Simulating the Hydrodynamics of Spouted Beds Using Continuum Computational Fluid Dynamics

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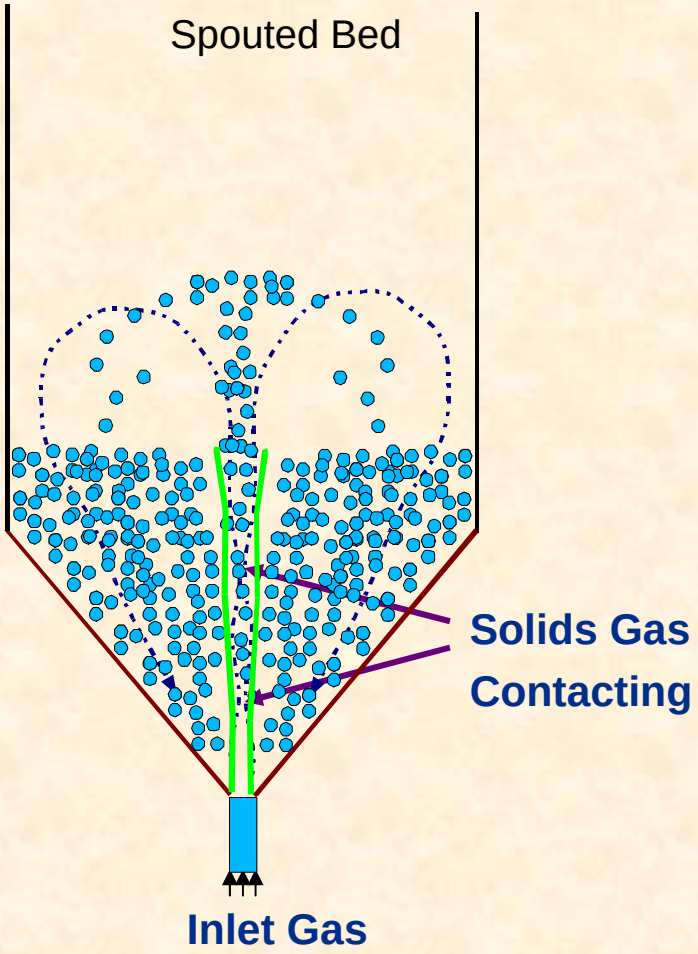
Spouted beds are a type of fluidized bed but they have unique features

- **Like other types of fluidized beds, spouted beds are good for:**
  - **multi-phase contacting**
  - **wide range of operating conditions**
  - **good mixing**
  - **particle surface exposure**

- **But also like other fluidized beds they can have problems:**
  - **unstable hydrodynamics, transients**
  - **sintering, agglomeration**
  - **direct measurements difficult**

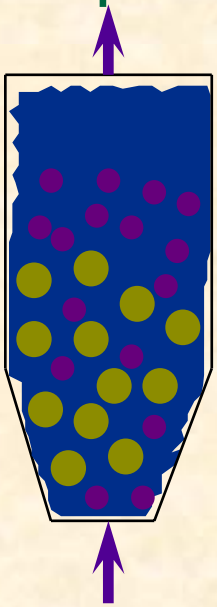
- **Unique features include:**
  - **Single, central primary gas inlet**
  - **Very dominant global circulation pattern (with distinctive pulsations)**
  - **Highly distinct lean flow (transport) and dense flow (defluidized) zones**



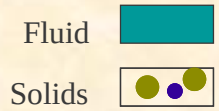
Our overall objective is to improve the capability for simulating spouted beds and spouted bed reactors

- **Spouted beds are used for many applications including particle coating, solids drying, and agglomeration**
- **Accurate simulations could greatly improve development of improved designs, controls**
- **Application of specific interest to ORNL is nuclear fuel particle coating (# 301a, Wed. @ 8:00 AM)**
- **Hydrodynamics is focus here, but heat and mass transfer and chemical reaction must also be considered depending on the application details**
- **Many issues remain to be resolved about appropriate selection of simulation parameters**

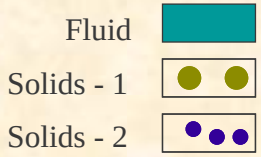
MFIX is a good candidate for spouted-bed CFD because of its detail, speed, maturity, open-source access, DOE support



- **Two Phases**



- **Three phases**



Size 1

Size 2

Continuity Equation

$$\frac{\partial}{\partial t}(\varepsilon_m \rho_m) + \nabla \cdot (\varepsilon_m \rho_m \vec{v}_m) = \sum_{l=1}^{M} R_{ml}$$

