The Effect of Closure Laws on the Simulation Results of MFIX Two-Fluid Model of Gas-Solid flows

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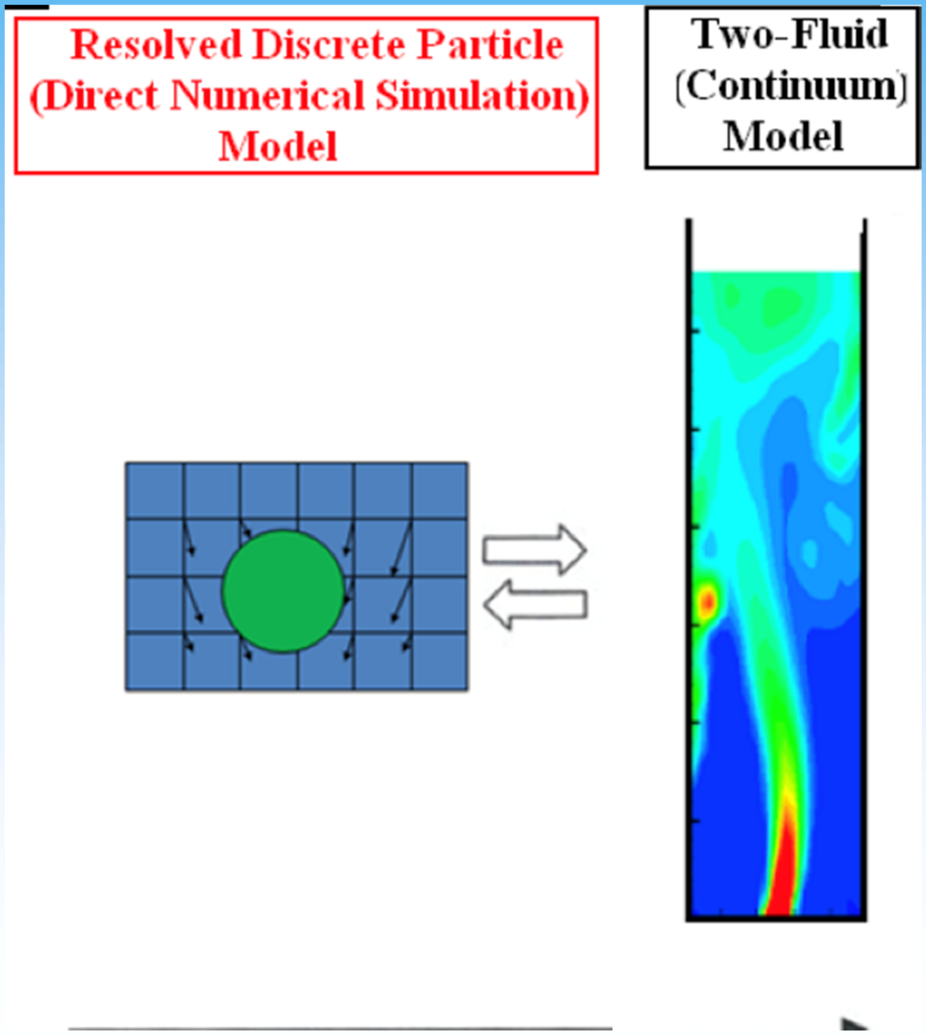
Multiscale Modeling for Particulate Flows

- To derive the drag correlation and heat transfer correlation based on the accurate result from direct numerical simulation (DNS)
- New correlation will be implemented into TFM to validate and improve results



Two fluid model in MFIX

- Momentum equation for gas phase

$$\left[\frac{\partial}{\partial t}\left(\varepsilon_g \rho_g U_{gi}\right)+\frac{\partial}{\partial x_j}\left(\varepsilon_g \rho_g U_{gj} U_{gi}\right)\right] = -\varepsilon_g \frac{\partial P_g}{\partial x_i} + \frac{\partial \tau_{gij}}{\partial x_j} - \sum_{m=1}^{M} I_{gmi} + f_{gi} + \varepsilon_g \rho_g g_i \qquad \text{(A4)}$$

  - Interphase momentum transfer

$$I_{gmi} = \beta_{gm}\left(u_{gi} - u_{mi}\right)$$

$$\beta_{gm} = 18\mu_g\left(1-\varepsilon_m\right)^2 \varepsilon_m \frac{F}{d_{pm}^2}$$

  - Various drag models for F

- Energy equation for gas phase

$$\varepsilon_g \rho_g C_{pg}\left[\frac{\partial T_g}{\partial t} + U_{gj}\frac{\partial T_g}{\partial x_j}\right] = -\frac{\partial q_{gi}}{\partial x_i} + \sum_{m=1}^{M}\gamma_{gm}\left(T_m - T_g\right) - \Delta H_g + \gamma_{Rg}\left(T_{Rg}^4 - T_g^4\right)$$

  - Interphase heat transfer

$$\gamma_{gm} = {C_{pg} R_{gm}} \Big/ \left[\exp\left(\frac{C_{pg} R_{gm}}{\gamma_{gm}^0}\right) - 1\right] \qquad \gamma_{gm}^0 = {6\kappa_g \varepsilon_m Nu_m} \Big/ {d_m^2}$$

$$Nu_m = \left(7 - 10\varepsilon_g + 5\varepsilon_g^2\right)\left(1 + 0.7\,\mathrm{Re}_m^{0.2}\,\mathrm{Pr}^{1/3}\right) + \left(1.33 - 2.4\varepsilon_g + 1.2\varepsilon_g^2\right)\mathrm{Re}_m^{0.7}\,\mathrm{Pr}^{1/3}$$

- Validation and improve these interface models

Summary of MFIX Equations (January 2012), NETL.

