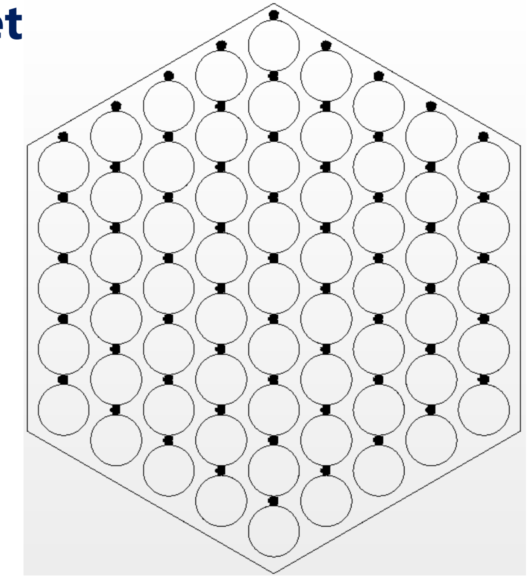
Geometry

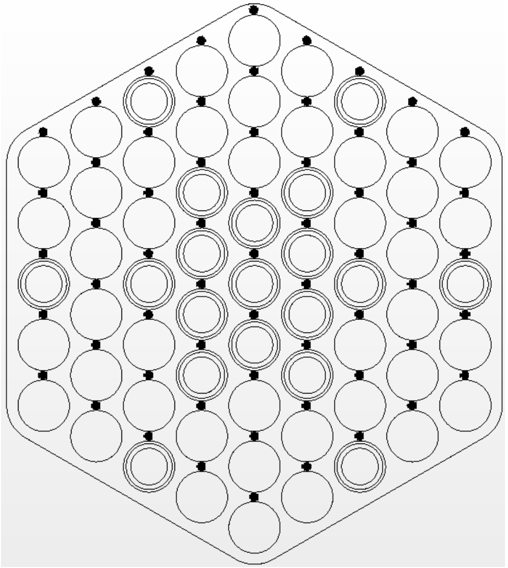
Isothermal

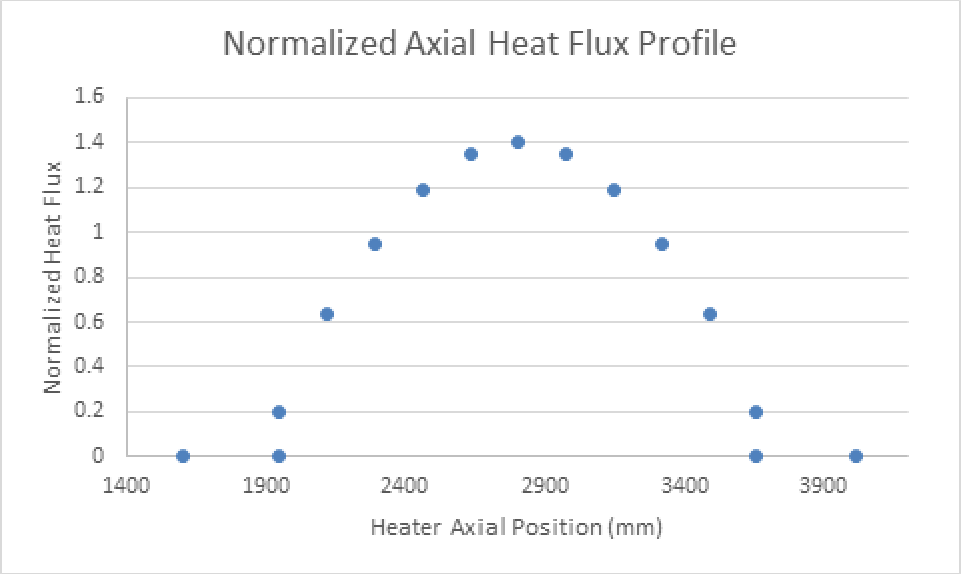




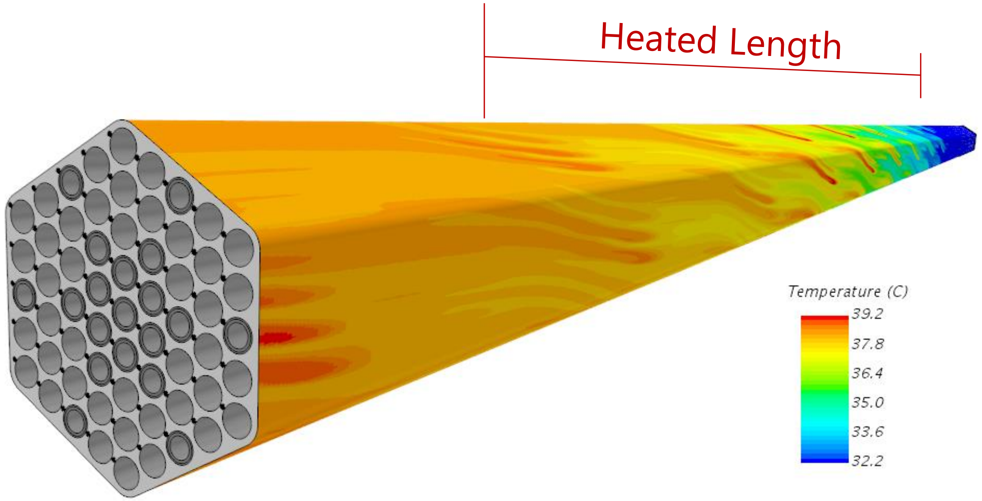
Pin Diameter = 15.9 mm
Wire Diameter = 3 mm
Duct Length = 1667 mm
Duct Wall Gap = 0.77% of flat-to-flat
3.5 wire pitches
P-Cymene
Re = 20,000
P/D = 1.189

Heated

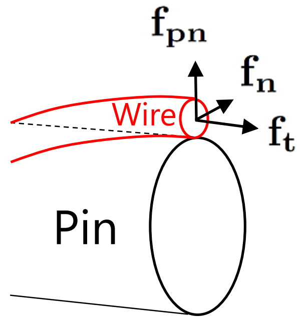




Pin Diameter = 9.5 mm
Wire Diameter = 1.73 mm
Duct Length = 3705 mm
Duct Wall Gap = 0.77% of flat-to-flat
13 wire pitches
6 heated pitches
19 heated pins (24 kW per pin)
Water
Re = 20,000
P/D = 1.18



Approach

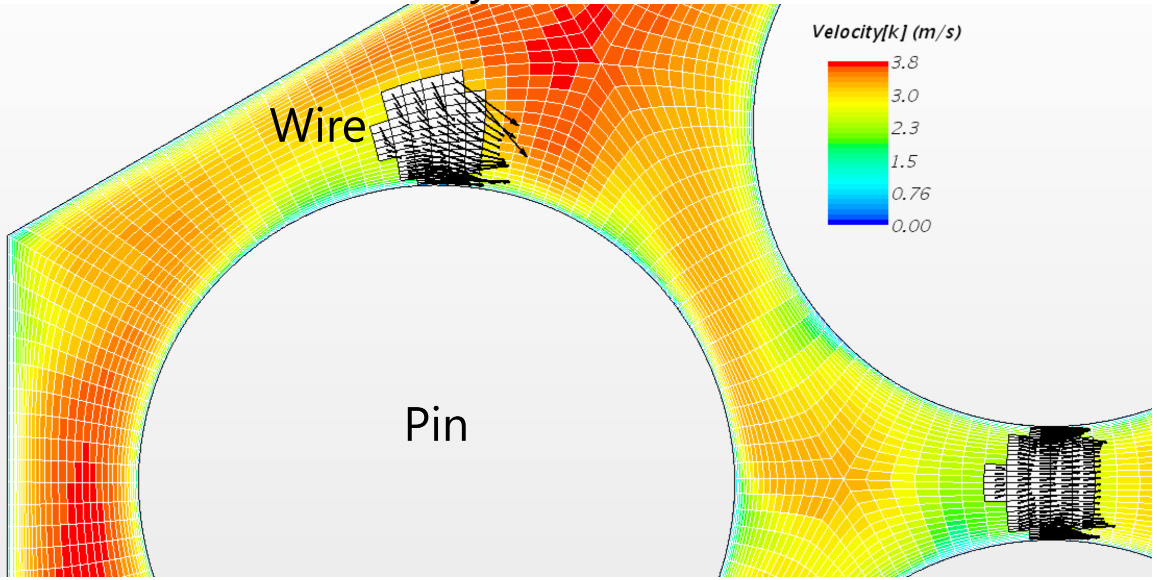


- Momentum Source to represent wire-wrapping
  - Applies body force per unit volume to the fluid momentum equation at cell locations of the wire wrap in place of a body-fitted mesh around the solid wire
  - Originally developed at Argonne National Lab [Hu & Fanning, 2011]
  - Forces are dictated by models based on the local velocity field
  - For the normal forces a multiplication coefficient is present to prevent flow through the wire surface. It's value is included in the sensitivity study