Momentum Equation

$$\frac{\partial}{\partial t}(\varepsilon_m \rho_m \vec{v}_m) + \nabla \cdot (\varepsilon_m \rho_m \vec{v}_m \vec{v}_m) = \nabla \cdot \overline{\overline{S}}_m + \sum_{l=1}^{M} \vec{I}_{ml} + \vec{f}_m$$

Stresses

Interaction Term

- Each phase treated as continuum fluid
- Constitutive equations determine phase flows and phase interactions
- Model posed as a series of PDEs simulating variations in space and time (Eulerian framework)
- Track local species, reaction rates, temperatures, gas & solids flows

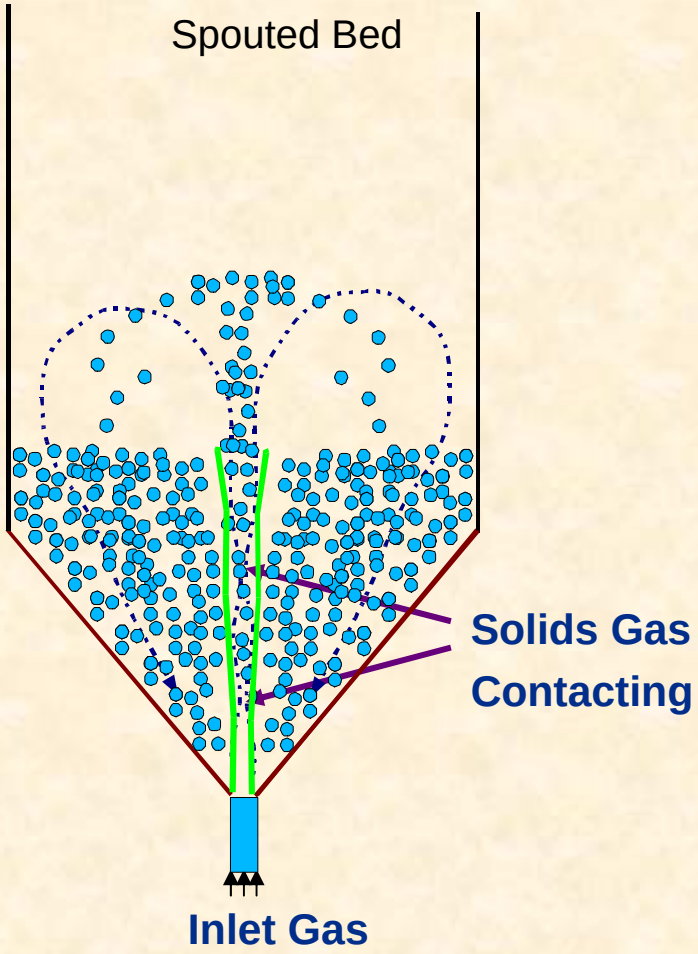
- Granular stresses modeled by granular kinetic theory (low density) and plastic flow theory (high density)
- Enhanced drag model describes gas-particle interaction
- Special post-processing allows mixing visualization, virtual particle tracking (simulates single particles)

Here we consider several simulation parameters that impact hydrodynamics

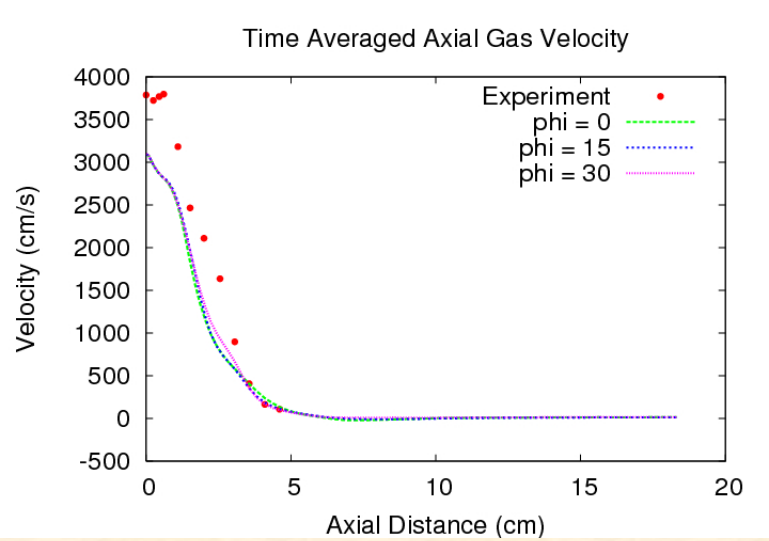
- **Particle-to-particle coefficient (*e*) of restitution**
  - **measures elasticity of particle-particle impacts**
  - **varied between 0.7 and 0.9 (higher value increases dissipation)**
  - **utilized where granular kinetic theory applicable for solids**
- **Angle of internal friction (ϕ) in dense flow**
  - **parameter describing shear-stress relationship in dense flow**
  - **varied between 0 and 30 degrees (higher value increases dissipation)**
  - **used only in regions where solids fraction is above critical value**
- **Representation of granular temperature**
  - **algebraic approximation, local equilibrium between production and dissipation**
  - **non-equilibrium PDE solved to account for transport**
- **Simulation grid resolution**
  - **non-uniform stretching**
  - **uniform grids with different spatial resolution**

