Investigation of the Effects of Mesh Topology on CFD Simulations of a Chemical Looping Air Reactor

Yong Liu[1,2], Justin Weber[1], N'dri Arthur Konan[1], Michael J. Gallagher, Jr.[1,2], Ronald Breault[1], E. David Huckaby[1]

[1]National Energy Technology Laboratory

[2]URS Corporation

Outline

I. **Introduction of ICMI (Industrial Carbon Management Initiative)**

II. **Cold Flow Simulations**
   i. Results
   ii. Motivation for Sensitivity Study

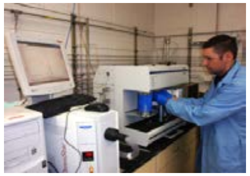
III. **Sensitivity Study**
   i. Mesh Topology
   ii. Turbulence Model
   iii. Spatial Discretization
   iv. Solid Phase Boundary Condition (specularity coefficient)

IV. **Conclusions & Future Work**

Activities

Integrated Experimental & Modeling Effort

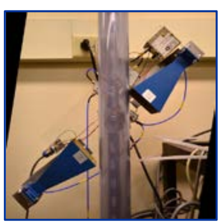
TGA and Mass-Spec



Lab-Scale Fixed Bed Reactor

Integrated Cold Flow Unit

Single Fluidized Bed Reactor



Microwave Sensor

Particle Reactivity
Reaction model development
via. parameter estimation

Bed Reaction Rate
Reaction model validation
Small scale validation of hydro, reaction and interactions

Circulating Hydrodynamics V&V
Solids Handling and Process Development

Solids Circulation Rate Measurement

Integrated Hot Reactive Unit

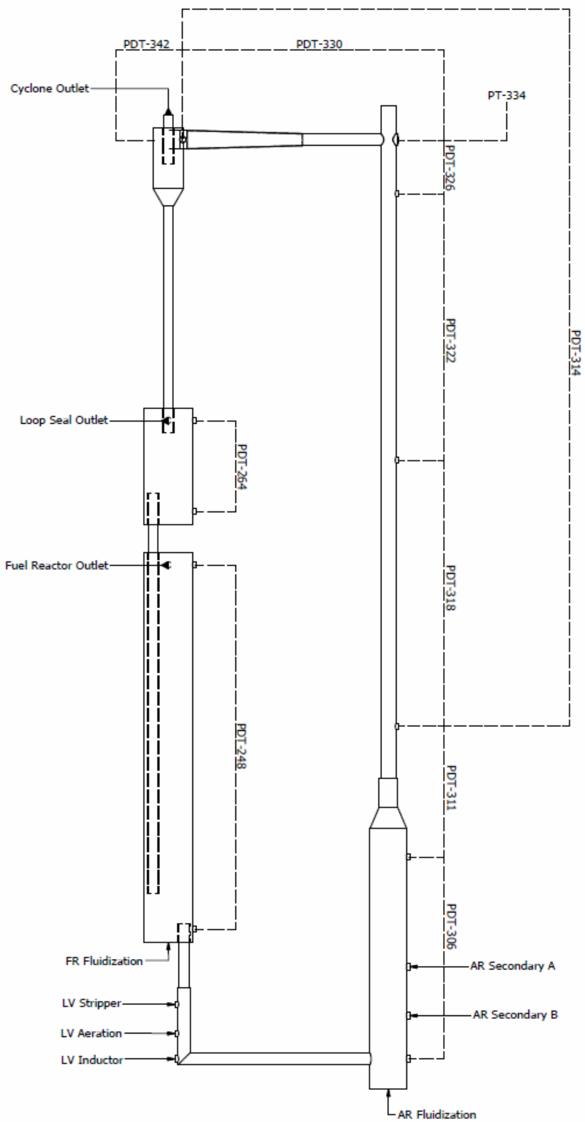
ICMI Modeling and Simulation Objectives

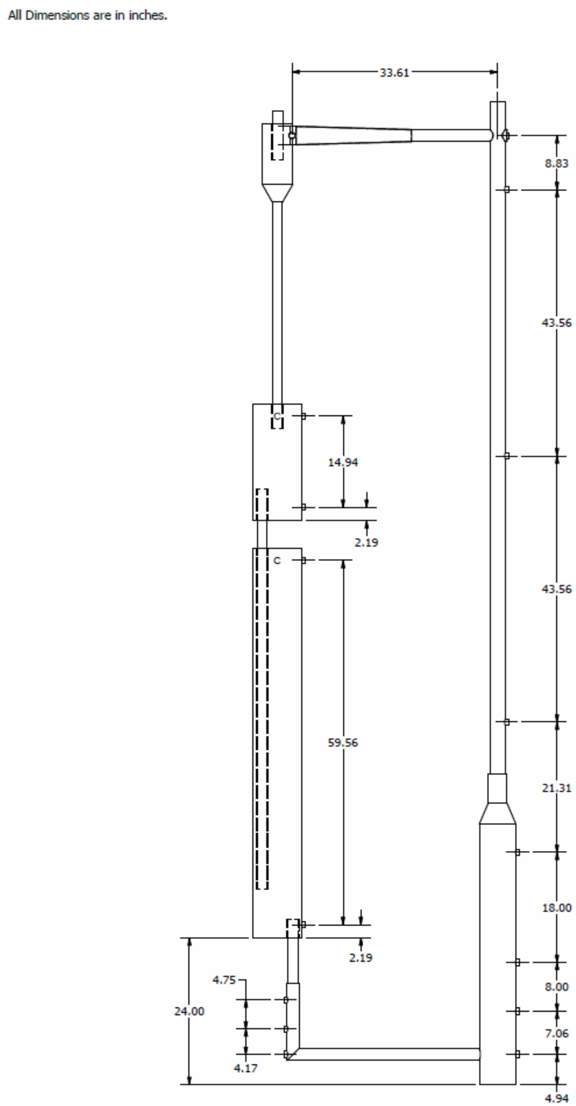
- **Implement** and calibrate physical sub-models to characterize CL process: granular flow, heat transfer, reactivity.

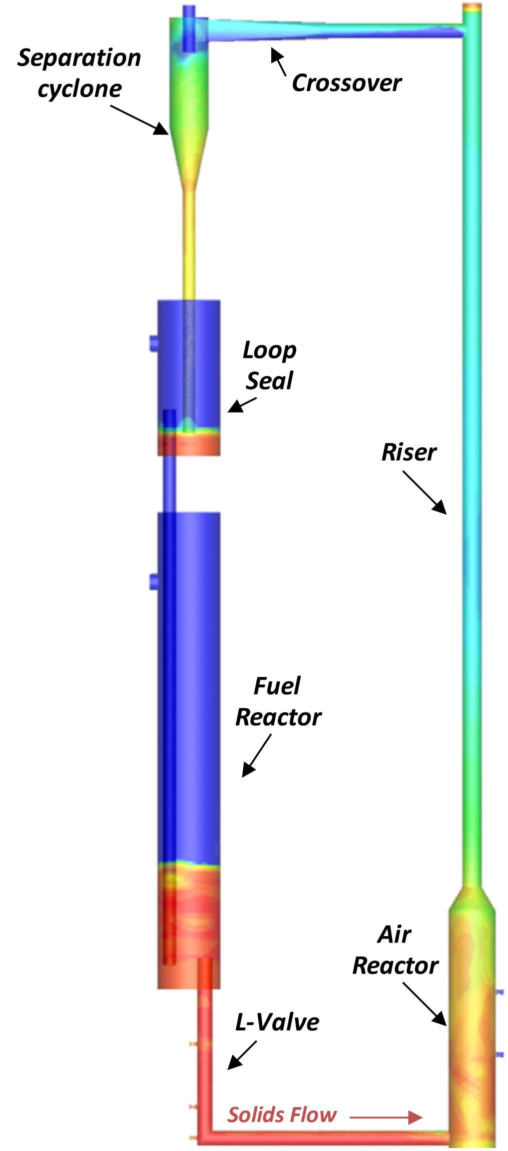
- **Validate** models using experimental data
  - provide estimates of the predictive capability.
  - provide guidance for the design and operational improvements to experimental program.

- **Apply** the models for exploration of pilot-scale and future industrial-scale designs of chemical looping reactors, which we expect will be larger and more geometrically complex.