Interface momentum and heat transfer

- Interface models in MFIX
  - Most of them based on experimental studies at high solid Fractions

  DRAG:
  - Ergun model
  - Wen-Yu model
  - Gidaspow model
  - Syamlal and O’Brien model
  - Hill-Koch-Ladd model

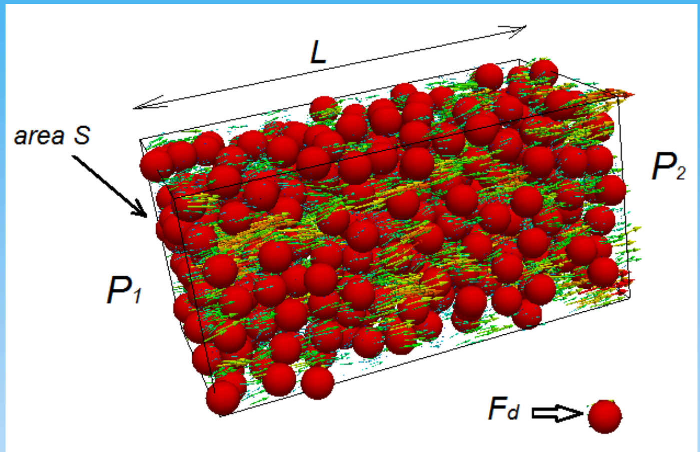
  HEAT TRANSFER:
  - Gunn model
  - Sun et al. model
- Improve interface models in MFIX
  - Use the resolved method: DNS

How to use DNS to compute drag

- Consider a control volume (CV) of N fixed particles
  - Flow is driven by pressure difference
  - Periodic boundary conditions
- Use DNS method *(Proteus*)* to solve flow in the CV
  - solid fraction $\phi = \frac{N\frac{\pi D^3}{6}}{Volume\ of\ the\ CV}$,

    $Re = \frac{\rho U D}{\mu}$, $U = flow\ average\ vel.$
  - Compute the average drag: $\bar{F}_d$
  - Dimensionless drag (Drag model)
    - $F = \frac{\bar{F}_d}{3\pi\mu D U}$
- Change the pressure (p1,p2) and number of particles N to vary Re and ϕ.
- Correlation (drag model):

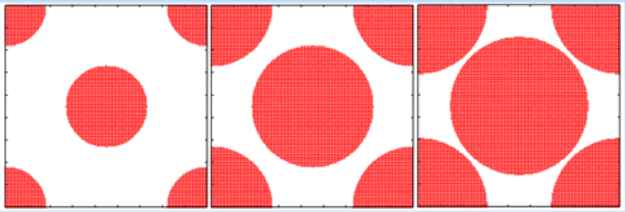
$$F = F(Re, \phi)$$



*Feng, Z.-G. and E. E. Michaelides, "***Proteus***: A direct forcing method in the simulations of particulate flow," *J. Comput. Phys.*, **202**: 20-51 (2005).

Validation case:
Flows over face-centered arrays of spheres

- A small cubic unit of size L is selected as computational domain.
  - Low Reynolds number (Re<0.01)
  - solid volume fraction $\phi = \frac{16\pi a^3}{3L^3}$
    - Highest solid fraction is 0.74 when spheres are in contact.
    - We are able to achieve converged results at solid fraction 0.658.
  - Grid up to 200x200x200 is used
    - Particle diameter is outlined by 136 nodes;
    - 57837 nodes assigned to the surface of a sphere
  - Dimensionless drag force $F = \frac{F_d(\phi)}{F_d(0)} = \frac{F_d(\phi)}{6\pi\mu a U}$



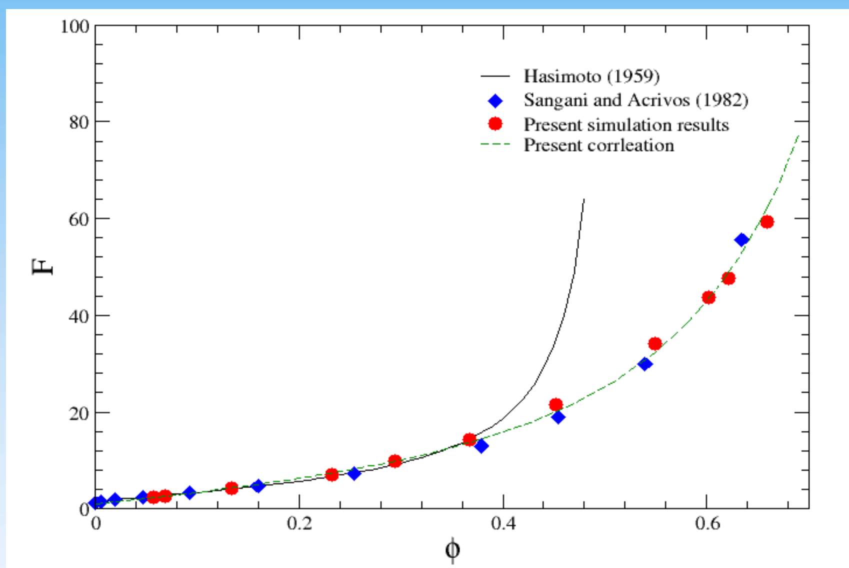
The void region(white) and solid region at a side surface of the computational cell Left: Φ=0.134; middle: ϕ=0.452; right: ϕ=0.659