$$\mathbf{f} = \mathbf{f_n} + \mathbf{f_{pn}} + \mathbf{f_t}$$

- $\mathbf{f}$: Body Force
- $\mathbf{f_n}$: Normal to the wire and tangential to the pin
- $\mathbf{f_{pn}}$: Normal to the pin and normal to the wire
- $\mathbf{f_t}$: Tangential to the centerline of the helically-wrapped wire

<u>Body force vectors</u>



- Momentum source is ideal for initial scoping studies of wire-wrap fuel assemblies
  - Medium fidelity approach reduces computational cost
  - Avoids complications due to body fitted meshing of wires
  - Quick turn-around time for design modifications

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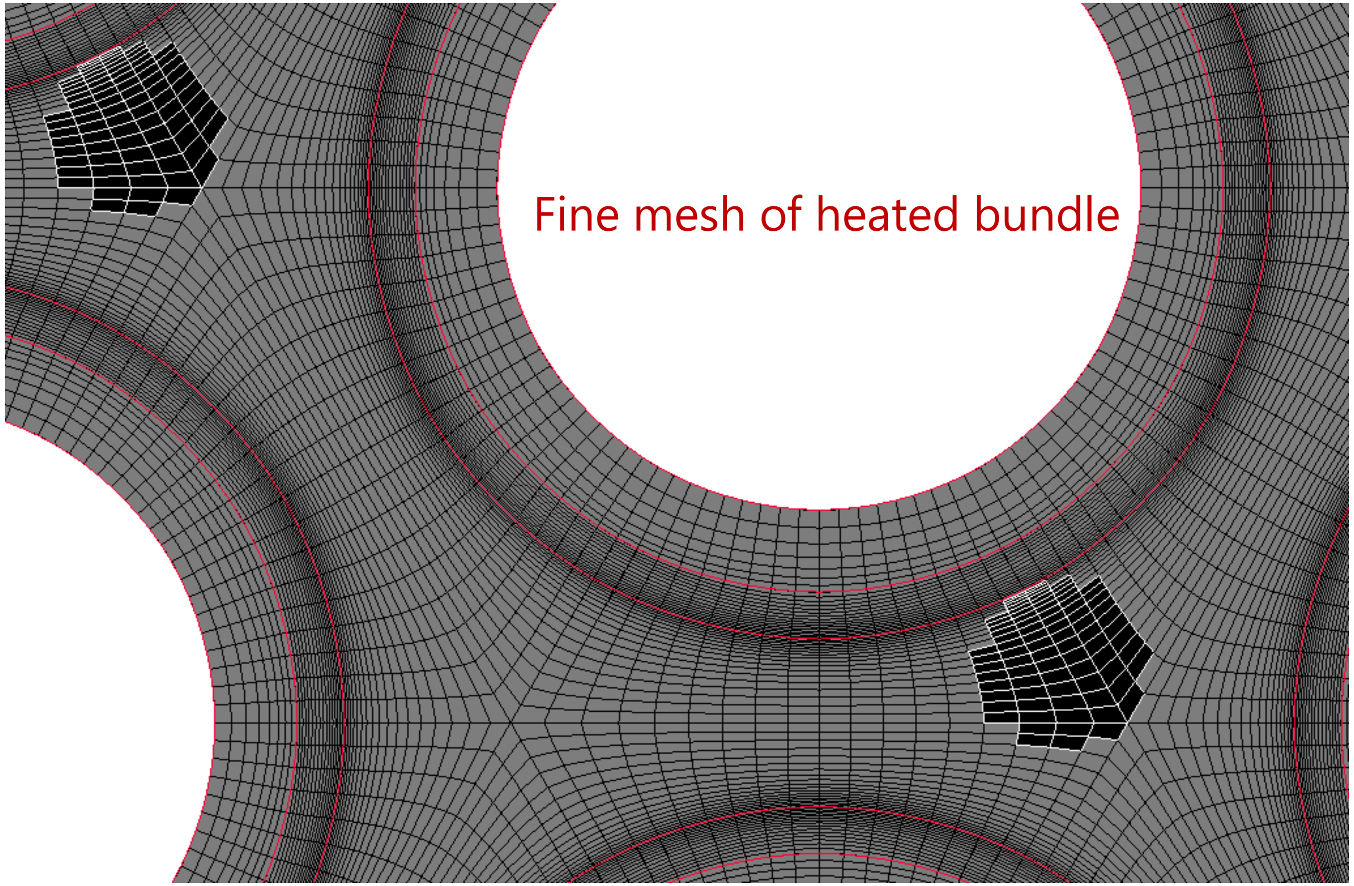
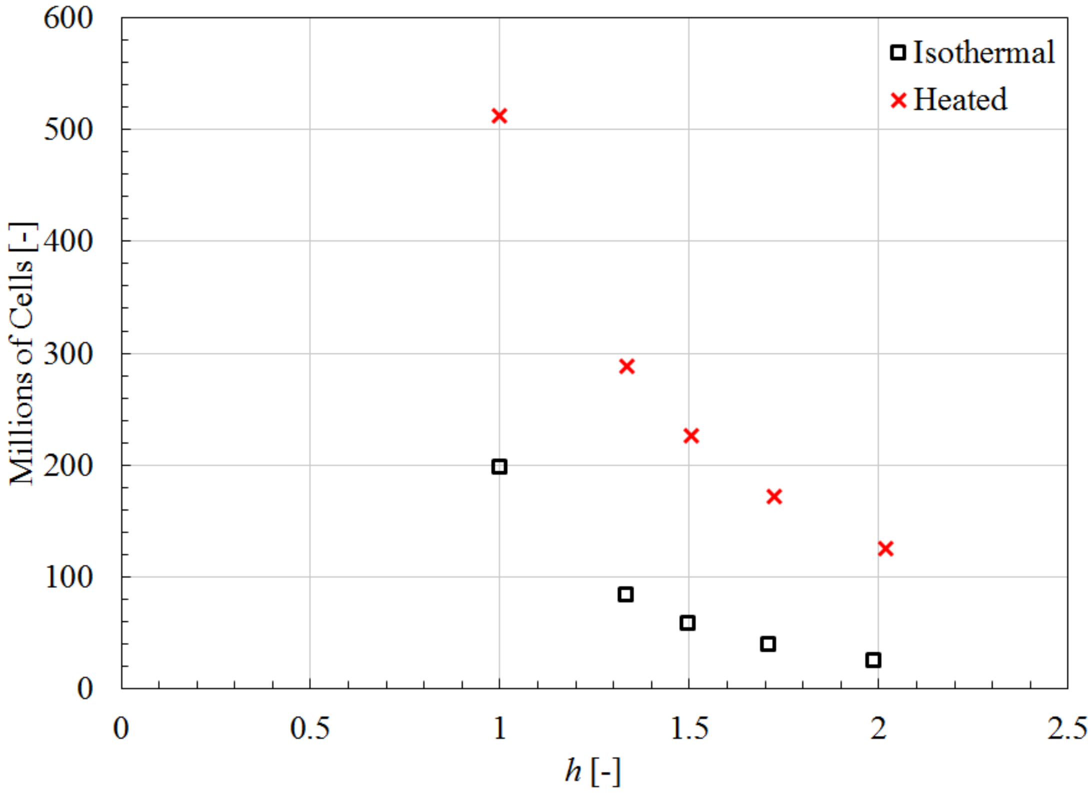
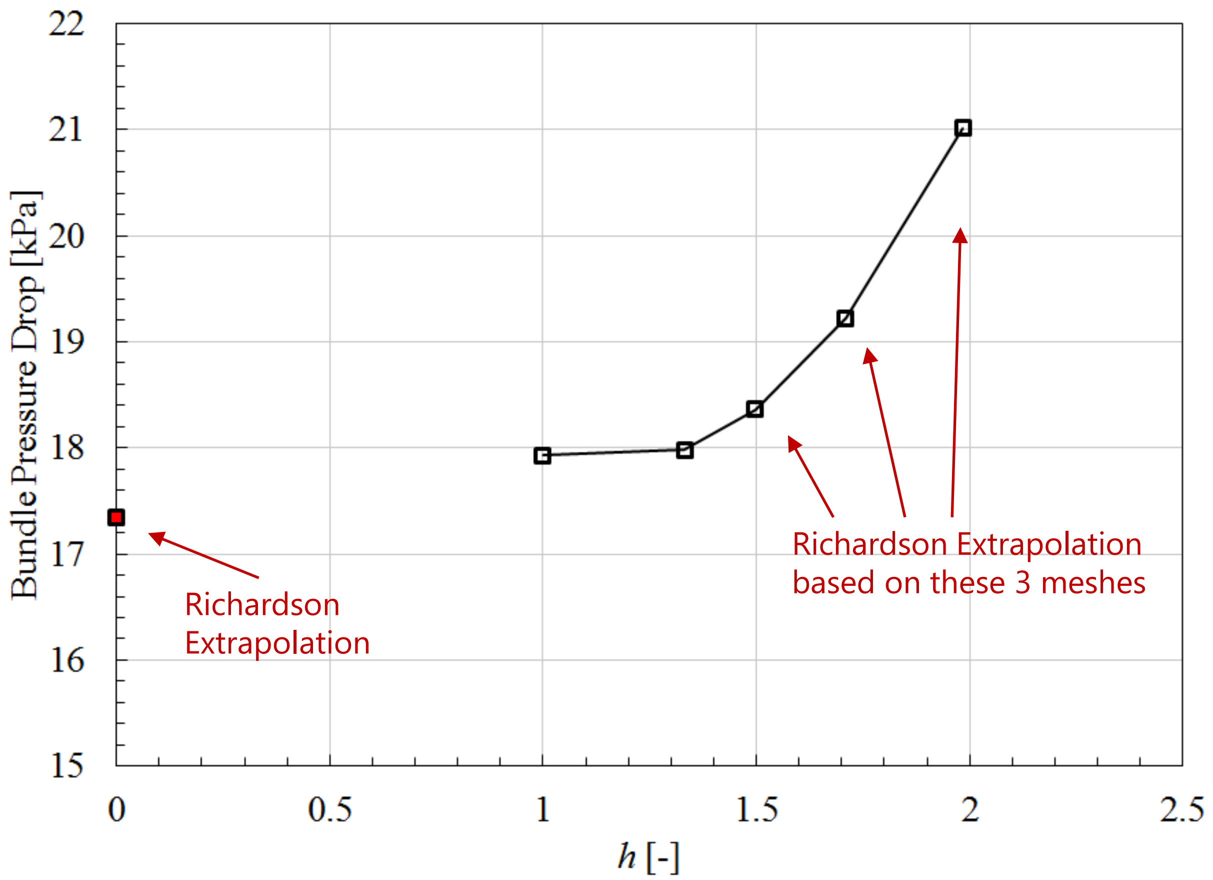
Meshes