Geometry of Chemical Looping System

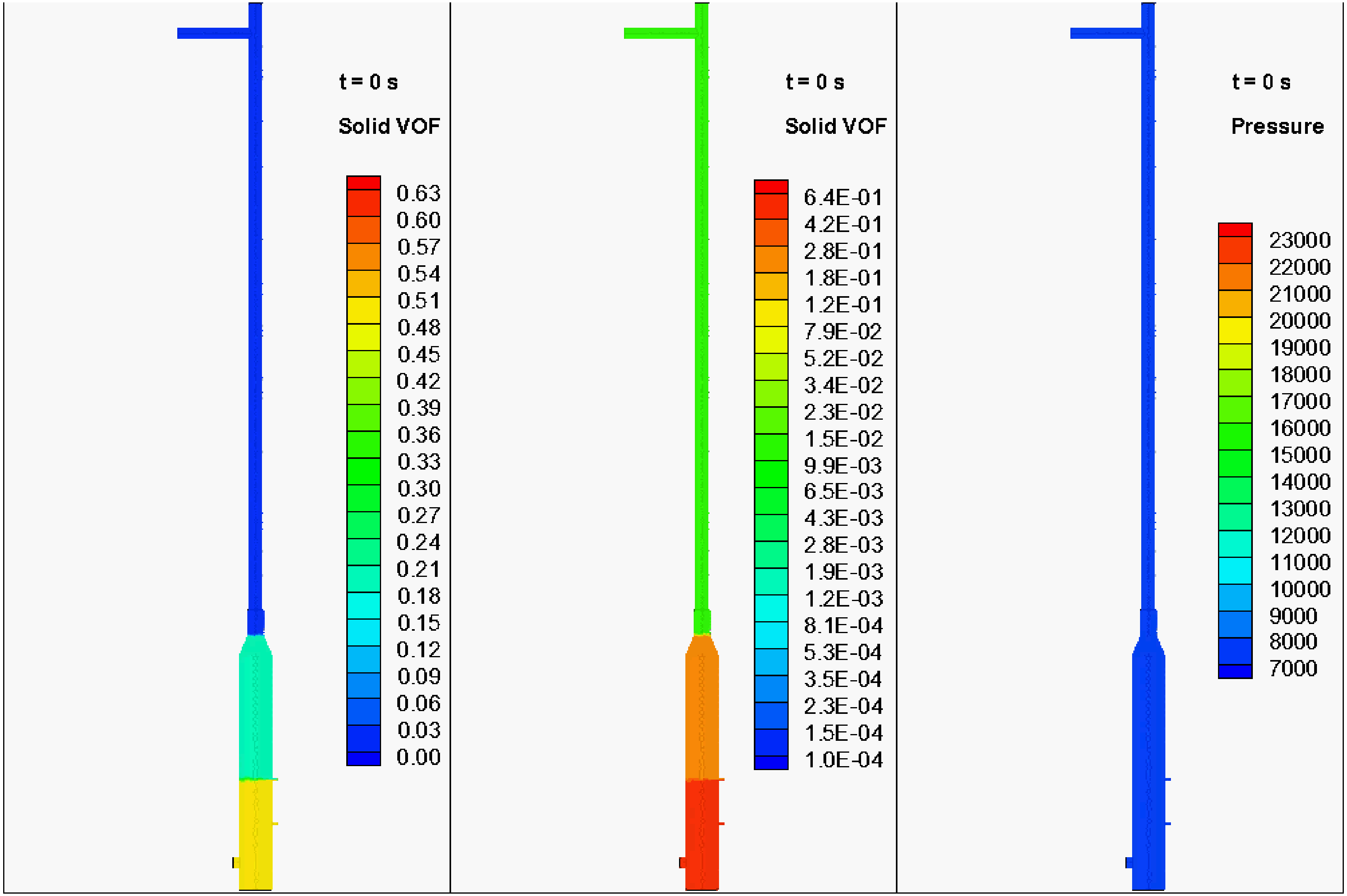




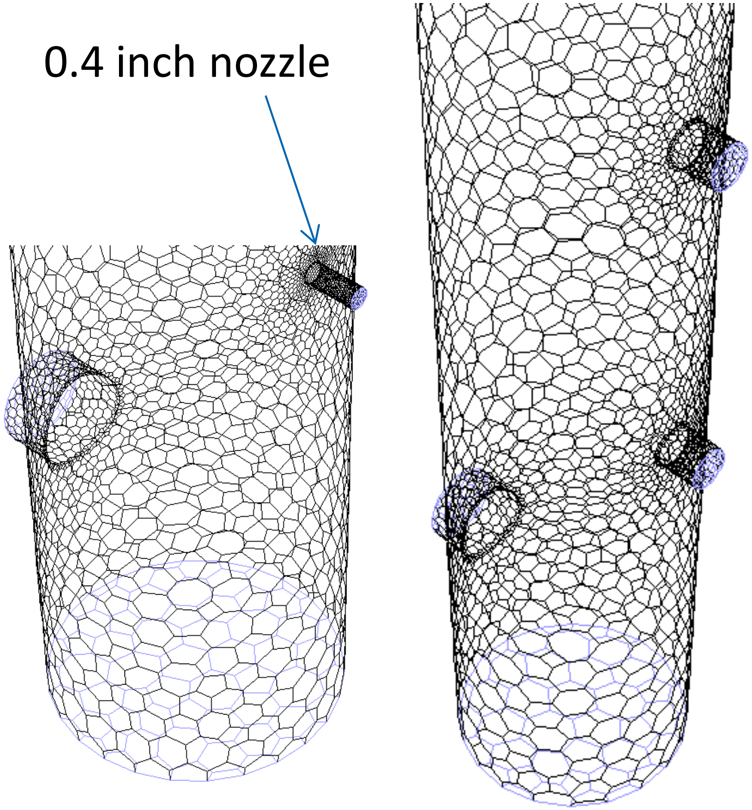


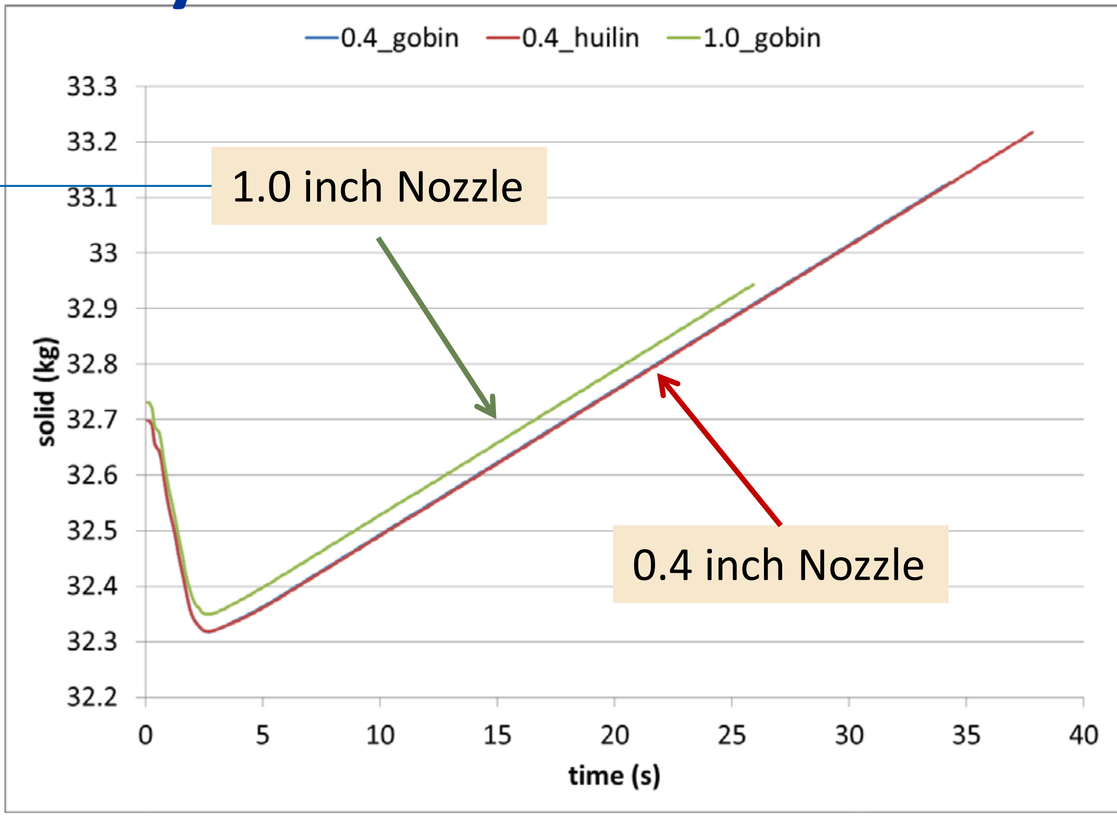
Boundary Conditions and Pressure Locations