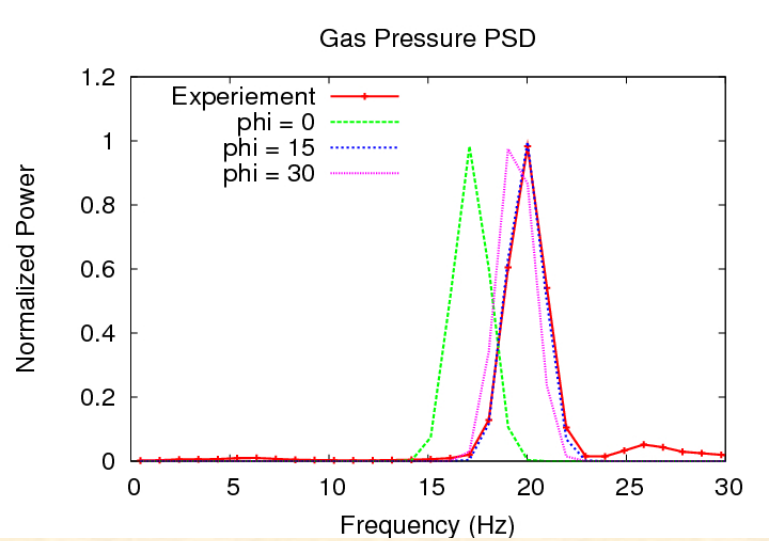
Spouted Bed

- **2 inch coater**
- **4 mm inlet**
- **54.5 gm of 500 micron Zirconia particles**
- **Air injected at 22 SLPM**

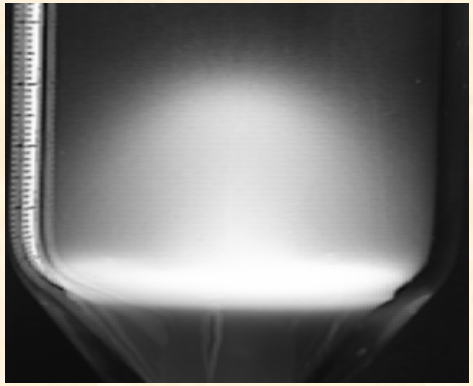


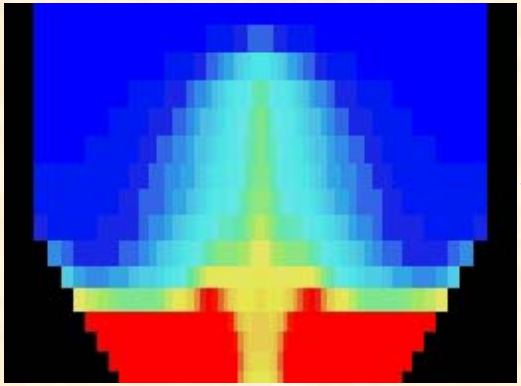
We find that both time-average and time-varying features should be considered in adjusting parameters to match experiments





Experiment

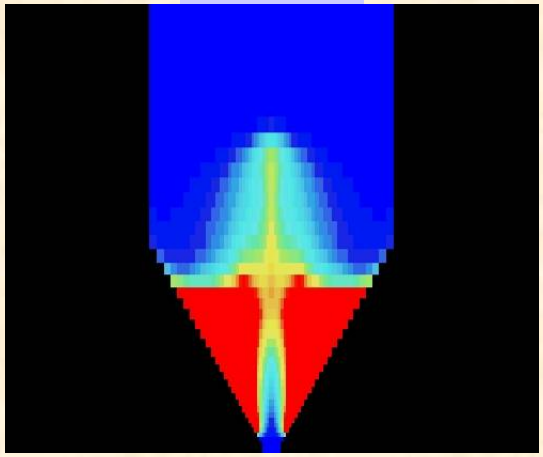




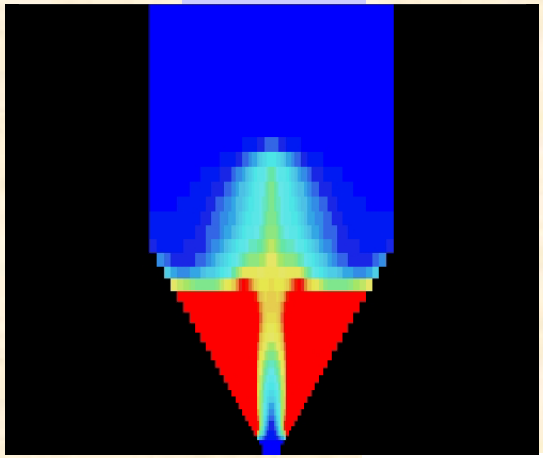
Simulation (ϕ = 15°)