- Fully structured meshes created with GridPro and systematically refined
- Using All-y^+ wall functions
- Average y^+ values less than 5.0 for all meshes





Isothermal Mesh Sensitivity



Observed Order of Accuracy	% Error between h=1.98 and RE	% Error between h=1.5 and RE	% Error between h=1.33 and RE	DE Estimate using h=1.33 Mesh [Pa]
4.32	21	6	3.7	642.5

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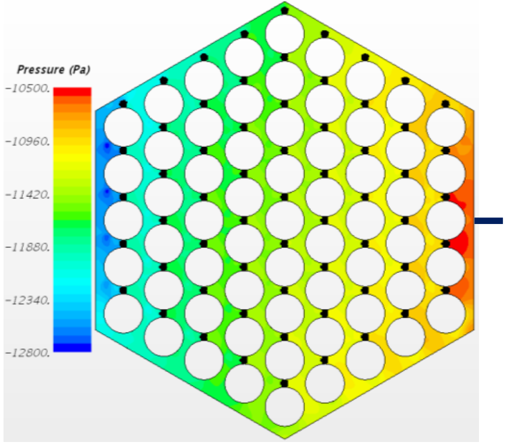
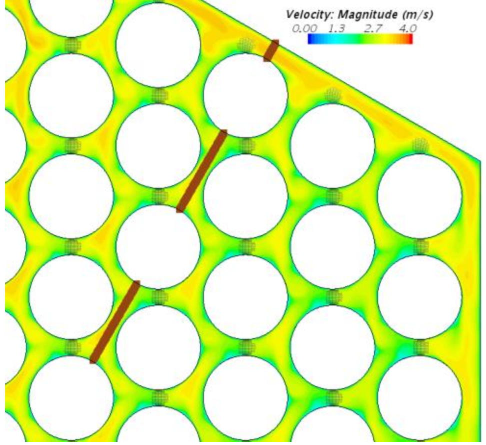
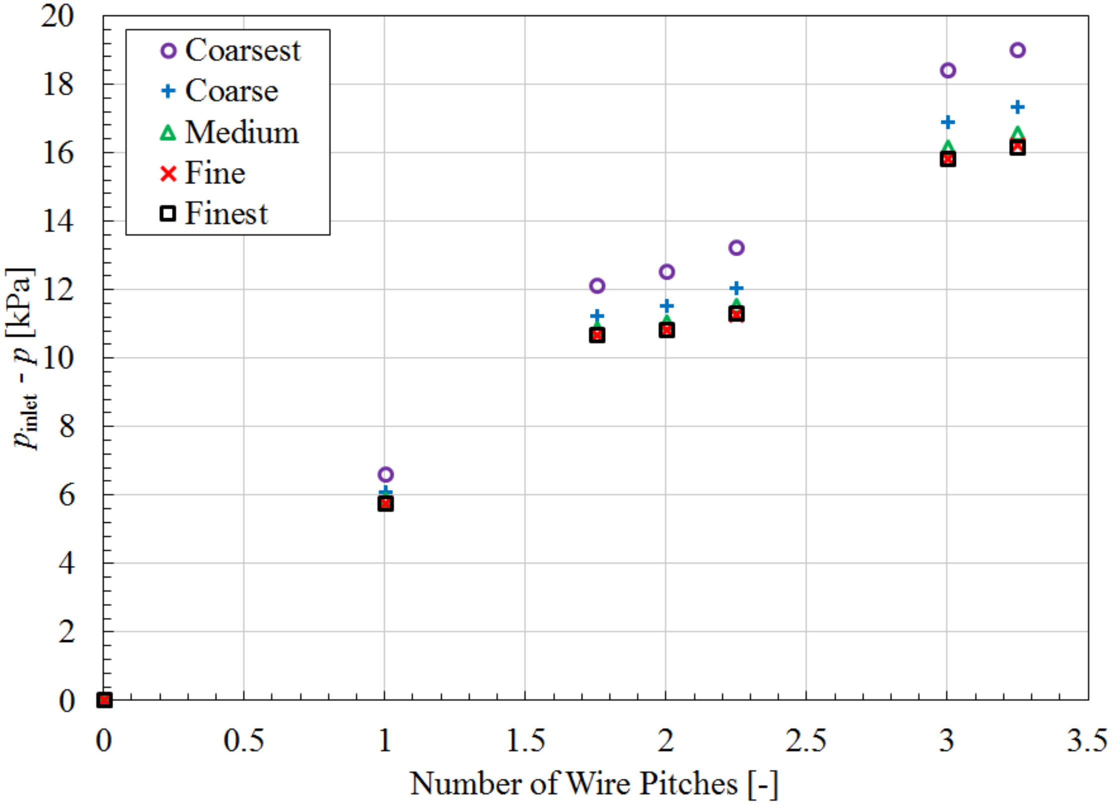
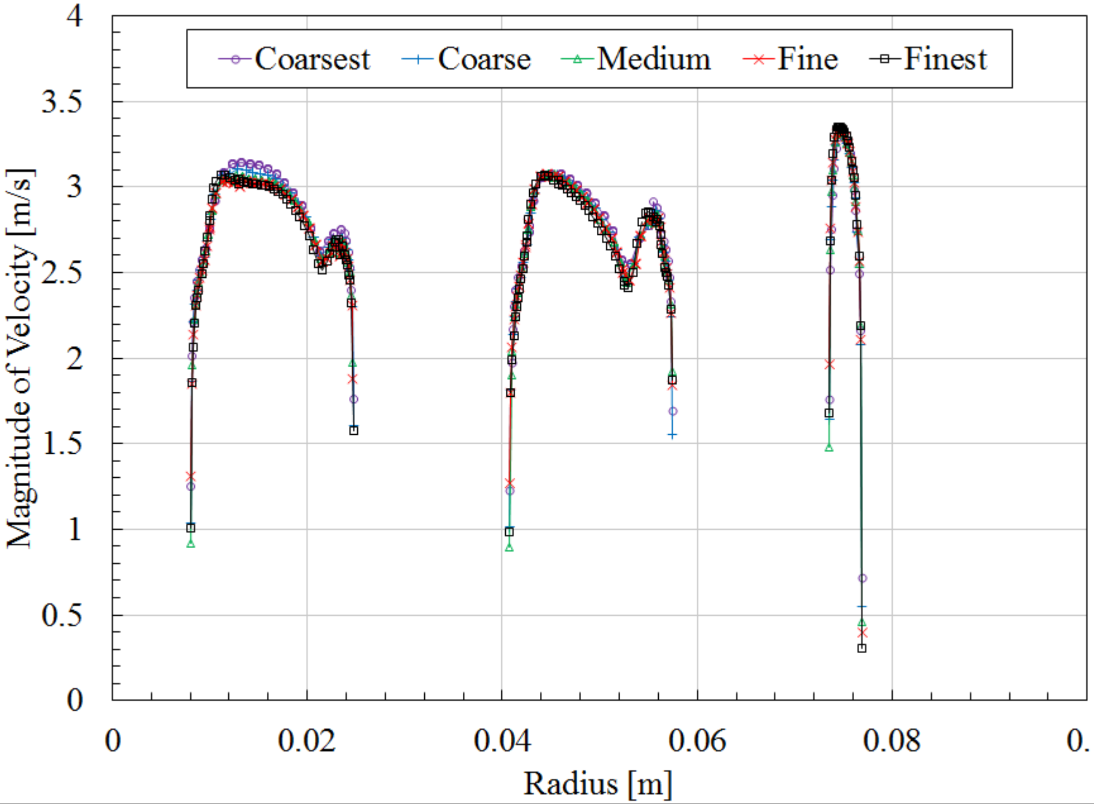
Isothermal Mesh Sensitivity