Air Reactor Simulation



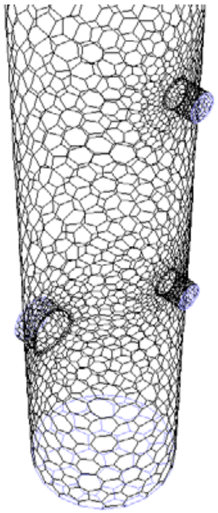
Effect of Secondary Nozzle Diameter

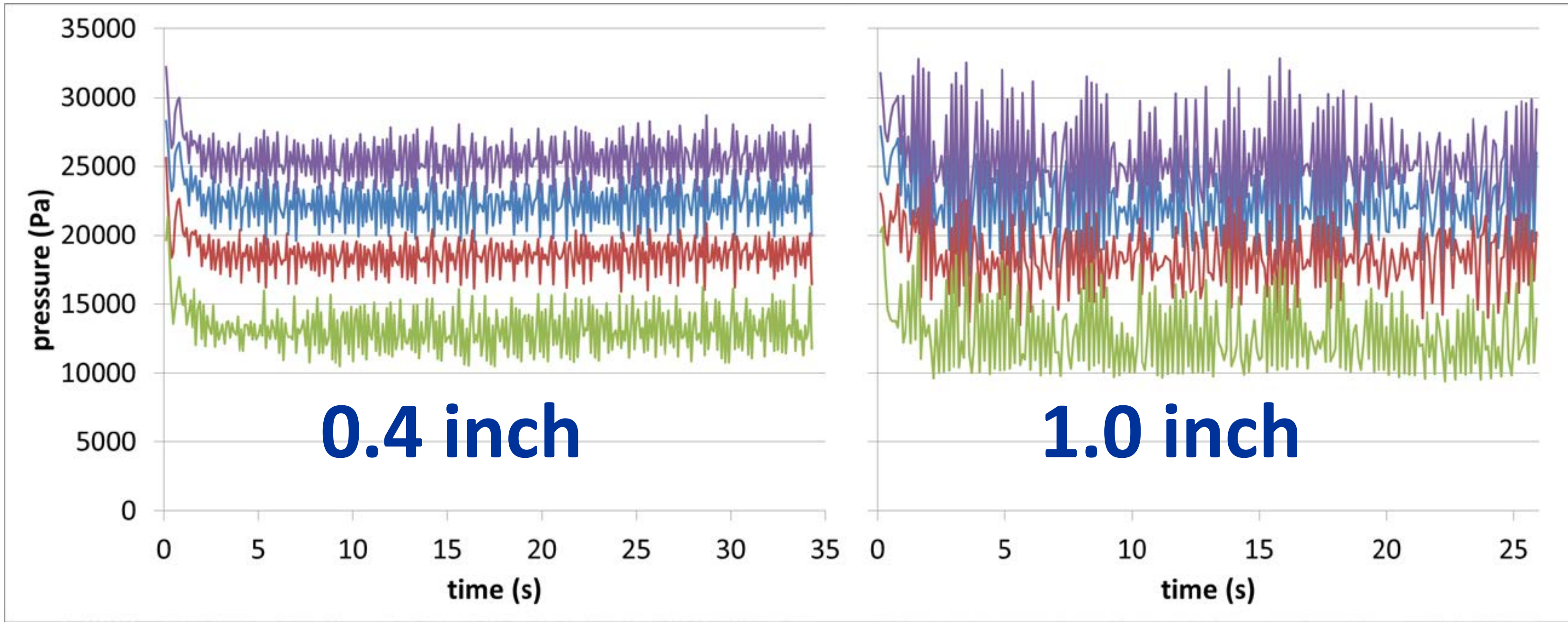




- Three simulation were performing using two drag laws and two secondary nozzle diameters.
- The drag law had a negligible effect on the evolution of the solid inventory.
- The nozzle diameter had a slight effect.

Effect of Secondary Nozzle Diameter

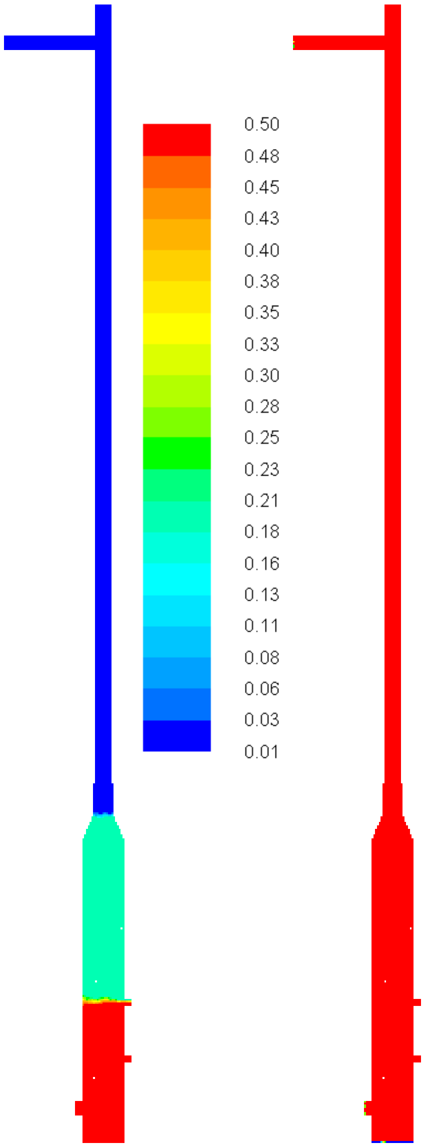


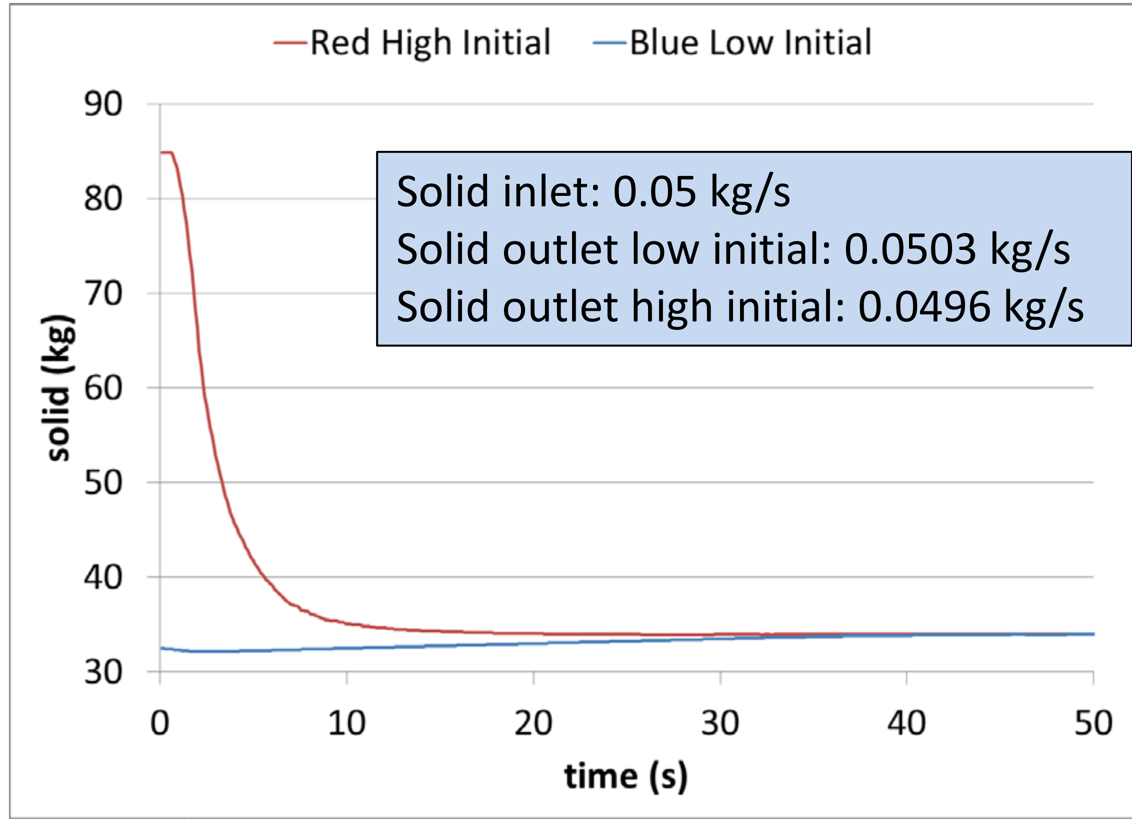


Purple: pressure at air inlet;
Red: pressure at bottom secondary;
Blue: pressure at solid inlet;
Green: pressure at top secondary;

- Secondary diameter does have effect on the solid circulation rate, pressure distribution.
- Smaller secondary inlet diameter results in smaller amplitude pressure fluctuations.