The particle-to-particle coefficient of restitution affects the spout dimensions

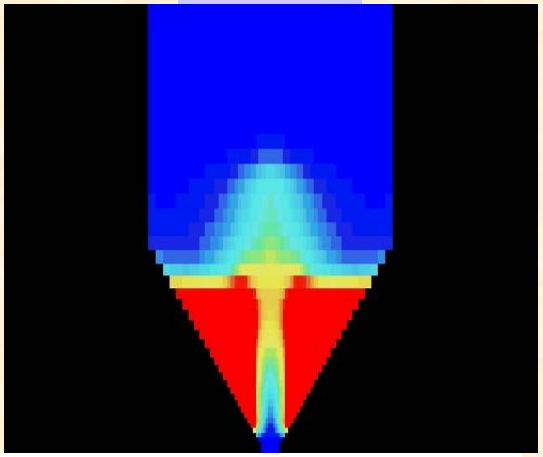
***e* = 0.7**

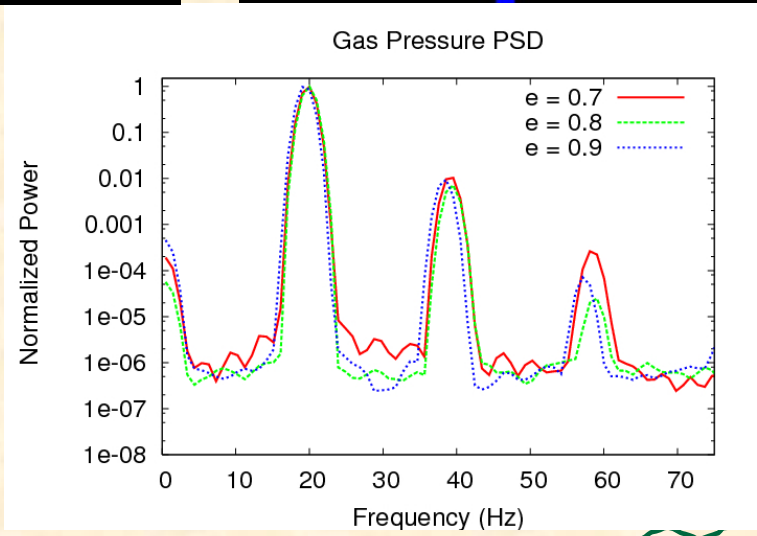


***e* = 0.8**



***e* = 0.9**



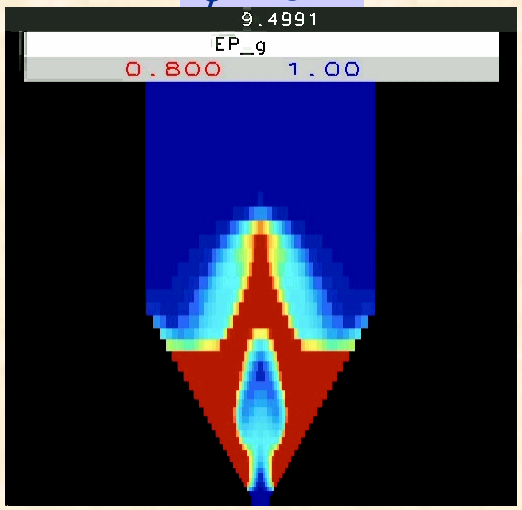


As *e* increases:

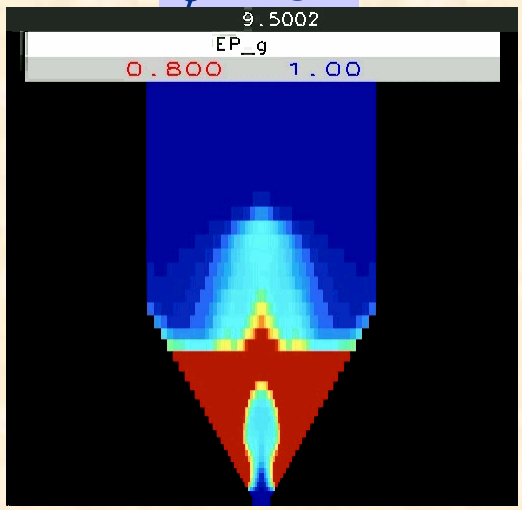
- **Spout height decreases**
- **Spout width increases**
- **No obvious effect on pulsation time scales**