Wall probe Δp show similar convergence to bundle Δp



Velocity magnitude profiles show little variation with mesh size

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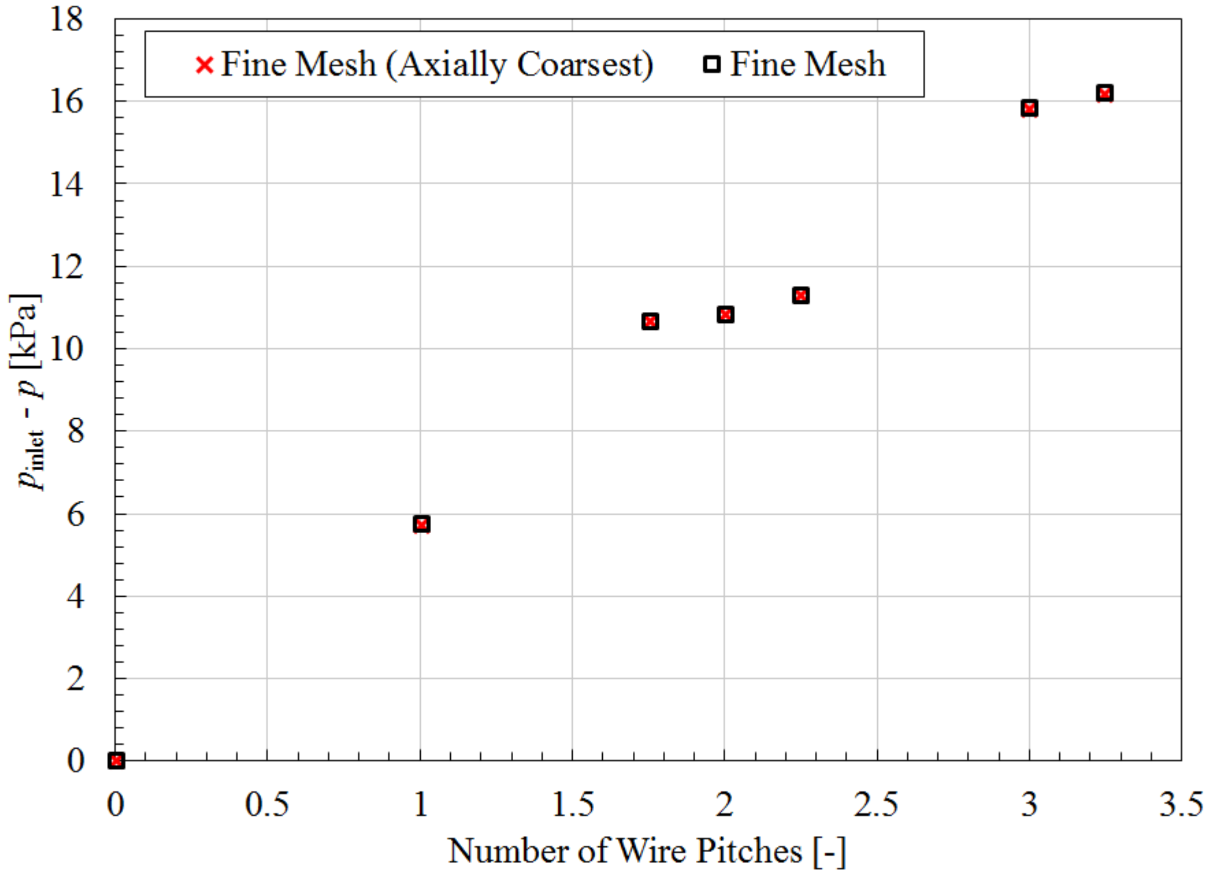
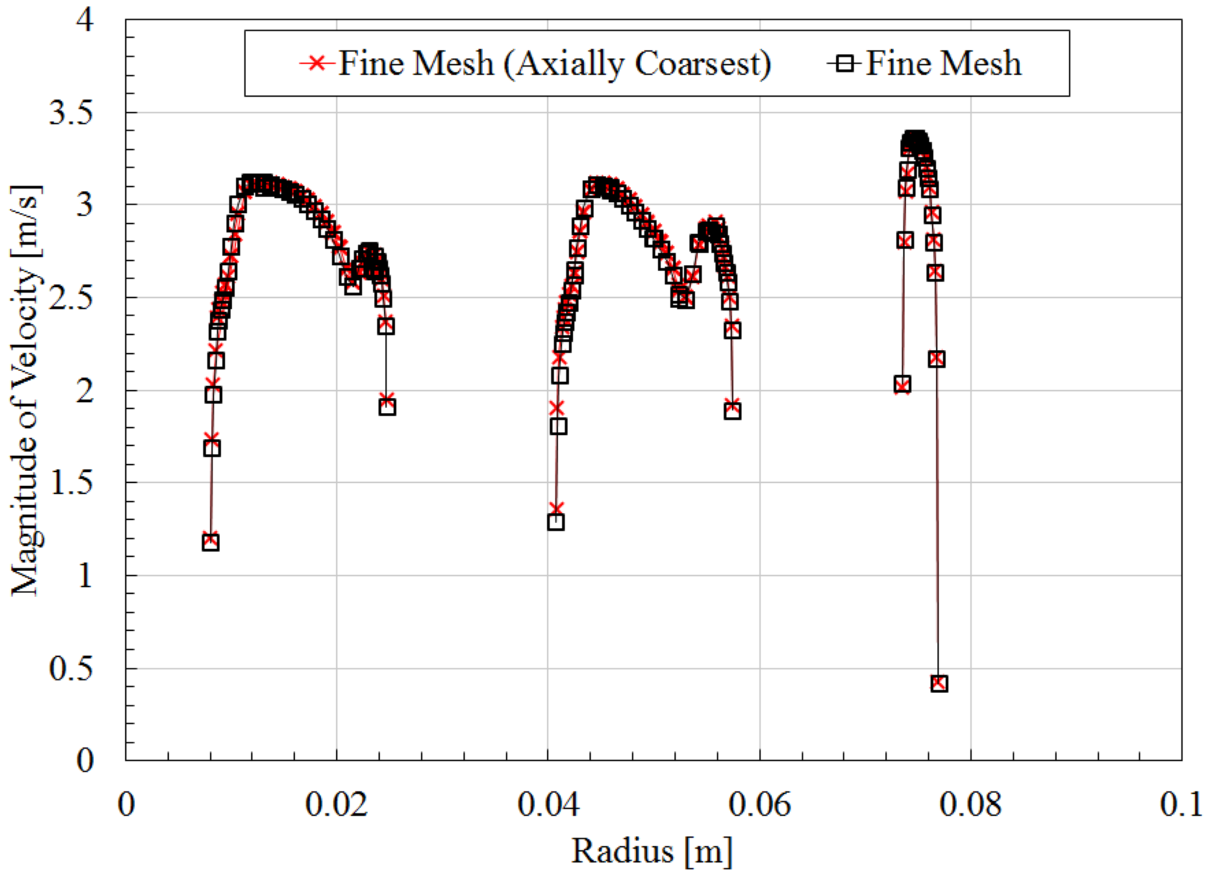
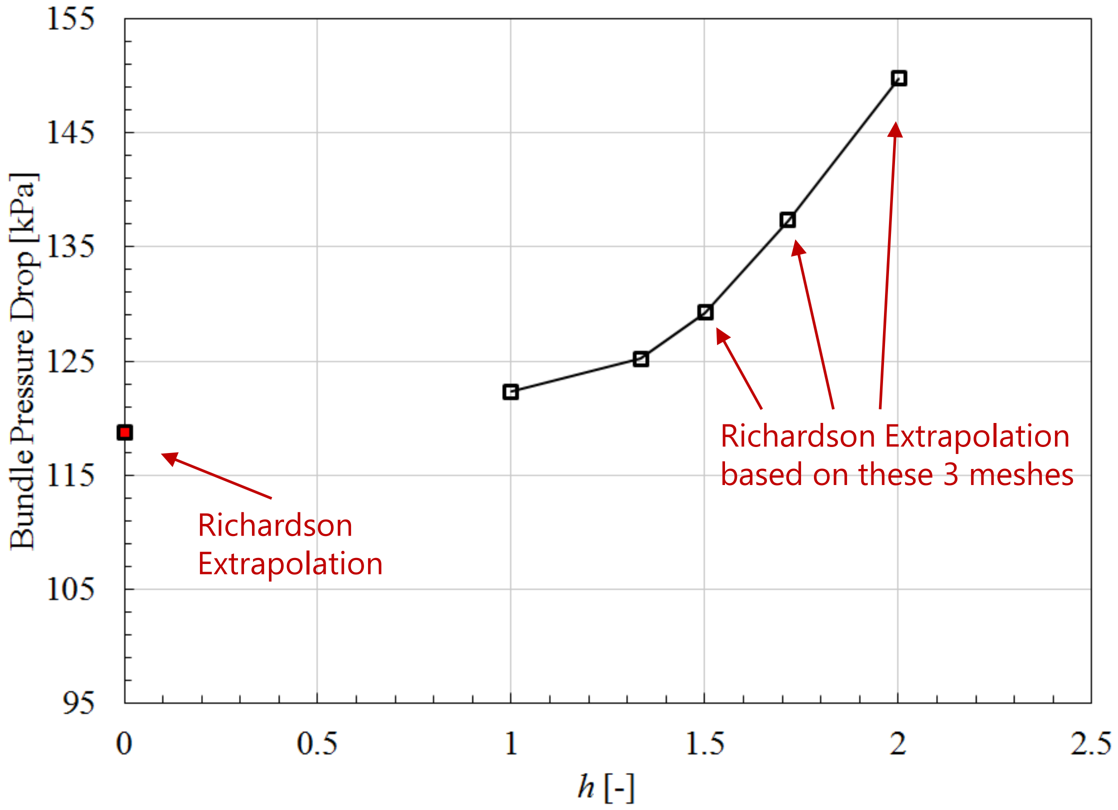
Axially Coarsening the Fine Mesh