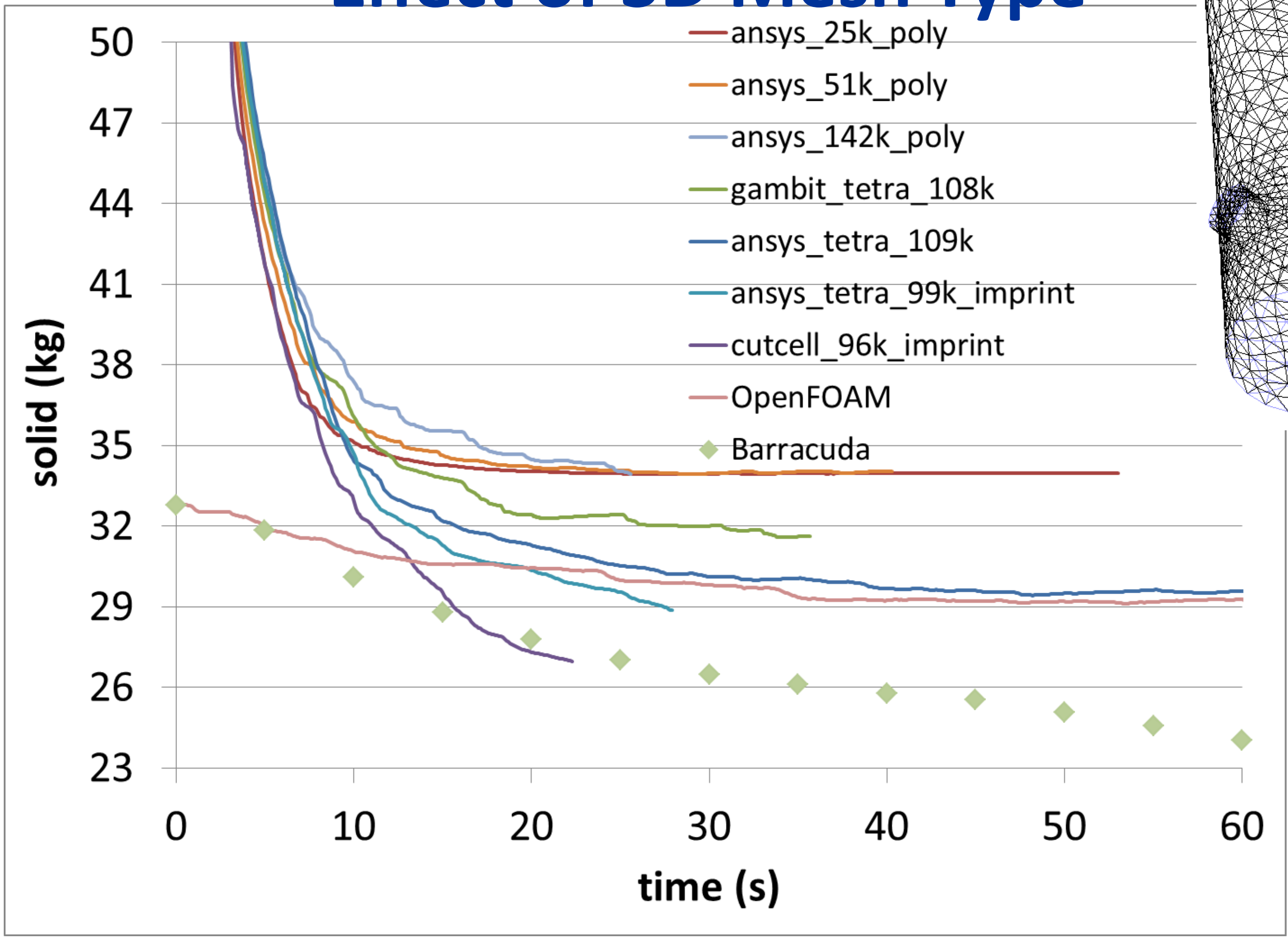
Effect of Initial Condition

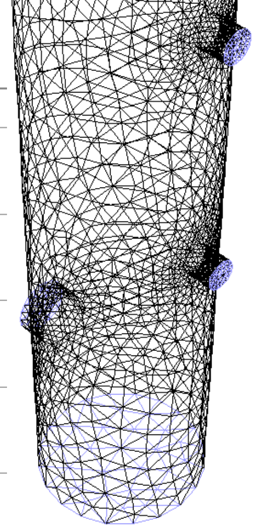


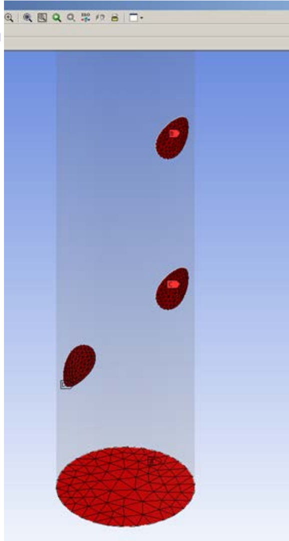


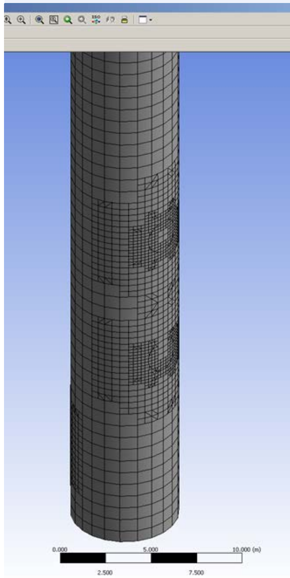
- Simulations were performed with two initial solid distributions
- High initial solid inventory simulation reaches a quasi-steady state much faster than the lower initial solid inventory simulation
- The two initial conditions lead to similar inventory at quasi-steady state

Effect of 3D Mesh Type



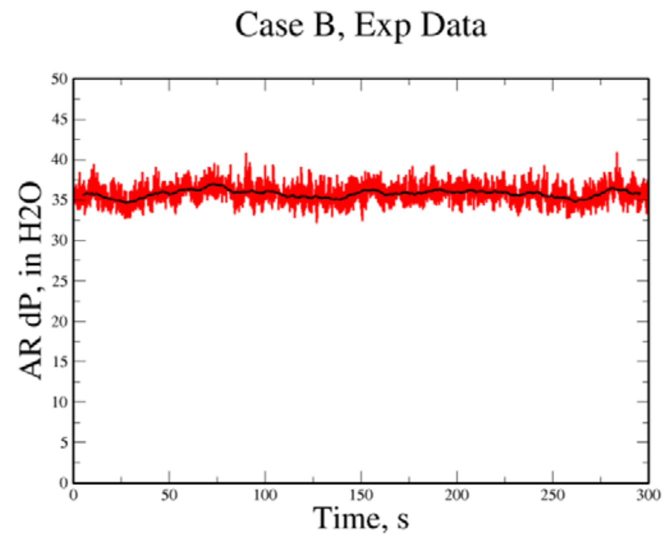


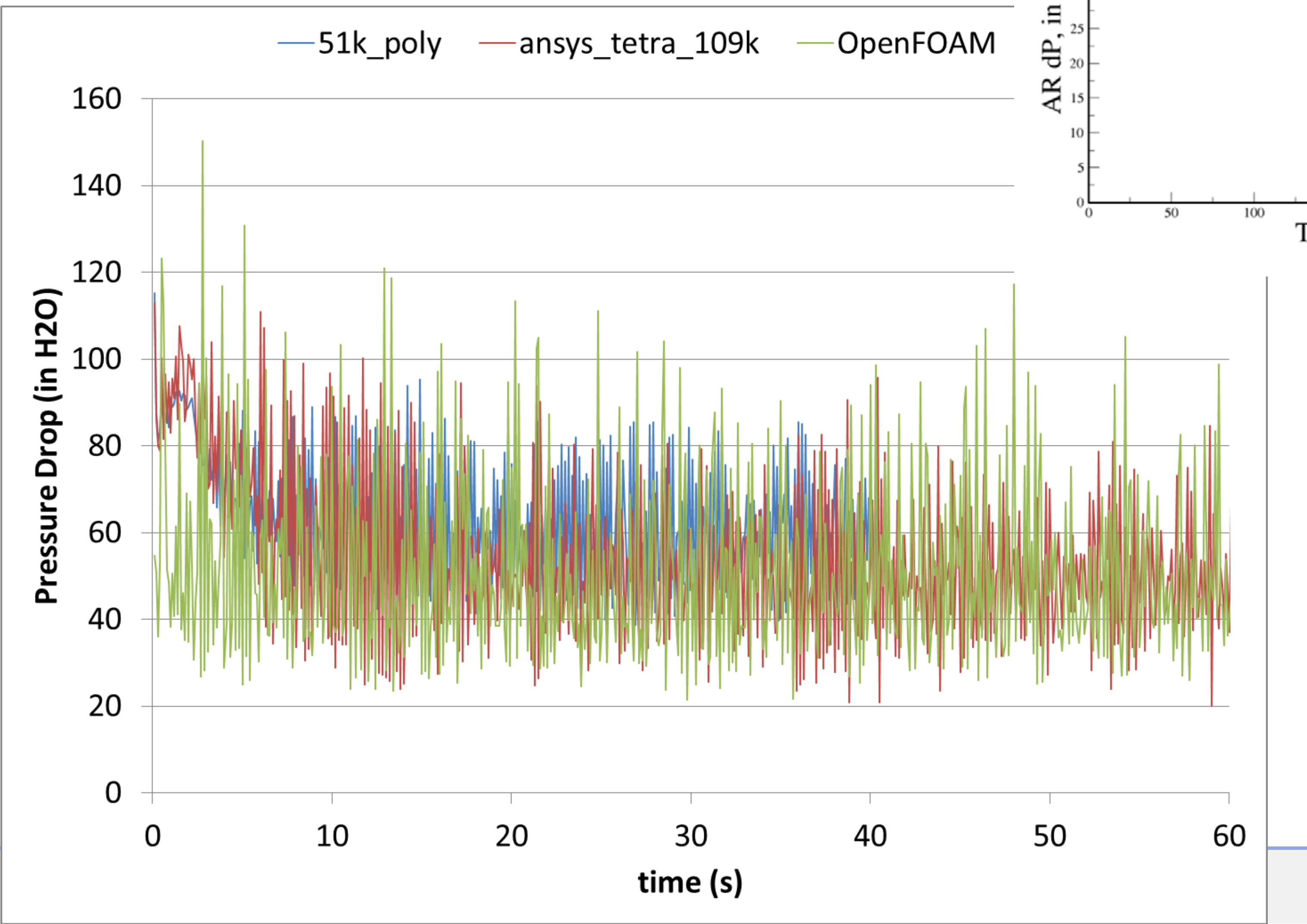


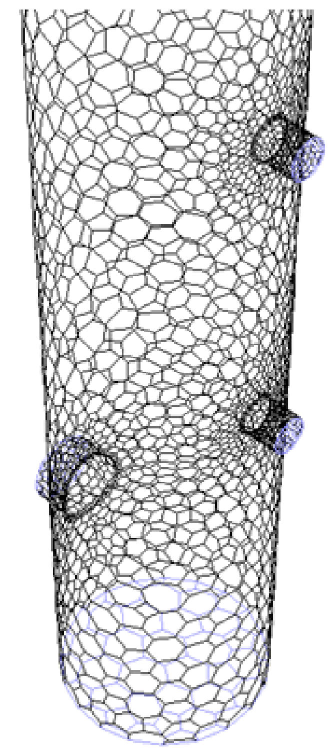


- Several meshes were created using different tools, topology and cell count.
- The tetrahedral mesh generated by different software (Ansys-meshing and Gambit) with similar numbers of mesh give different inventory.
- Polyhedral mesh appears to be converging to a different solution than other mesh topology

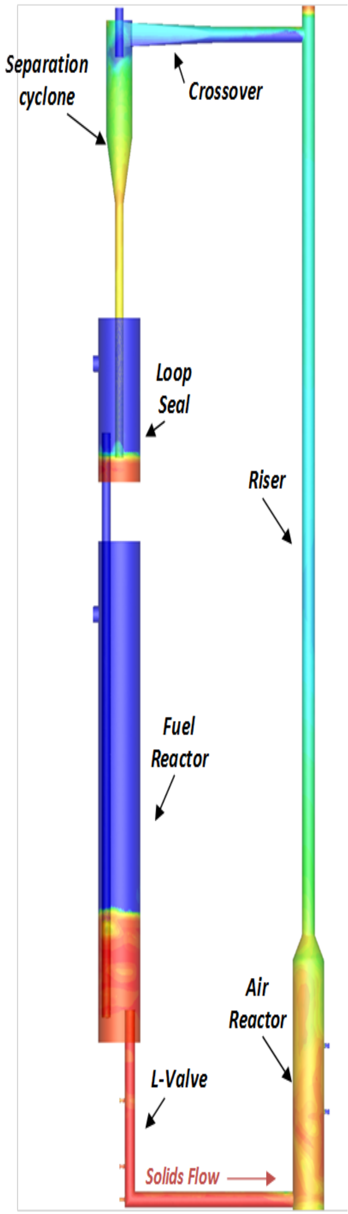
Pressure Drop vs. time for Different Meshes