The angle of internal friction changes the stability of the central core

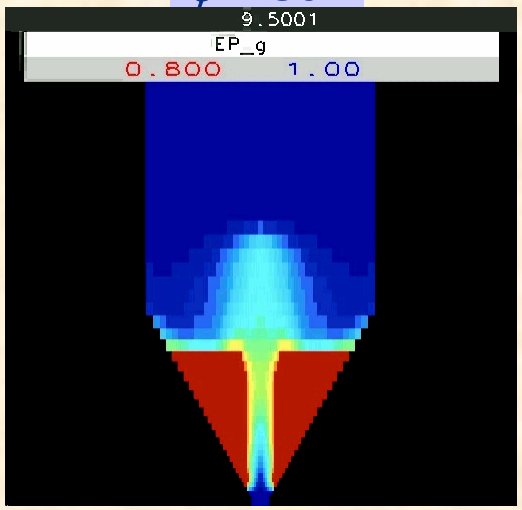
$\phi = 0°$

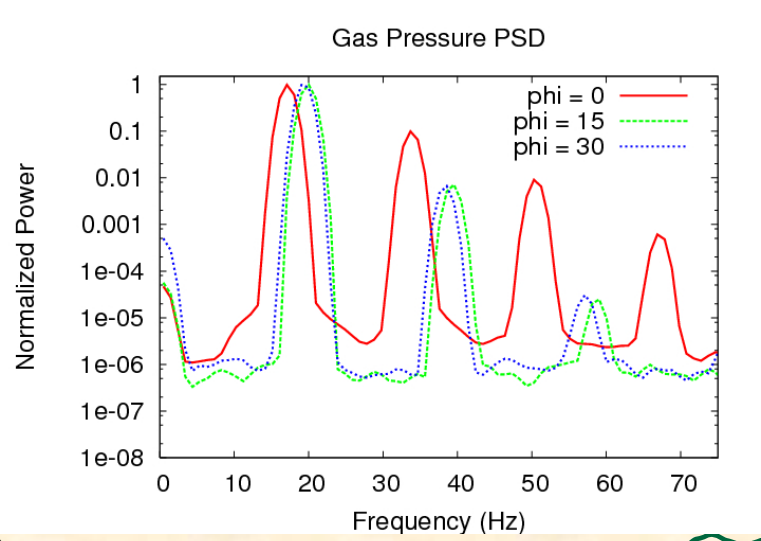


$\phi = 15°$



$\phi = 30°$



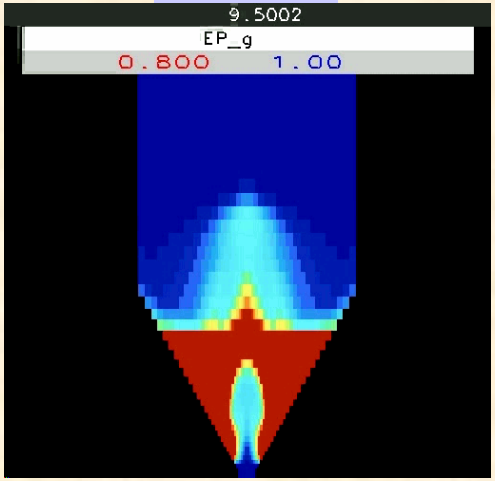


As ϕ increases:

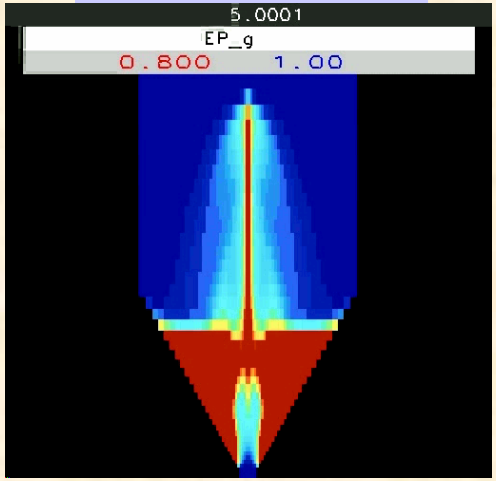
- **Central core more stable**
- **Pulsation rate increases**
- **Solids circulation reduced**