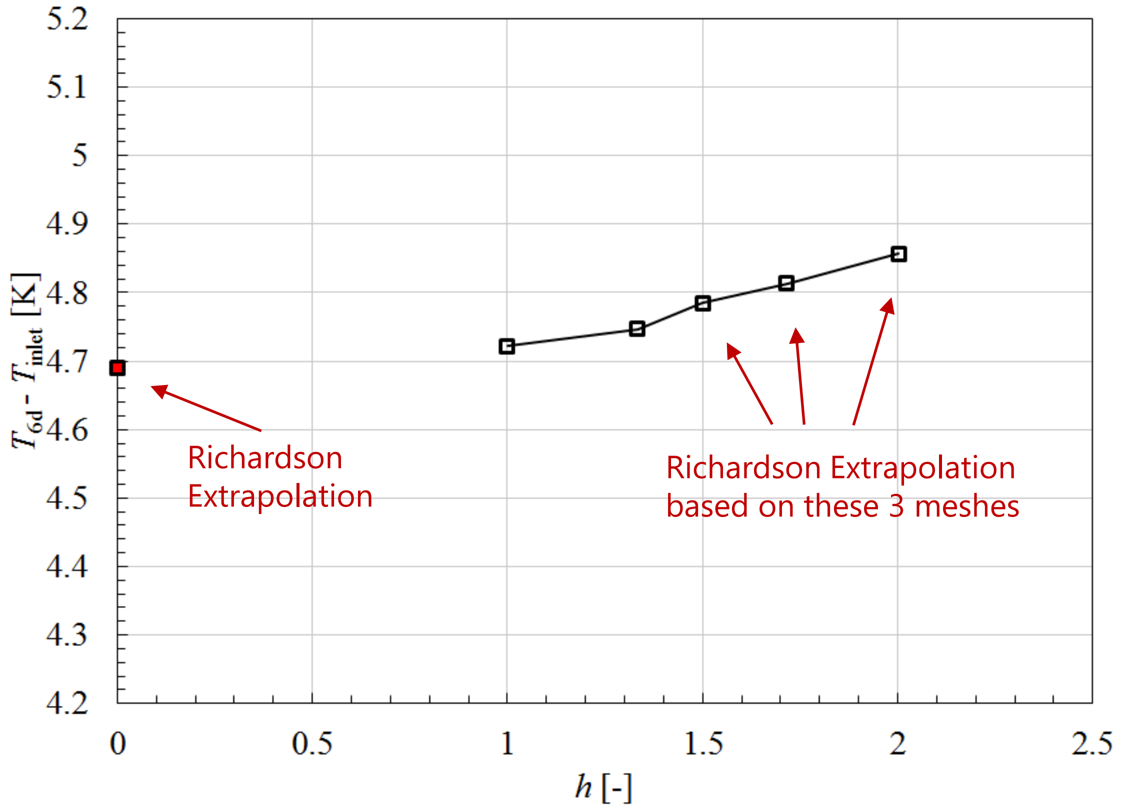




Axially coarsening fine mesh to number of axial cells in the coarsest mesh gives same results
Cell reduction of 27 million cells (32 % reduction)

Heated Mesh Sensitivity





Observed Order of Accuracy	% Error between h=2.0 and RE	% Error between h=1.5 and RE	% Error between h=1.33 and RE	DE Estimate using h=1.33 Mesh [Pa]
1.92	26.16	8.86	5.46	6485

Observed Order of Accuracy	% Error between h=1.98 and RE	% Error between h=1.5 and RE	% Error between h=1.33 and RE	DE Estimate using h=1.33 Mesh [K]
2.05	3.56	2.03	1.21	0.057

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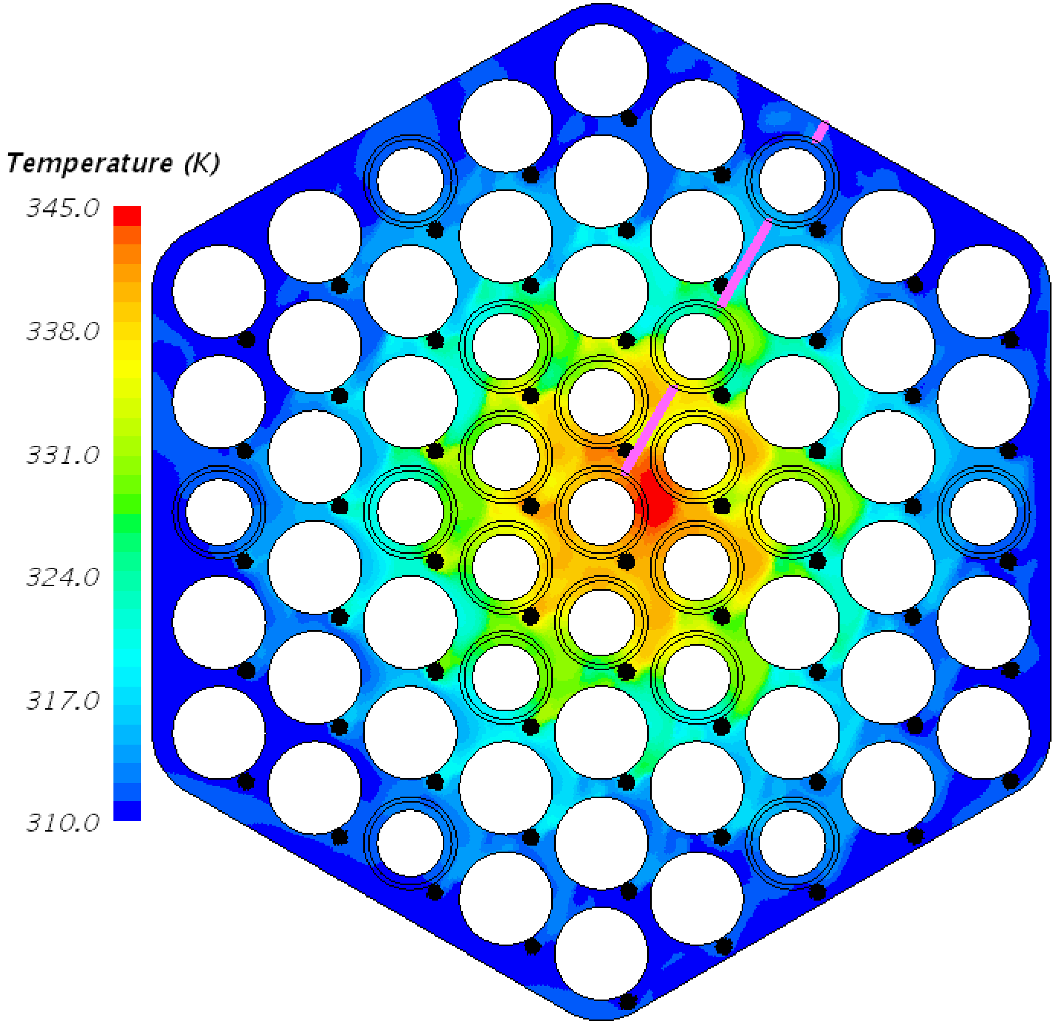
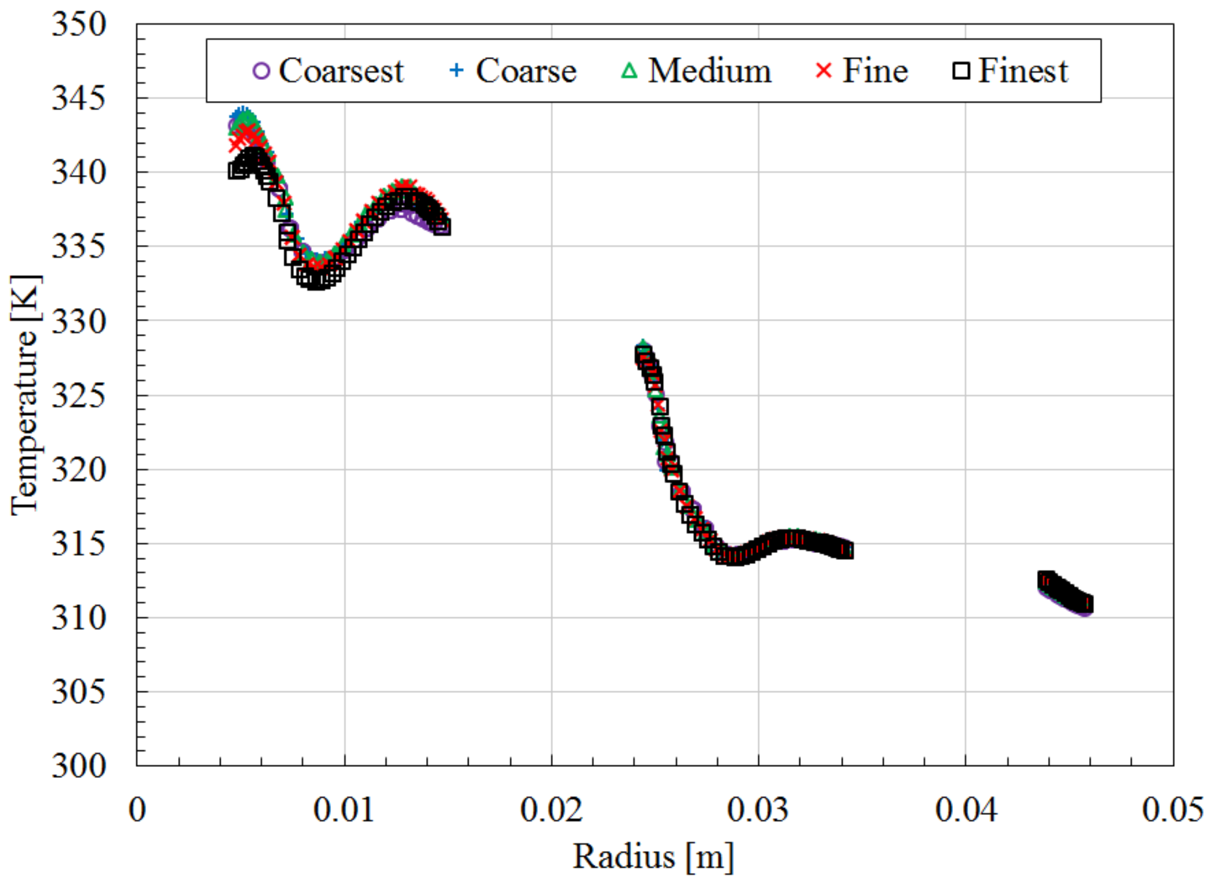
Heated Mesh Sensitivity