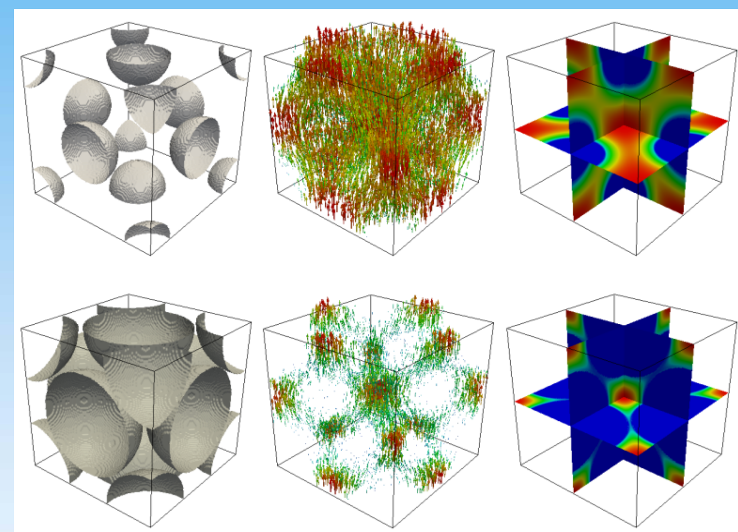
- Theoretical solution for Stokes flows at low solid fraction(<0.2)* $F = \frac{1-\phi}{1-1.791\sqrt[3]{\phi}+\phi-0.302\phi^2+\cdots}$

Hasimoto, H., "On the periodic fundamental solutions of the Stokes equations and their application to viscous flow past a cubic array of spheres," *J. Fluid Mech*., 5:317-328 (1959).

Validation results

- Flow structures for face-centered cases





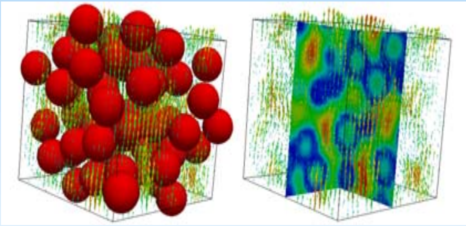
Flow over face-centered arrays of spheres at solid fractions 0.134 and 0.659: (a) pore structure; (b) flow velocity vector; (c) flow velocity (magnitude) contour.

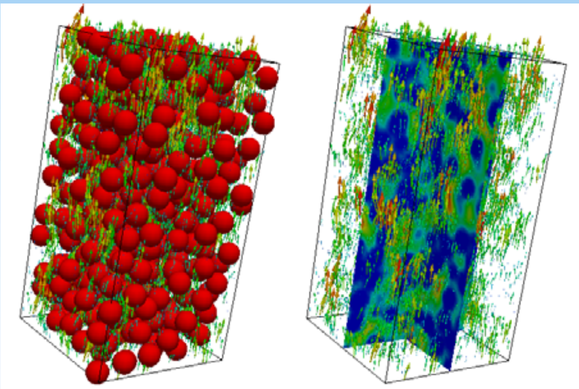
- Correlation of $C_d \sim \phi$

$$F(\phi) = 10\frac{\phi}{(1-\phi)^2} + 12\phi\sqrt{1-\phi} + 1.$$

Flows over random arrays of spheres

- Randomly distributed spheres
  - Using 60~405 spheres; solid fraction Φ=0.05~0.63.
  - Different Reynolds number by changing pressure gradients, 0<Re<300.