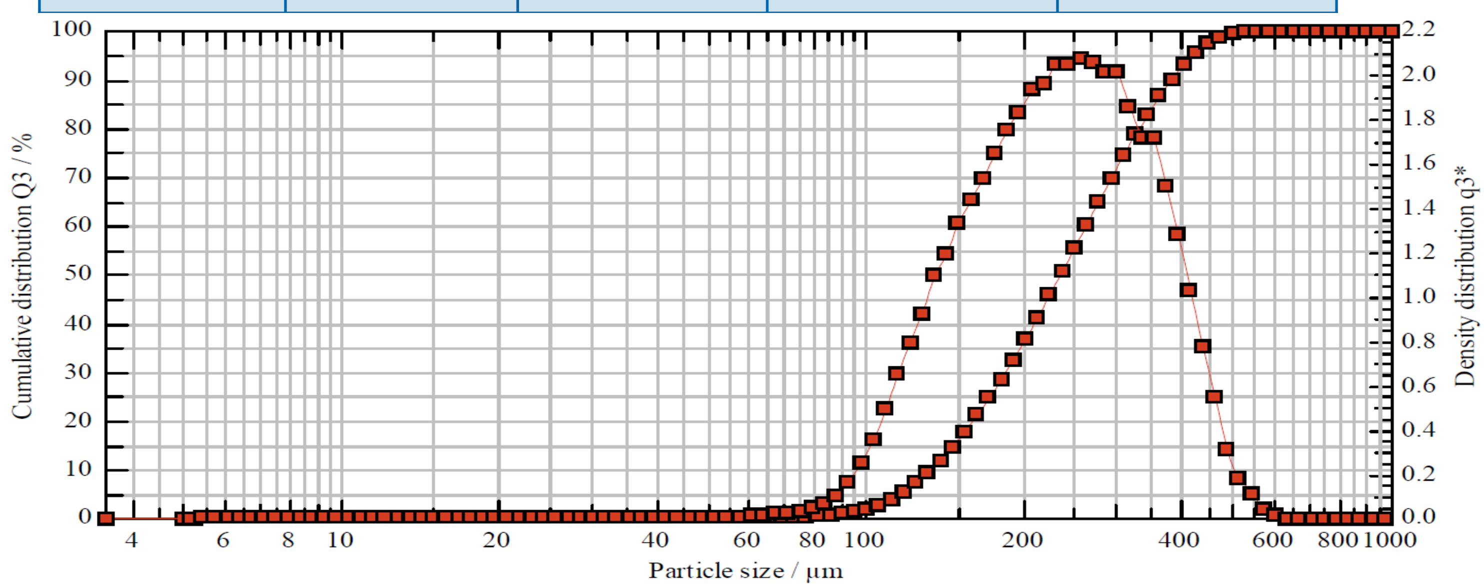




Particle Redistribution



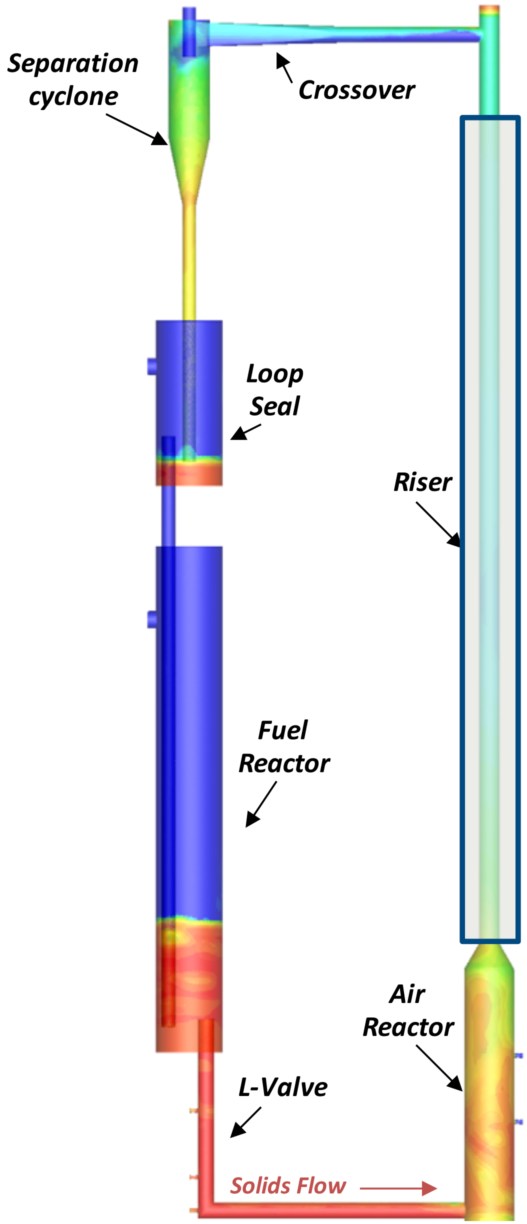
	Original (micron)	Loop Seal (micron)	Fuel Reactor (micron)	Air Reactor (micron)
X10	**149.20**	**108.06**	**111.71**	**148.25**
X50	234.26	194.39	194.08	247.19
X90	381.20	343.73	325.45	375.36
SMD	209.95	170.54	171.87	221.97
VMD	247.14	211.31	207.12	255.24

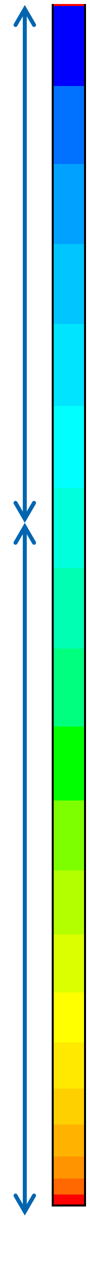


Motivation of 2D Study

- Initial Air Reactor simulations showed a dependence on mesh topology (polyhedral, tetrahedral, Cartesian…) even as the mesh was refined.
- However,
  - Geometric complexities make it difficult isolate the specific influence of cell topology
  - Simulations are too costly for mesh independent solutions
- **Perform 2D simulations of a simplified configuration to explore the sensitivity to cell topology and several other parameters**