Probe points just above heated region



Temperature profiles show little sensitivity to mesh refinement

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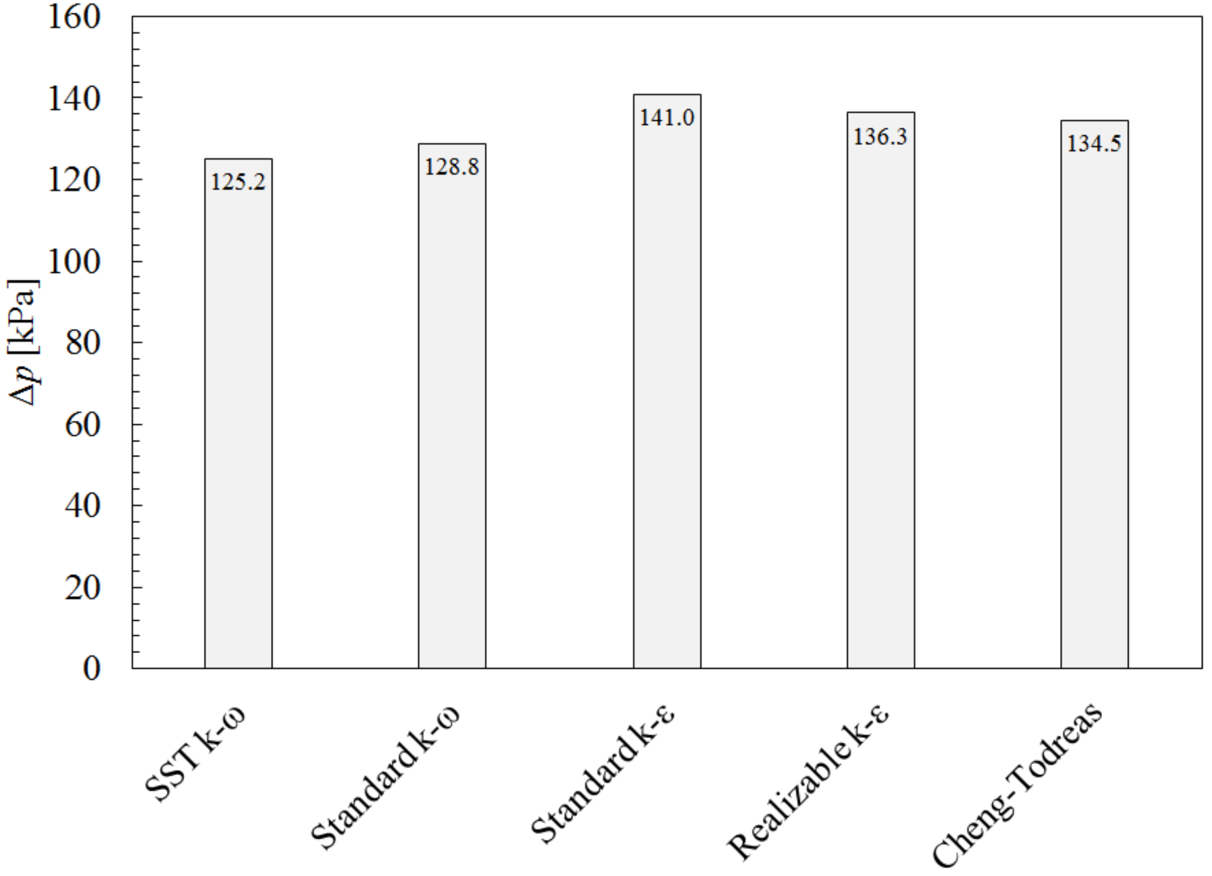
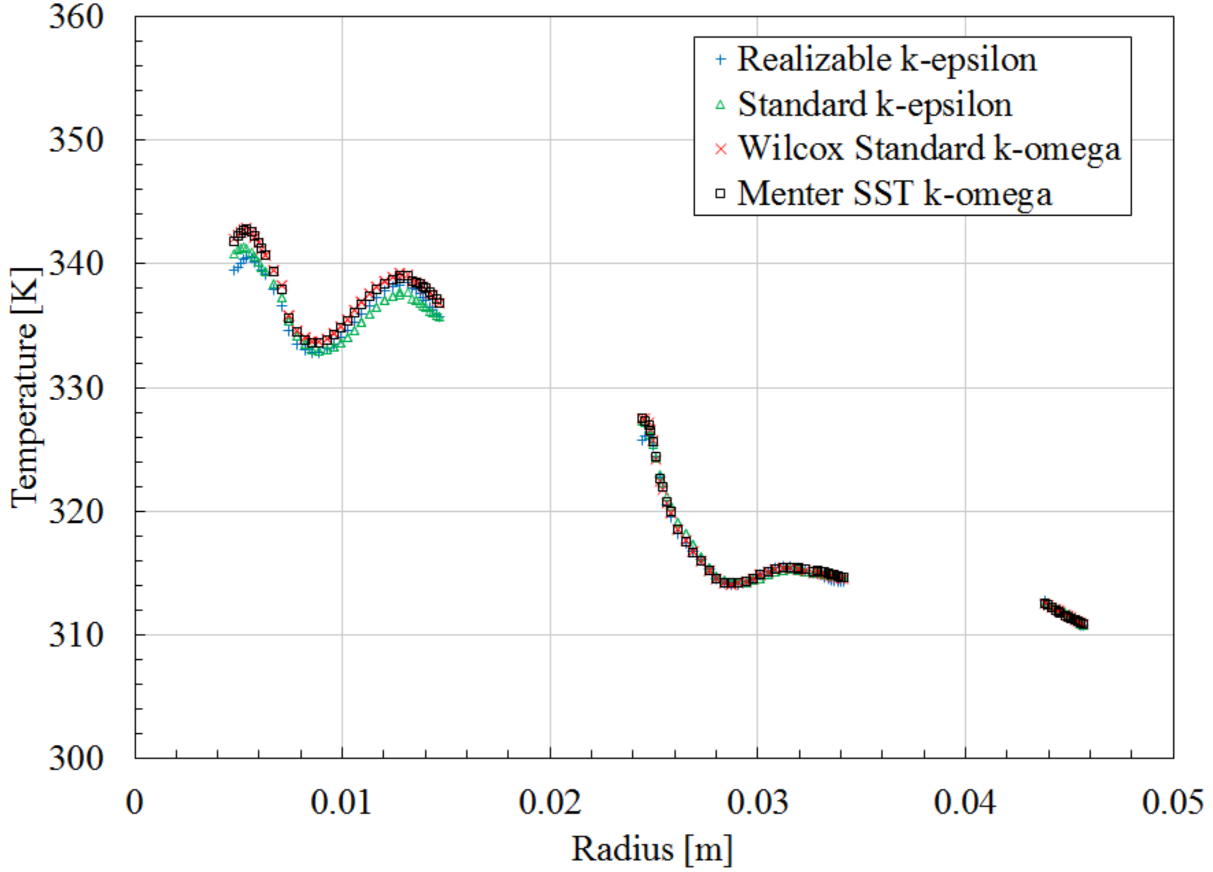
Heated Turbulence Model Sensitivity (Fine Mesh)