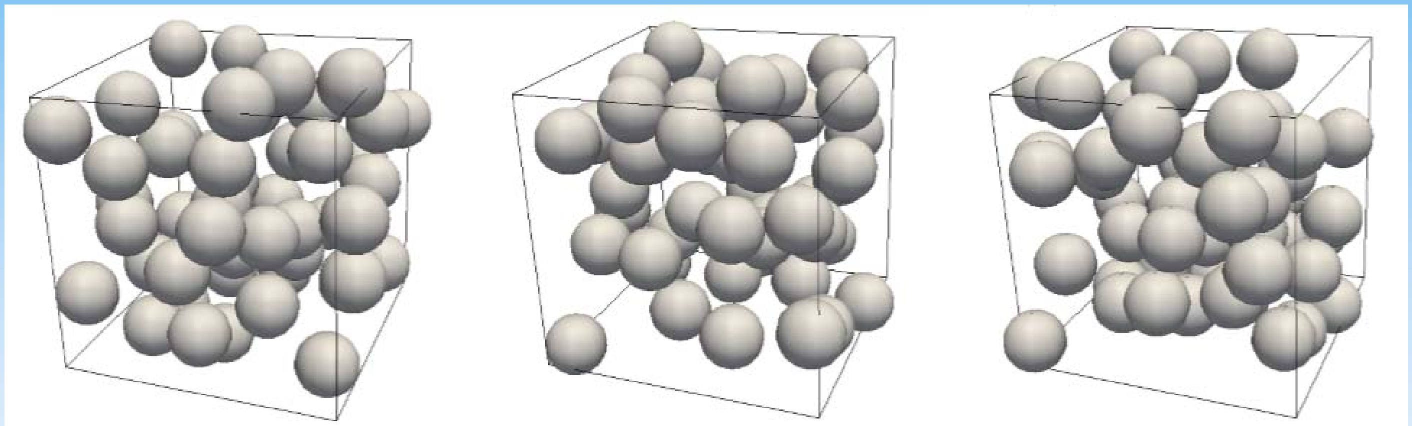


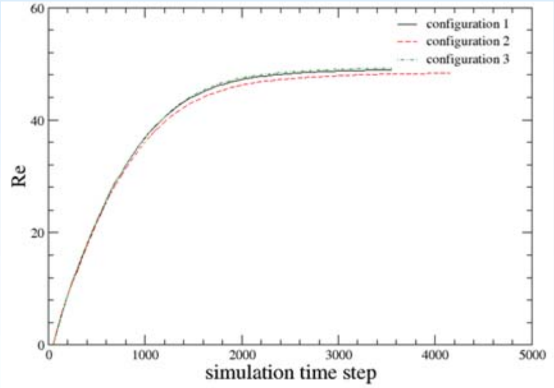


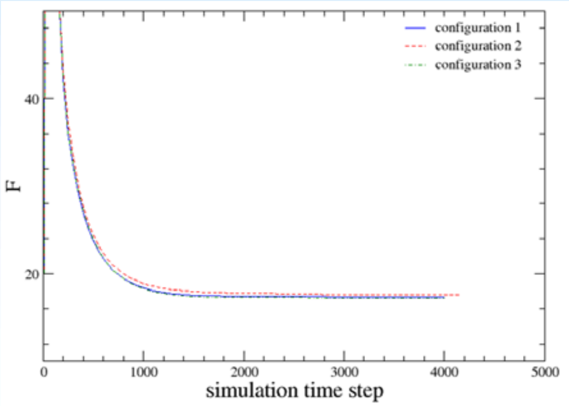
LEFT: Flow over a random distributed 60 spheres; RIGHT: Flow over 405 spheres. The same pressure gradients are applied. Solid volume fraction for both cases: ϕ=0.345.

Influence of sphere configurations

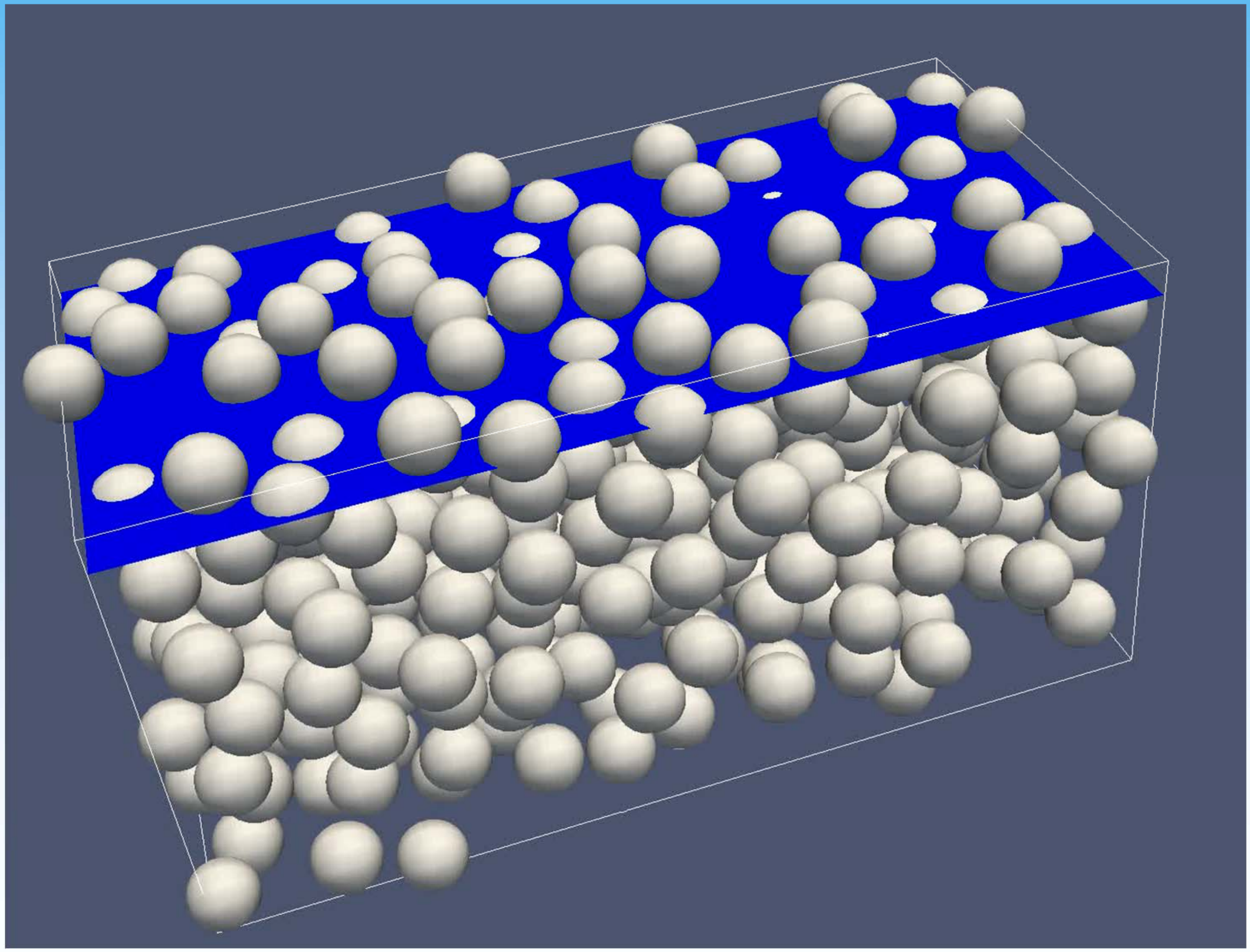
- Three different random configurations of 50 spheres placed in a cube (solid fraction 0.2873)
- Applied the same pressure gradient