2D Configuration

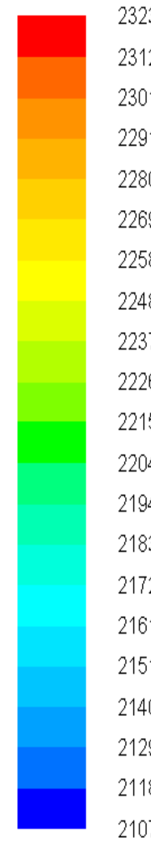




top pressure drop

bottom pressure drop

Pressure

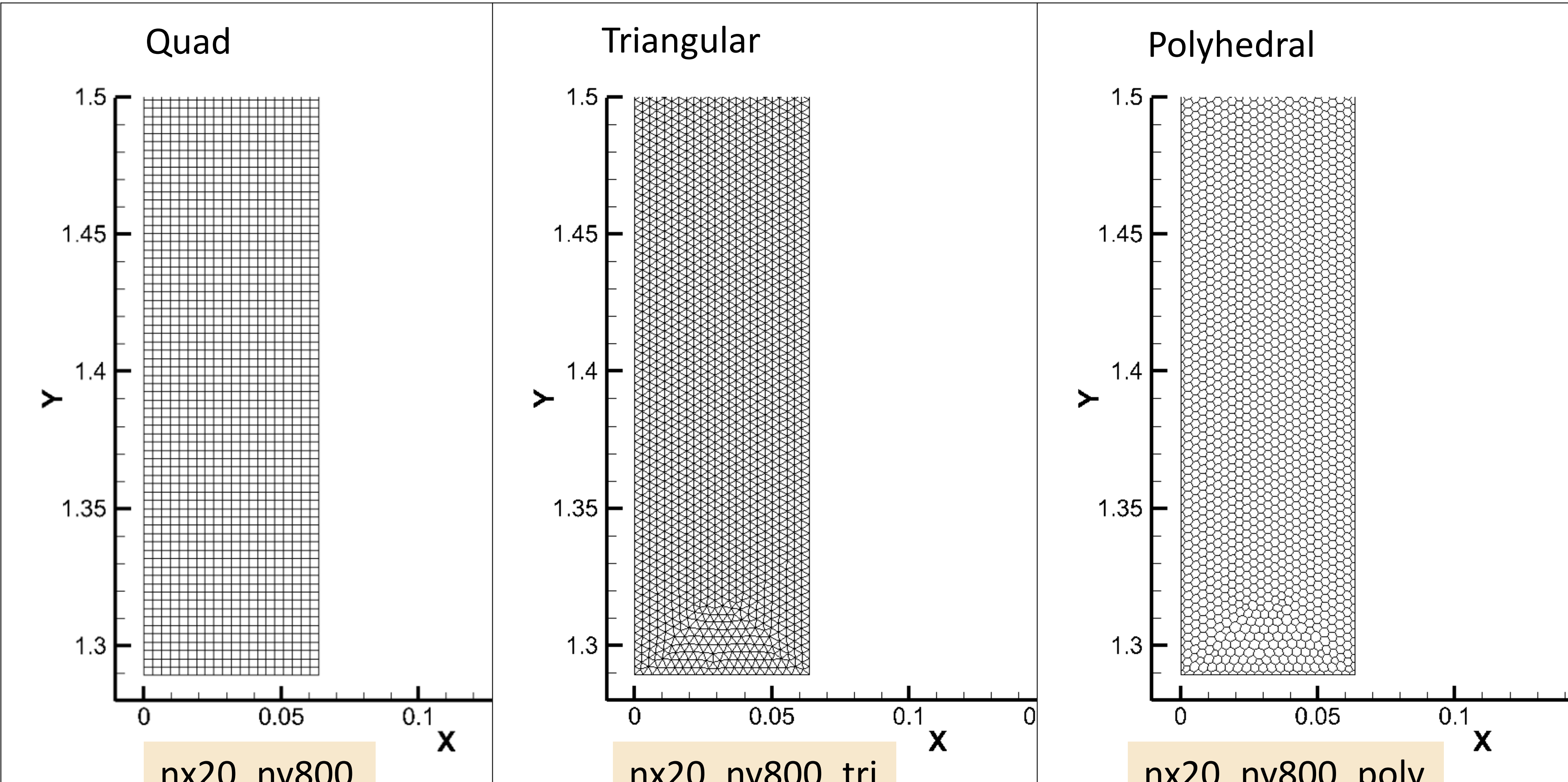


Width
2.5 inch

Height
146 inch

mdot_solid = 0.064167 kg/s
mdot_g as = 0.030527 kg/s
Inlet Solid VOF = 0.00517

Mesh Topology at the Bottom of the Domain



nx20_ny800
16000 cells

nx20_ny800_tri
38094 cells

nx20_ny800_poly
19868 cells

- **Label indicate number of cells along the "X" and "Y" edges**

Model Parameters and Sub-models

Physical Properties	
Air	Ideal Gas
Diameter (micron)	234
Density (kg/m^3)	4701
Particle-Particle Restitution Coefficient	0.9
Particle -Wall Restitution Coefficient	0.8
Particle-Wall Specularity Coefficient	0.1
Drag	Huilin/ Gobin

Granular Model	
Granular Temperature	PDE
Granular Viscosity	Syamlal-OBrien
Granular Bulk Viscosity	Lun-et-al
Frictional Viscosity	Not Used
Frictional Pressure	Not Used
Granular Conductivity	Syamlal-Obrien
Solids Pressure	Syamlal-Obrien
Radial Distribution	Lun-et-al
Elasticity Modulus	Derived

Numerical Discretization	
Transient	Bounded 2nd-order implicit
Gradient	Least Squares
Momentum	MUSCL
Volume	2nd-order upwind
Energy	MUSCL

Turbulence Model	
k-epsilon	Realizable
Multiphase	Dispersed
Options	Drift Force
Near-Wall	Enhanced-wall treatment

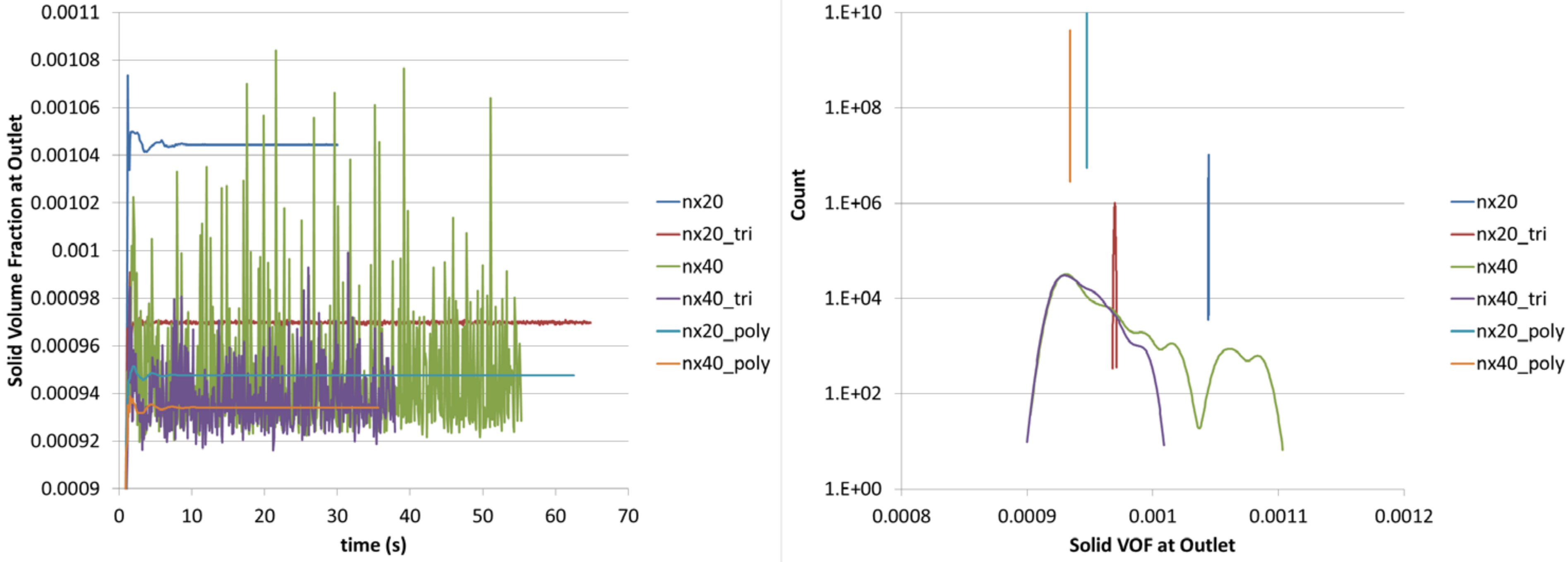
Boundary Conditions	
Momentum	Specularity Coefficient Model
Multiphase	Johnson-Jackson
Gas	No-Slip
Thermal	No Heat Flux

Effect of Mesh Typology on CFD Simulations

Topology	**Mesh**	**VOS @ y = 59 in**	**VOS @ y = 103 in**	**ΔP (Pa) Bottom**	**ΔP (Pa) Top**
Experiment				**112.94**	**57.02**
Quad	20x800	1.45e-3	1.02e-3	91.12	73.36
Quad	40x1600	1.45e-3	0.99e-3	91.94	70.48
Tri	20x800	1.44e-3	1.00e-3	92.57	70.80
Tri	40x1600	1.43e-3	0.98e-3	92.40	69.21
Poly	20x800	1.45e-3	0.98e-3	93.78	69.44
Poly	40x1600	1.45e-3	0.97e-3	93.46	68.60

- The point of comparison with the experiment is to insure that the simulations are in the same flow regime.
- The point is that the results should be completely independent of topology and they are not, which implies lack of mesh independence.
- High order discretization; Solid Wall B.C. Specularity Coefficient = 0.1

Effect of Mesh Typology on CFD Simulations



nx40 quad; average=9.46e-4;
deviation=0.293e-4

nx40_tri; average=9.39e-4
deviation=0.150e-4

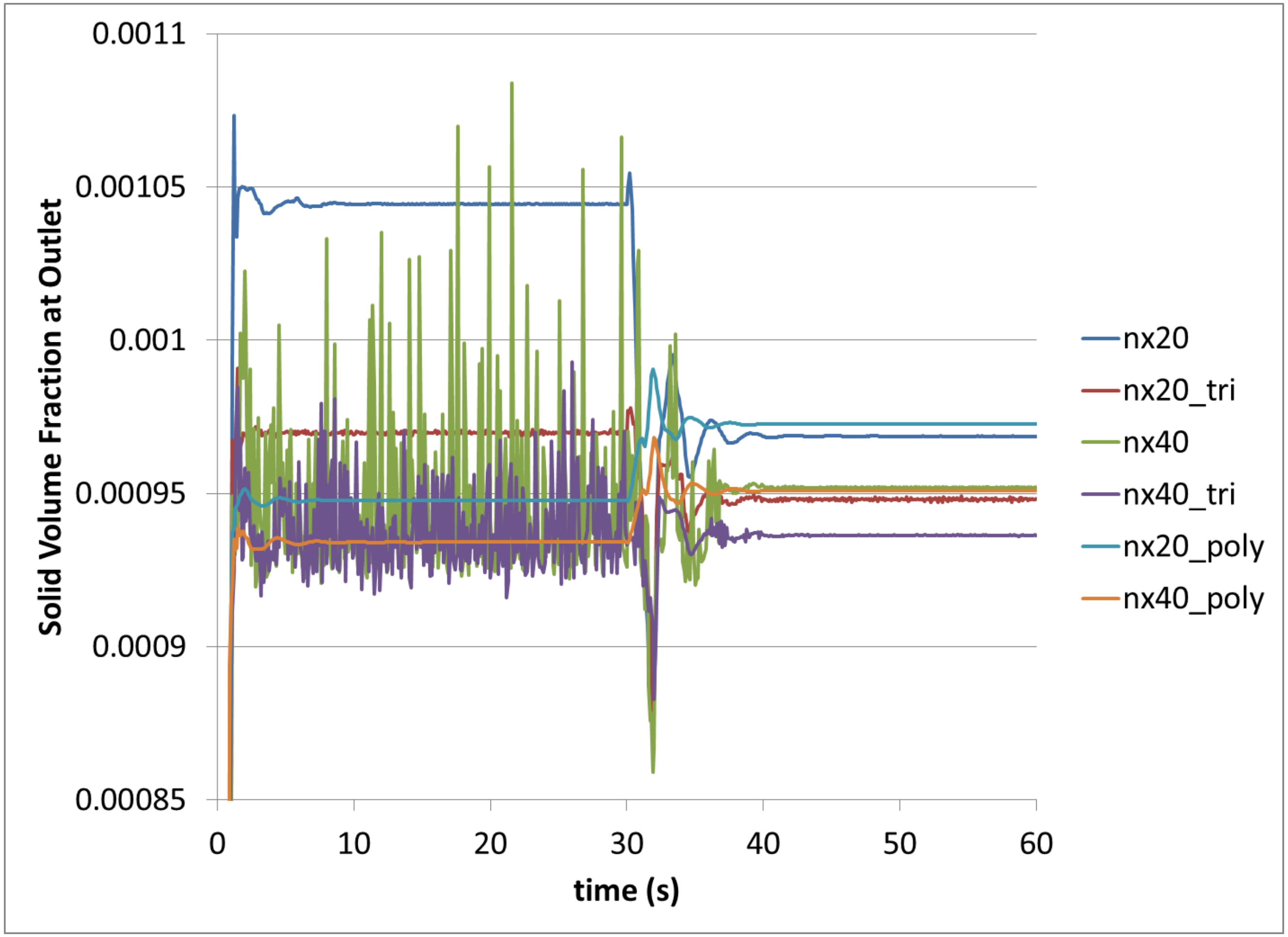
- The Figure shows that the solid volume fraction at the outlet fluctuates for fine mesh (nx40_ny1600).
- The quad mesh fluctuates more than the tri-angular mesh.
- The poly meshes results are always smooth.
- High order discretization; Solid Wall B.C. Specularity Coefficient = 0.1