The treatment of granular temperature impacts the radial transport of energy

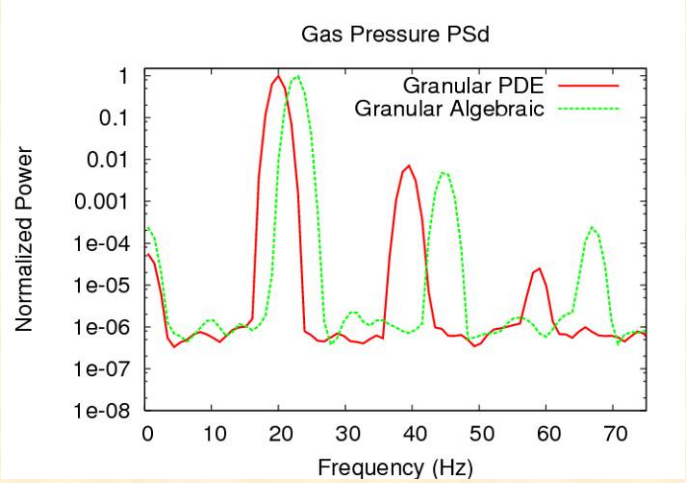
PDE



Algebraic

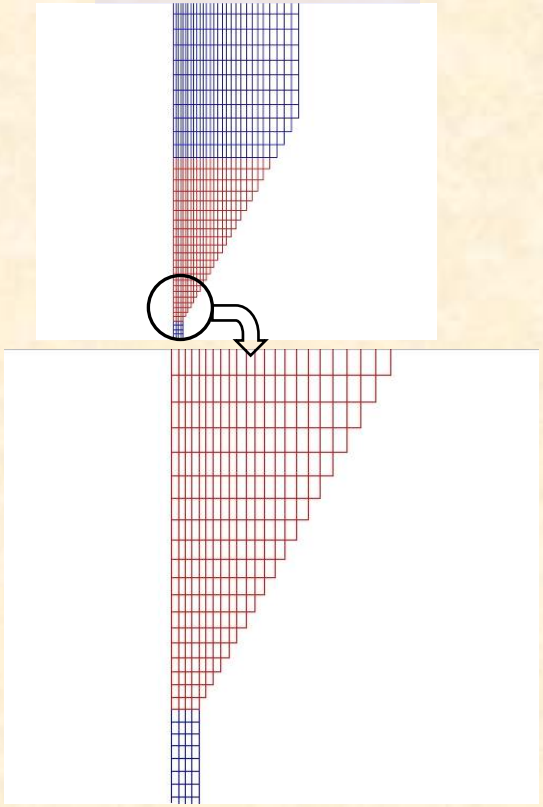


- **Algebraic form reduces radial energy transport, lengthens spout**
- **PDE form allows more natural interaction between core and outer annulus**
- **Pulsations rate increases for algebraic form**

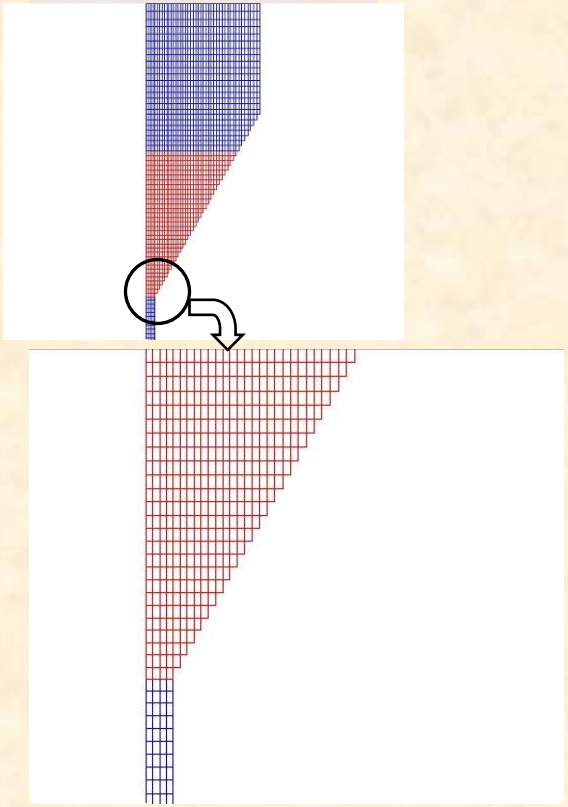


The various grids used here were intended to resolve different parts of the dynamics