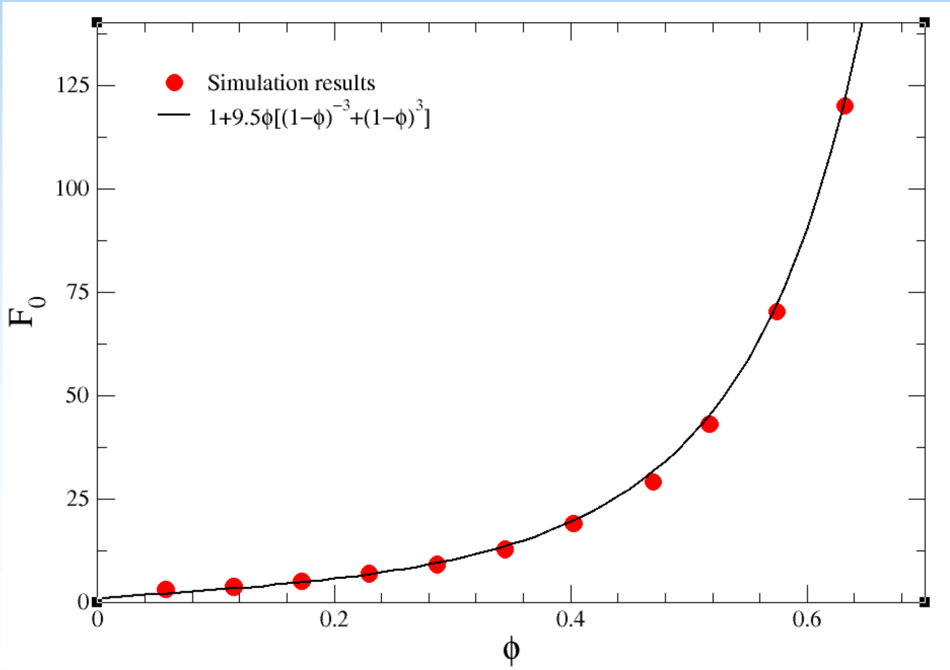


Flow in a random arrays of spheres (Animation)



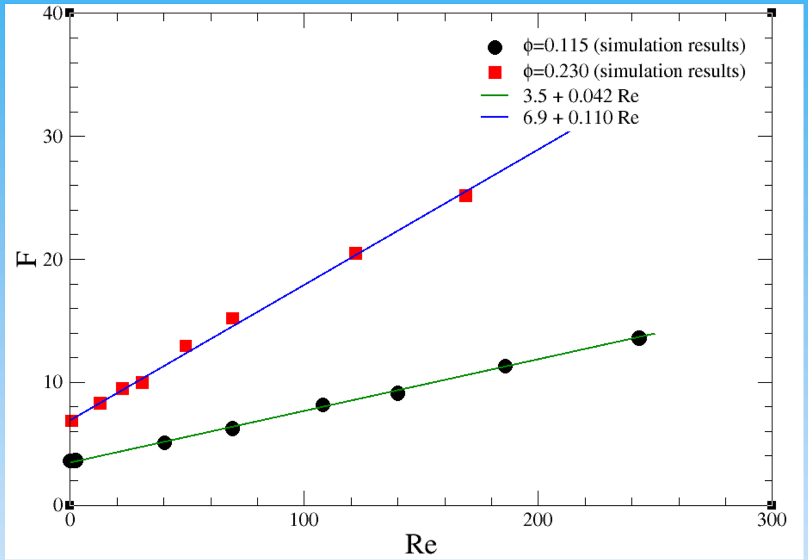
Drag vs. solid fraction and Reynolds number

- In general, it is found $F = F_0 + m\,\mathrm{Re}$
  - F_0 and m are only functions of solid fraction.
- At very low Re<<1, $F_0 = 1 + 9.5\phi/(1-\phi)^3 + 9.5\phi(1-\phi)^3$