Effect of Turbulence Model

Topology	Mesh	ΔP (Pa) Bottom	ΔP (Pa) Top	ΔP (Pa) Bottom Turbulence	ΔP (Pa) Top Turbulence
Experiment		**112.94**	**57.02**	**112.94**	**57.02**
Quad	20x800	91.12	73.36	96.20	73.71
Quad	40x1600	91.94	70.48	96.38	73.20
Tri	20x800	92.57	70.80	95.64	72.49
Tri	40x1600	92.40	69.21	96.30	72.79
Poly	20x800	93.78	69.44	102.47	78.59
Poly	40x1600	93.46	68.60	100.73	76.67

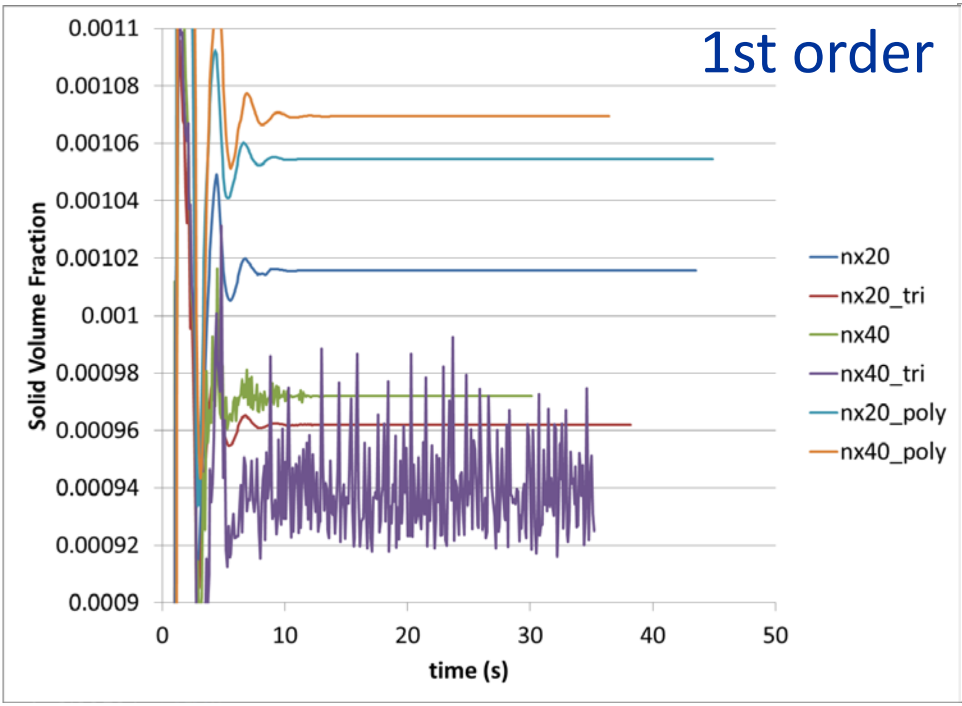
- The turbulence model was “turned on” after 30s.
- The turbulence model result in slightly higher pressure drop.

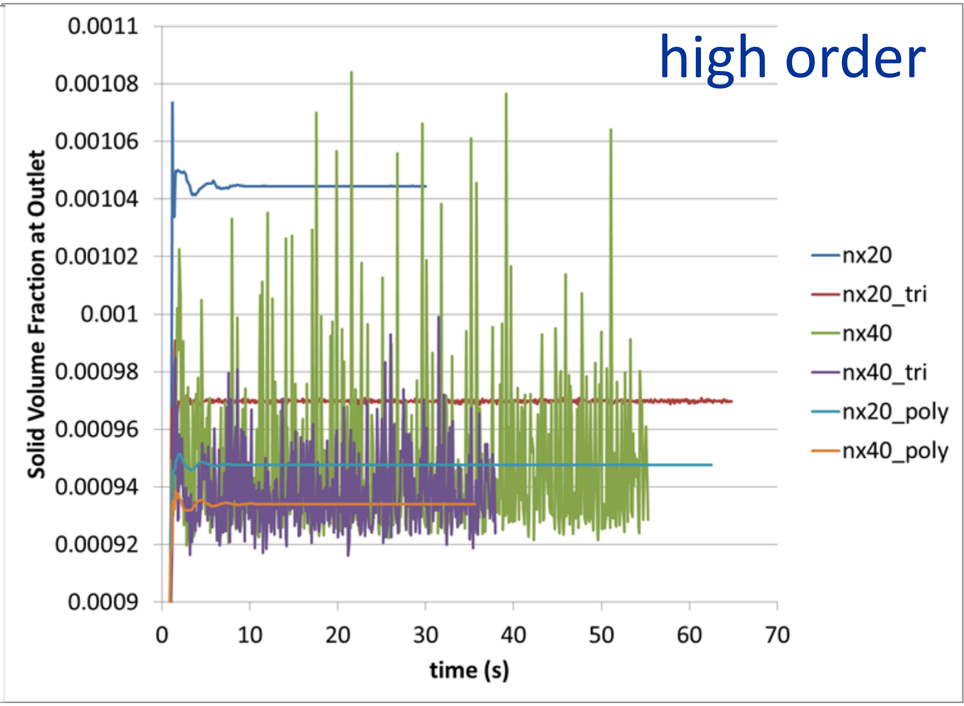
Effect of Turbulence Model



- The turbulence model was “turned on” after 30s.
- The turbulence model reduces the fluctuation of solid vof at the outlet.

Effect of Numerical Discretization





1st order nx40_tri
average=9.40e-4
deviation=0.166e-4

high order nx40
average=9.46e-4
deviation=0.293e-4

high order nx40_tri
average=9.39e-4
deviation=0.150e-4

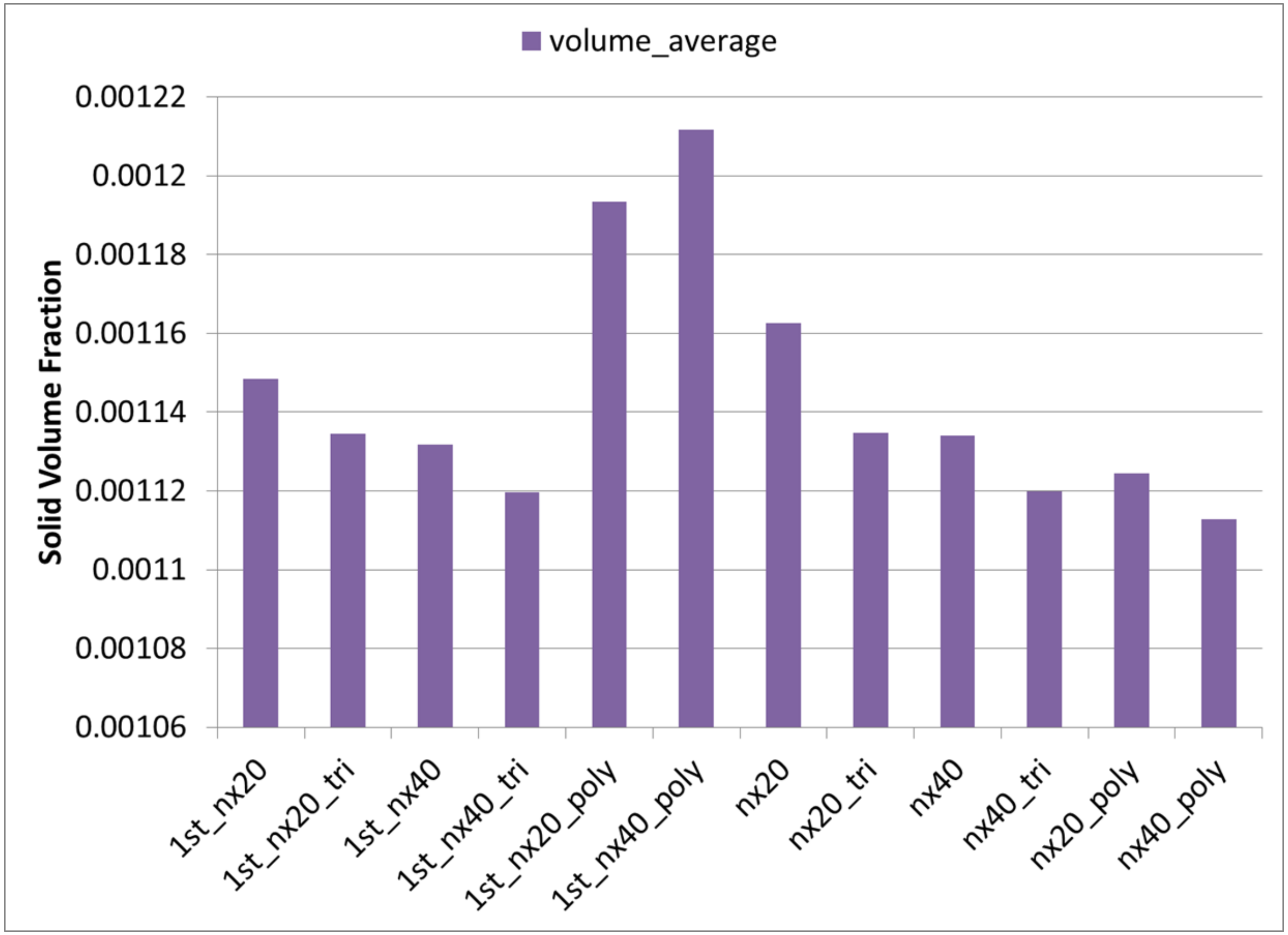
- High order discretization results in more fluctuation for quad mesh nx_40 than 1st order upwind discretization.
- The quad mesh fluctuates more than the tri-angular mesh.