All turbulence models predict Δp within ~7% of well-known bundle Δp correlation



Temperature profiles show slight variation with choice of turbulence model

Isothermal bundle pressures show similar sensitivity to choice of turbulence model

Isothermal bundle velocity field shows little sensitivity to choice of turbulence model

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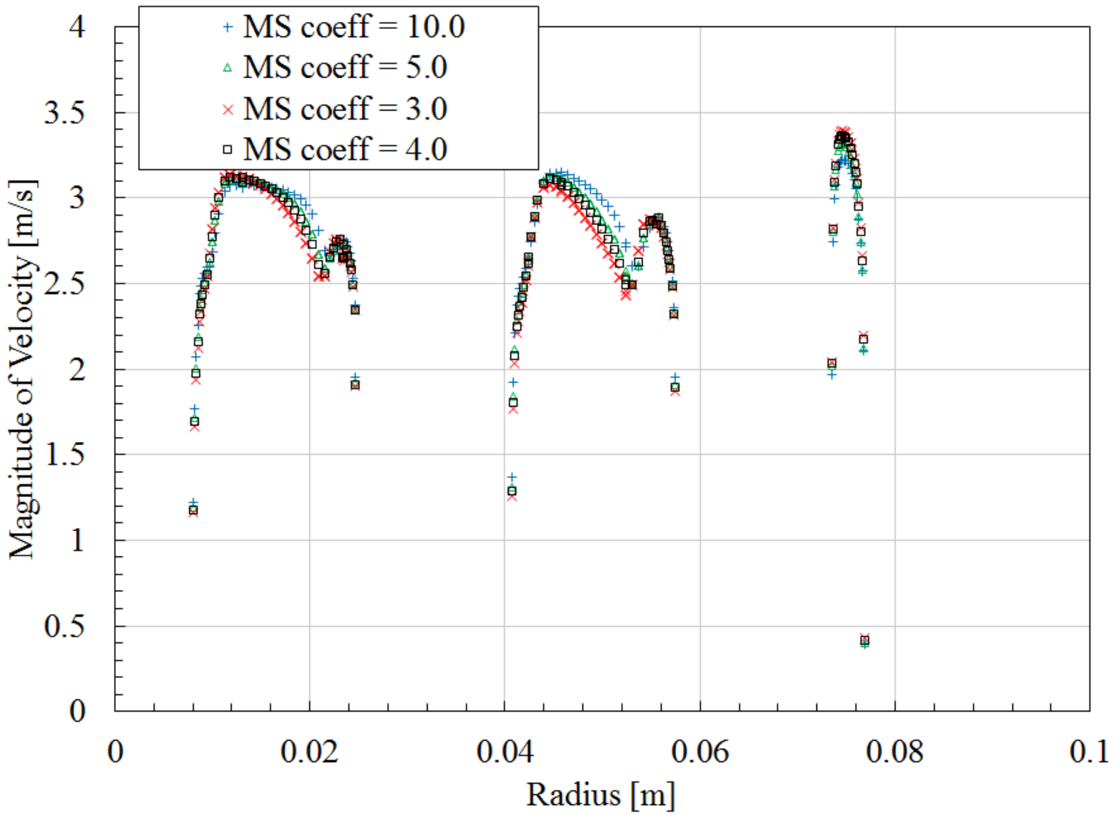
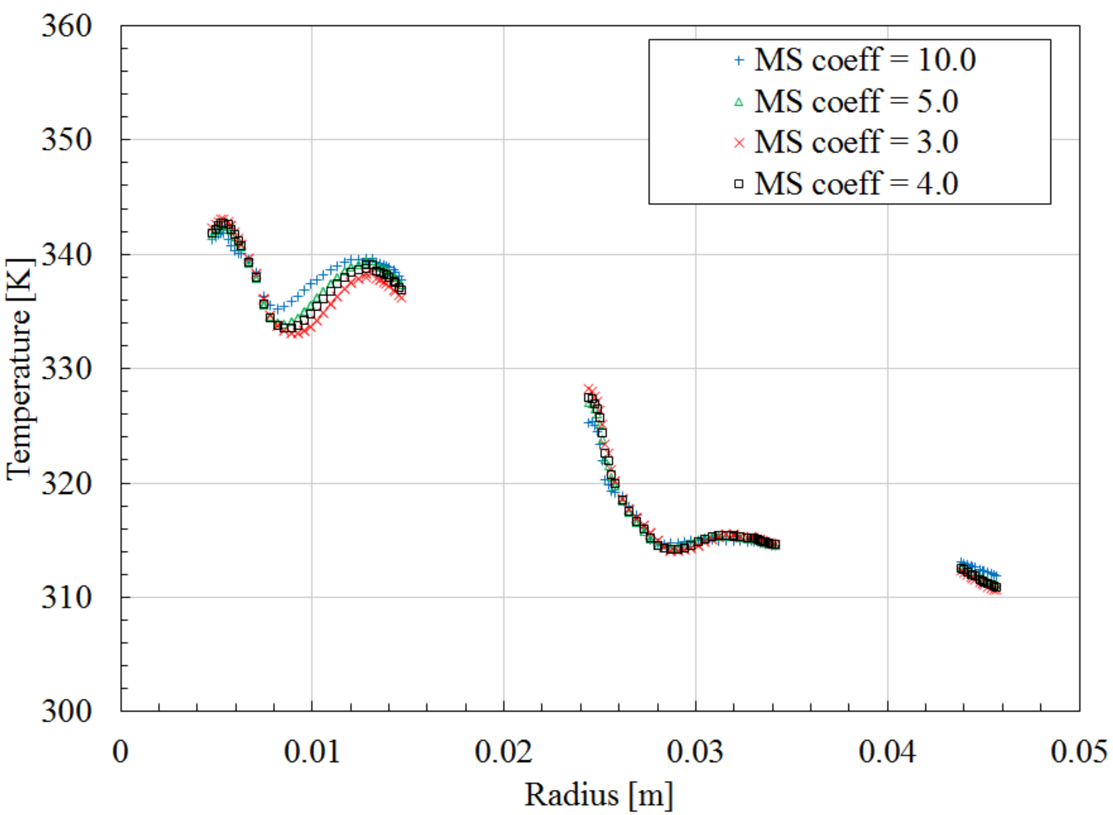
Momentum Source Coefficient Sensitivity (Fine Mesh)

- No appreciable change in pressure values due to varying momentum source coefficient
- Slight variations in velocity and temperature profiles with coefficient value



Isothermal Bundle



Heated Bundle

Summary & Future Work

- Summary
  - Method of Manufactured Solutions code verification approach implemented into Star-CCM+
  - Results show convergence and may have uncovered an issue with 2nd-order schemes
  - Solution verification of non-deformed isothermal and heated bundles completed and discretization error estimated from converged solutions
  - Turbulence model sensitivity tests show little variation in velocity and temperature fields; pressure drop results are close to accepted correlation
  - Temperature & velocity fields show some sensitivity to value of momentum source coefficient

- Future Work
  - Expand on code verification & work with CD-Adapco to fix issues
  - Simulate deformed bundle geometries for pre-tests
  - Use verification and sensitivity studies to determine pre-test blind results
  - Perform solution validation and further post-test simulations after test results become available

Acknowledgements

- TerraPower
- AREVA
- Argonne National Lab
- Texas A&M University
- Department of Energy

This material is provided to support the Department of Energy [National Nuclear Security Administration] Award Number [DE-NE0008321]

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