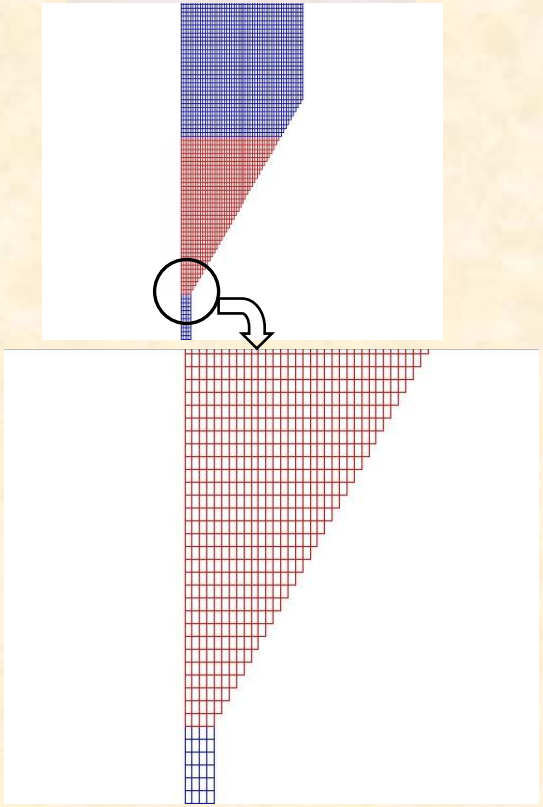
Coarse Mesh
28x80 (2240)



Fine Mesh
44x160 (7040)

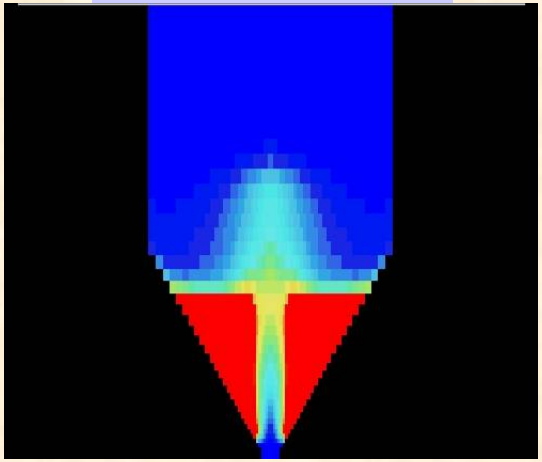


Uniform Mesh
51x172 (8772)

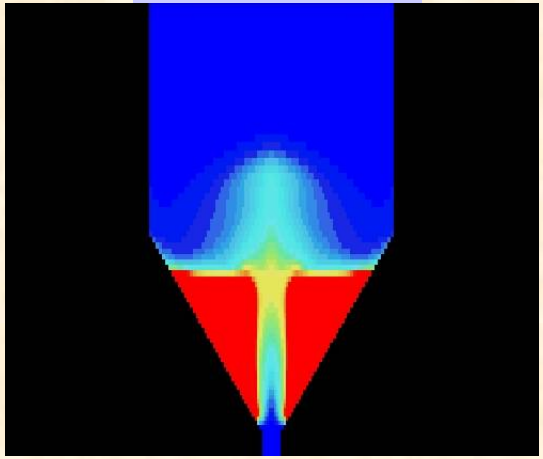


Simulation grid needs to be selected such that different regions are correctly resolved

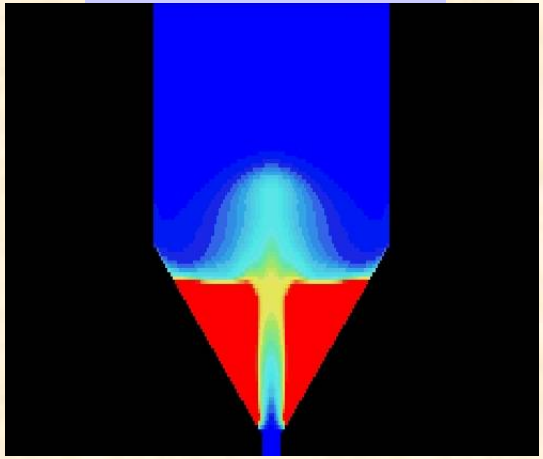
Coarse Mesh



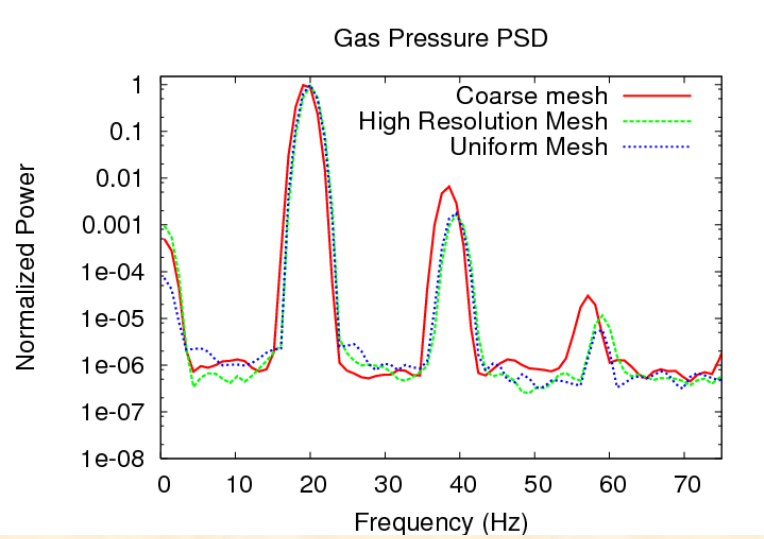
Fine Mesh



Uniform Mesh



- **Mixing dynamics in spout, core, and annulus need to interface properly**
- **Minimum mesh is of order of individual particle size**
- **Pulsation rate is almost the same**