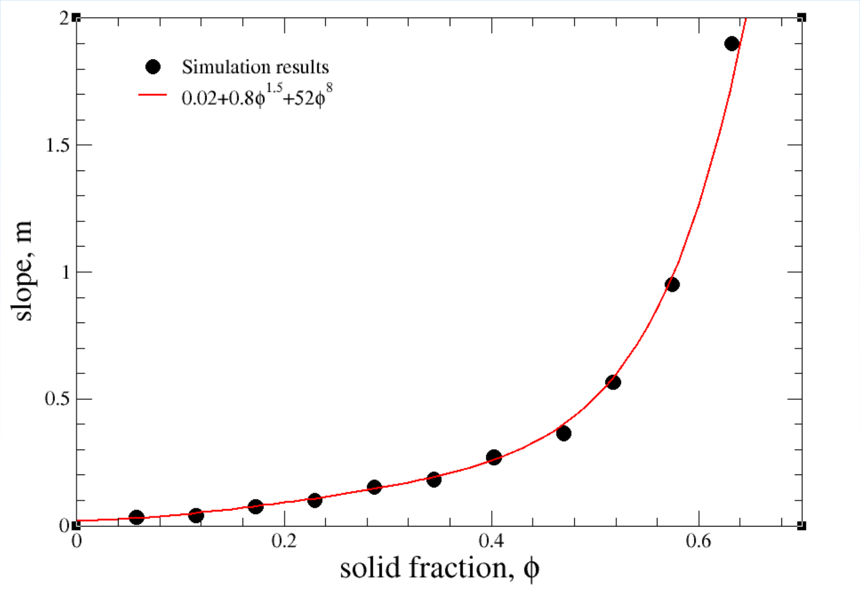


Drag vs solid fraction and Reynolds number

- Slope m for each solid fraction



- Slope vs. solid fraction



$$m = 0.002 + 0.8\varepsilon_s^{1.5} + 52\varepsilon_s^{8}$$

New drag correlation

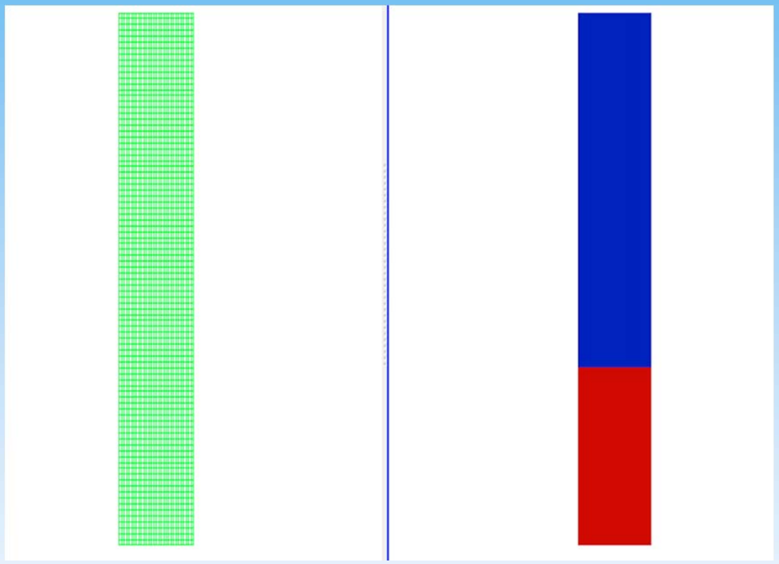
- Final correlation for the drag model:

$$F = 1 + 9.5\phi/(1-\phi)^3 + 9.5\phi(1-\phi)^3 + (0.002 + 0.8\phi^{1.5} + 52\phi^8)\mathrm{Re}$$

  - Based on over 150 simulation data.
  - Applicable to solid fraction 0.05~0.63 and Reynolds number 0~300.
  - Easy to be implemented in MFIX

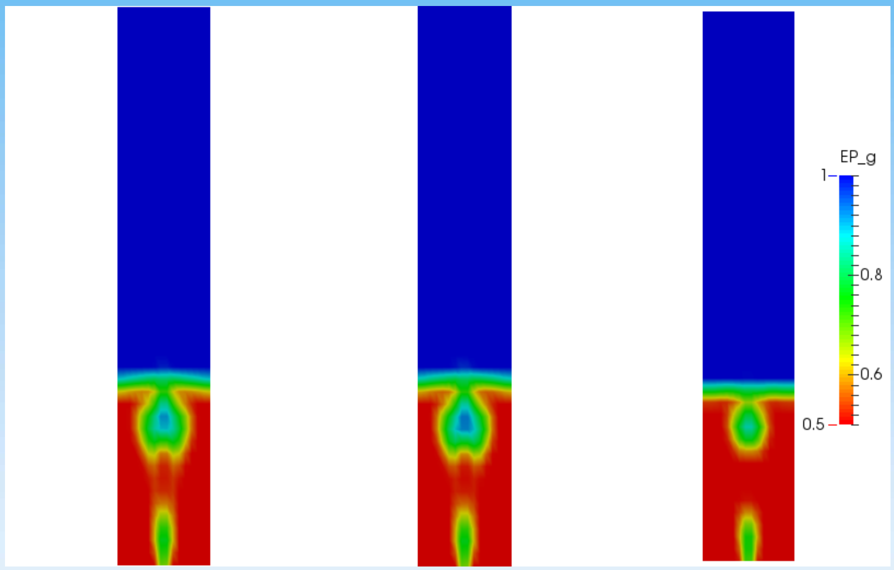
Implementation of drag model

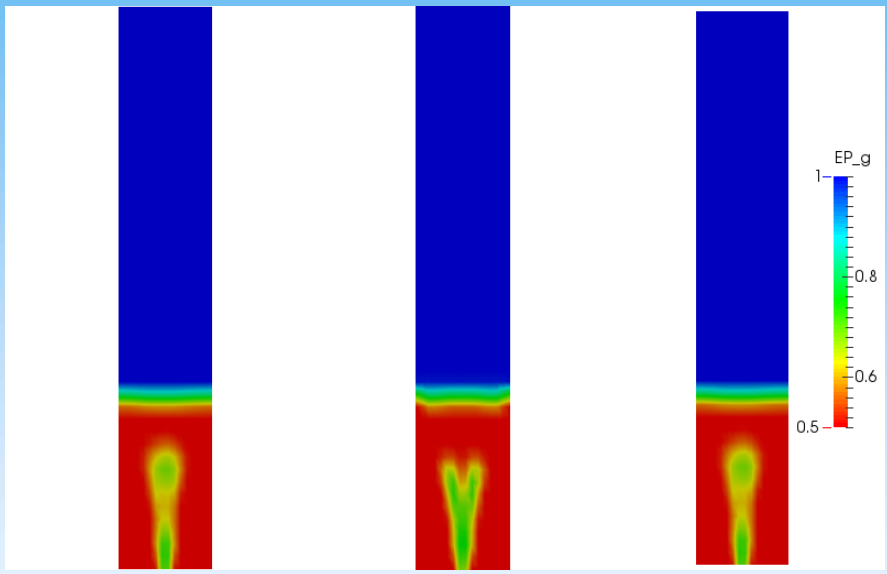
SIMULATION AND MODEL PARAMETERS	
Bed height	90cm
Bed width	15cm
Static bed height	30cm
Grid resolution	30x90
Gas density	1.205kg/m^3
Gas viscosity	1.8e^{-5}s/m^2
Particle density	2700kg/m^3
Particle diameter	0.4cm
Initial volume fraction	0.499
Angel of internal fraction	30
Restitution coefficient	0.9
Friction coefficient	0.3
Background velocity	2.6m/s



Tsuji, Y., et al. (1993). "Discrete particle simulation of two-dimensional fluidized bed." Powder technology **77**(1): 79-87.