Effect of Numerical Discretization

Topology	Mesh	ΔP (Pa) Bottom 1st order	ΔP (Pa) Top 1st order	ΔP (Pa) Bottom high order	ΔP (Pa) Top high order
Experiment		**112.94**	**57.02**	**112.94**	**57.02**
Quad	20x800	91.97	71.76	91.12	73.36
Quad	40x1600	93.58	70.22	91.94	70.48
Tri	20x800	93.19	70.14	92.57	70.80
Tri	40x1600	92.86	69.32	92.40	69.21
Poly	20x800	103.44	86.85	93.78	69.44
Poly	40x1600	111.37	94.07	93.46	68.60

- 1st order discretization results in higher mean pressure drop than high order upwind discretization for poly mesh while discretization has little effect for quad and tri-angular mesh.
- Different meshes give similar results using high order discretization.
- For 1st order discretization, poly mesh predicts higher pressure drop than quad and triangular mesh.

Effect of Numerical Discretization



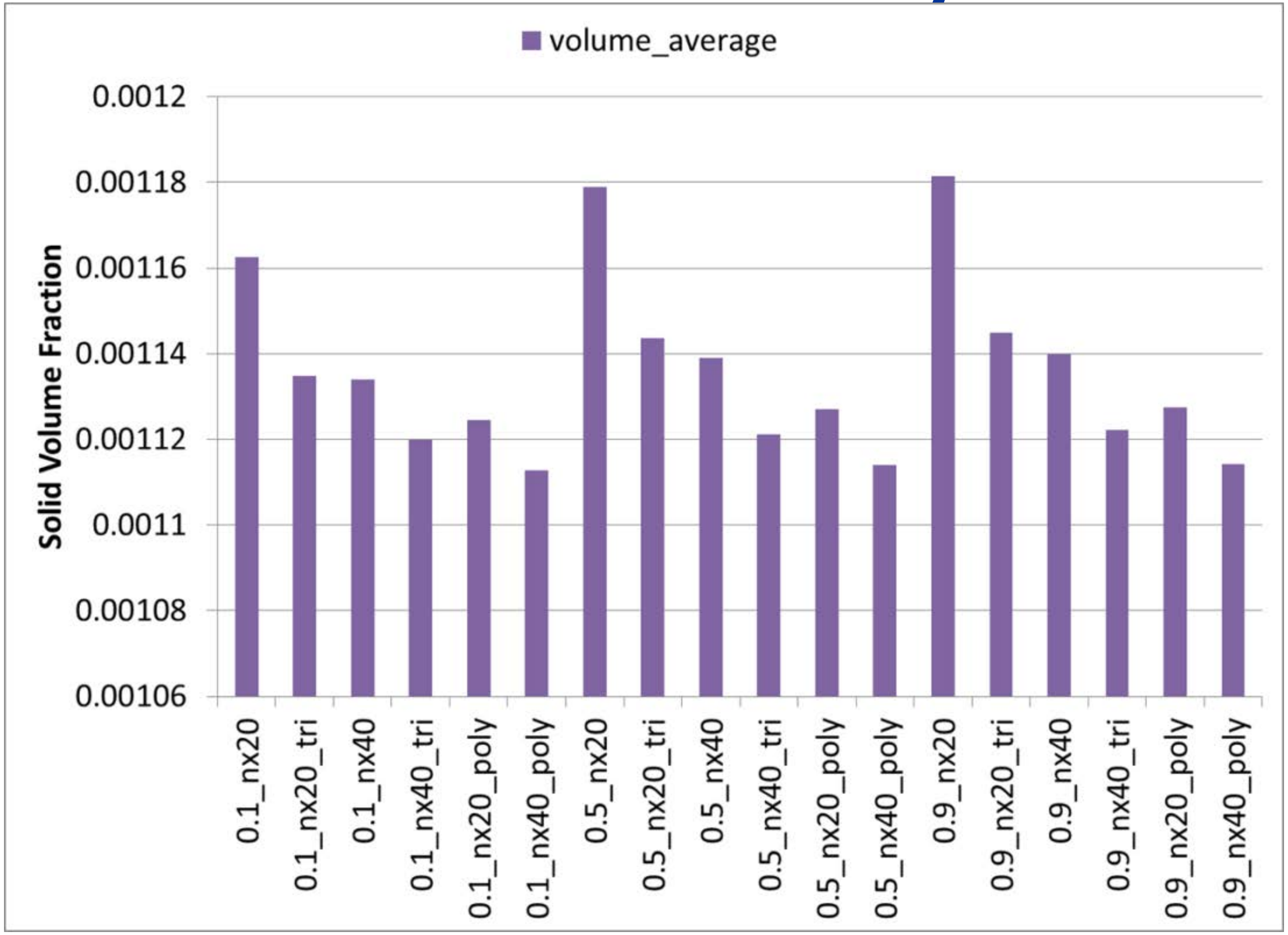
- 1st order discretization results in higher solid inventory as shown by the volume average solid vof. For poly mesh, the maximum difference is less than 10%.

Effect of Solid Wall Boundary Conditions

Topology	Mesh	ΔP (Pa) Bottom 0.1	ΔP (Pa) Top 0.1	ΔP (Pa) Bottom 0.5	ΔP (Pa) Top 0.5	ΔP (Pa) Bottom 0.9	ΔP (Pa) Top 0.9
Experiment		**112.94**	**57.02**	**112.94**	**57.02**	**112.94**	**57.02**
Quad	20x800	91.12	73.36	91.63	75.94	91.72	76.34
Quad	40x1600	91.94	70.48	92.53	71.55	92.63	71.72
Tri	20x800	92.57	70.80	93.27	71.44	93.39	71.57
Tri	40x1600	92.40	69.21	92.69	69.59	92.69	69.83
Poly	20x800	93.78	69.44	94.27	69.88	94.33	69.95
Poly	40x1600	93.46	68.60	93.66	68.86	93.70	68.90

- High specularity coefficient results in slightly higher pressure drop because of higher drag between solid and wall.

Effect of Solid Wall Boundary Conditions



- High specularity coefficient results in higher solid inventory because of higher drag between solid and wall.
- For given specularity coefficient, the highest differences are between quad mesh and poly mesh. The maximum differences are around 6.3%.

Conclusions – Air Reactor

- **Simulations over predict the amplitude and frequency of pressure fluctuations**
  - but .. the data acquisition (DA) system samples at 1Hz.
- **Solid inventory**
  - High initial solid inventory simulations equilibrate to quasi-steady state much faster
  - The quasi-steady inventory is independent of the initial condition.
- **Polyhedral mesh simulations**
  - are less sensitive to the cell count
  - predict higher solid inventory than the tetrahedral mesh.
- **Simulations using a smaller secondary inlet diameter results have smaller amplitude pressure fluctuations.**

Conclusion – Sensitivity Study

- **Cell Topology**
  - Poly simulations are "smoother"
- **Turbulence Model**
  - Reduces the amplitude the outlet solid volume fraction. fluctuation
  - The turbulence model result in slightly higher pressure drop.
- **Spatial Discretization**
  - 1st order discretization results in higher solid inventory
  - For poly mesh, the maximum difference is less than 10% when different discretization are used.
- **Specularity Coefficient**
  - Increased solid inventory with larger value because of higher drag between solid and wall.
  - For given specularity coefficient, the highest differences are between quad mesh and poly mesh. The maximum differences are around 6.3%.

Future Work

- **Air Reactor Simulations**
  - Additional operating conditions
  - Mesh Refinement
  - Sub-grid Model

- **Sensitivity Study**
  - Further mesh refinement
    - Unlikely that results are mesh independent
  - Additional operating conditions and modifications to the configuration
    - Need to have 2D simulations in an operating regime which is closer to the experiments
    - Larger spatial and temporal variation in volume fraction and pressure

Acknowledgment

- **The technical discussions with George Richards, Stephen P. Carpenter and other ICMI team members are highly appreciated.**

- ***This work was performed in support of the National Energy Technology Laboratory's ongoing research for the Industrial Carbon Management Initiative under the RES contract DE-FE0004000.***

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ICMI Project

Chemical Looping Model Development and Simulation

Thank You!

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ICMI Industrial Carbon Management Initiative

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