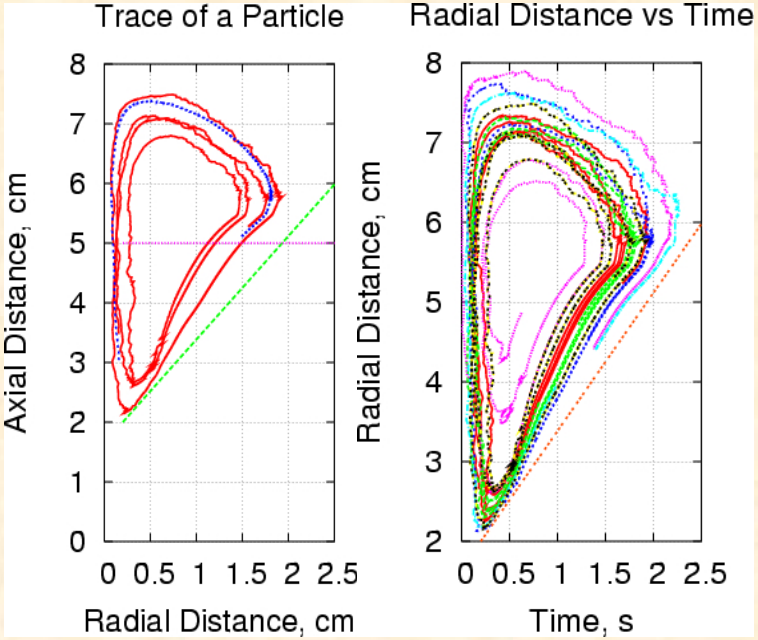


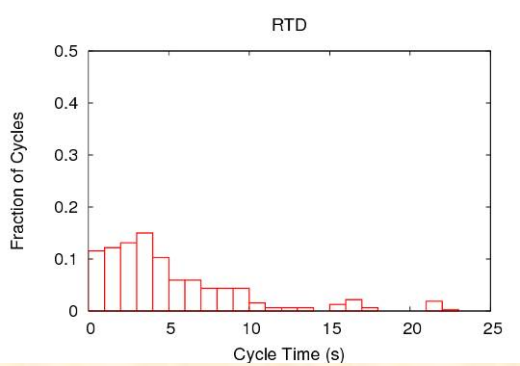
For experimental spouted-bed studies in conjunction with the nuclear-fuels coating, we have arrived at a specific set of recommended simulation parameter values

- **Particle-to-mesh Ratio: 1 to 6**
- **e = 0.8**
- **ϕ = 15°**
- **PDE equation for granular temperature**
- **Blended Kinetic Theory/Schaeffer formulation (# 62d)**
- **Boundary Conditions**
  - **Mass inlet at the bottom**
  - **Pressure outlet at the top**
  - **No-slip walls for gas; Johnson and Jackson condition for solids**

We have developed a new 'Virtual Tracer' algorithm that can help reveal differences in time-varying mixing dynamics

- **Lagrangian tracking in an Eulerian field**
- **Procedure**
  - **Identify the computational cell in which a tracer seed lies**
  - **Extract the solids velocities in that cell**
  - **Also account for the fluctuation component**
  - **Advance the tracer in time and space**
  - **Constraints at the wall, center line and the fountain zone**





Example particle residence time distribution in main circulation loop

Additional studies including several other prominent computational parameters are needed

- **Wall coefficient of restitution**
- **Numerical integration approximations (high order vs. low order)**
- **More variations of grid resolution**
- **Different boundary conditions**
- **Frictional stress formulations**

Conclusions

- **Proper selection of simulation parameters is quite important for accurately simulating spouted-bed hydrodynamics.**
- **In general appropriate values of these parameters must be determined by some degree of calibration with experiments.**
- **Matching time-averaged quantities is necessary but not sufficient; time-varying features should also be matched.**
- **In the long run, it may be necessary to develop non-averaged or local values of parameters such as those studied here to properly account for the observed behavior.**

Thank you for your attention!!

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