Implementation of drag model





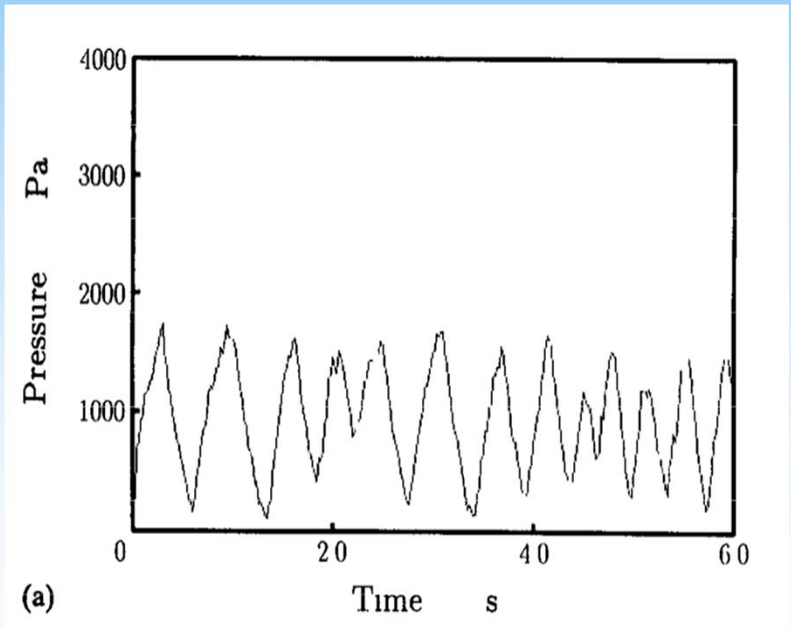
t=0.4 secs

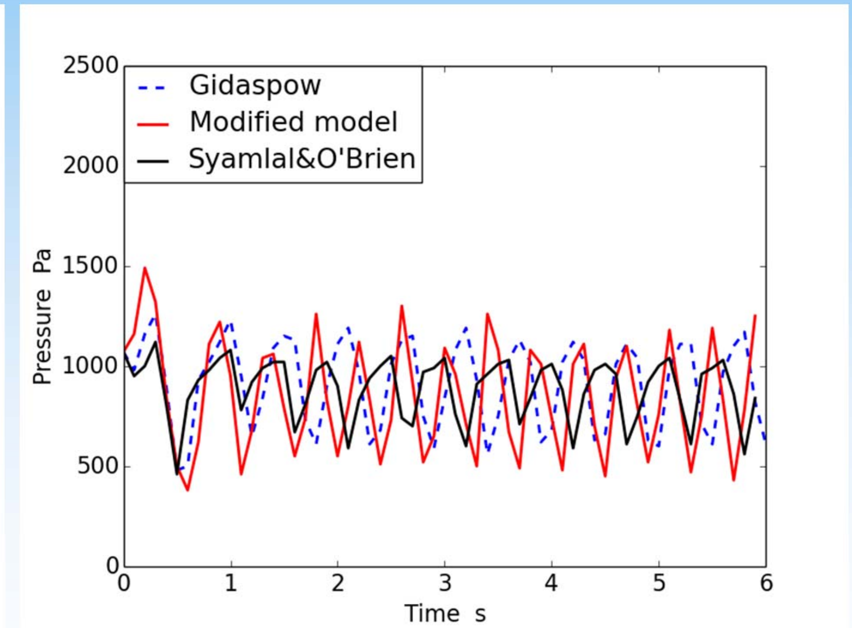
t=4 secs

From left to right: Gidaspow, our modified model, and Syamlal&O'Brien

Comparison with experimental data

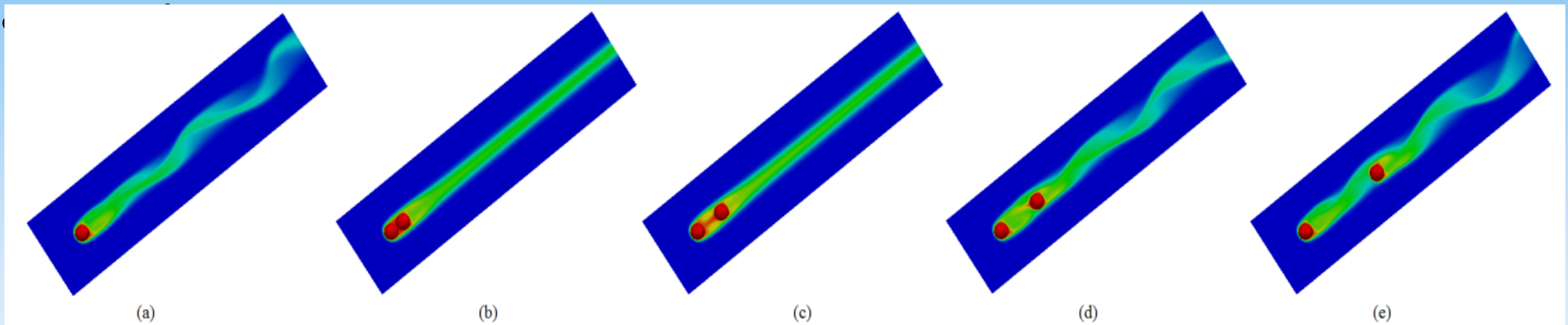
Gas pressure at 20cm height from experiment (left) and from the MFIX two fluid simulation (right). All three model correctly predicted the time average pressure; the fluctuation frequency generally agrees with the experimental data. Result is in consistence with the findings of smaller bubble sizes by Syamlal-O'Brien model that produces less violent pressure fluctuations as the bubble bursts. Overall our modified model has more accuracy in terms of the fluctuation amplitude.

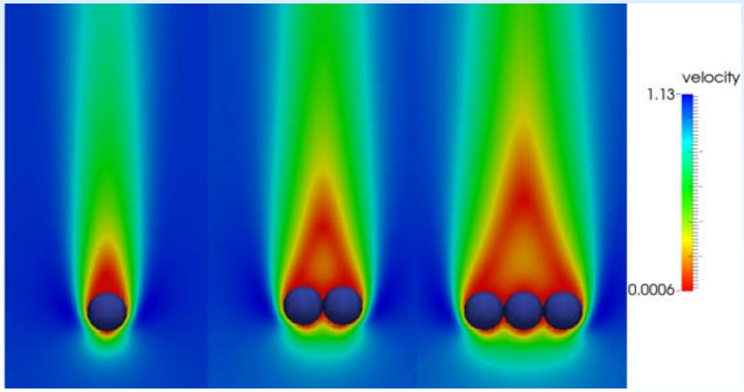




Heat transfer correlation

- DNS based *Proteus* method is extended to solve heat transfer
- Follow the same procedures of deriving drag model to develop new closure law for interphase heat transfer (in progress)





Interphase heat transfer model

Current heat transfer model: Gunn's model

Interphase heat transfer

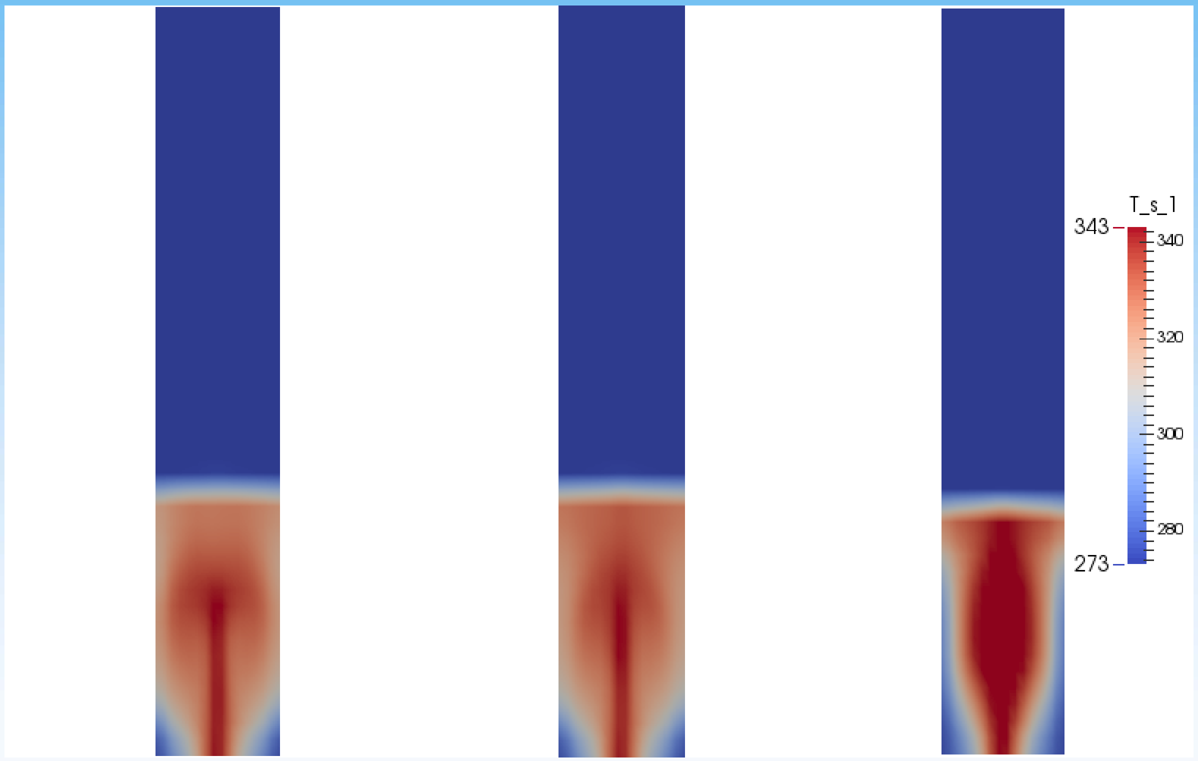
$$\gamma_{gm} = \frac{C_{pg} R_{gm}}{\left[\exp\left(\frac{C_{pg} R_{gm}}{\gamma_{gm}^{0}}\right) - 1\right]}$$

$$\gamma_{gm}^{0} = \frac{6\kappa_g \varepsilon_m Nu_m}{d_m^2}$$

$$Nu_m = \left(7 - 10\varepsilon_g + 5\varepsilon_g^2\right)\left(1 + 0.7\,\mathrm{Re}_m^{0.2}\,\mathrm{Pr}^{1/3}\right) + \left(1.33 - 2.4\varepsilon_g + 1.2\varepsilon_g^2\right)\mathrm{Re}_m^{0.7}\,\mathrm{Pr}^{1/3}$$

Importance of closure laws to heat transfer

Drag model can have significant impact on temperature distribution by affecting the flow structure:



Temperature of solid phase at 6 second after a simulation fluidized bed with heated bottom inlet (1000K) in the middle, Gidaspow(left), our modified model(middle) and Syamlal&O'Brien model(right) incorporating Gunn's heat transfer model

Conclusions

- MFIX two-fluid model simulation requires the use of drag model and heat transfer model, and the choice of drag model can significantly influence MFIX simulation results
- The Koch-Hill drag model underestimates the gas-solid momentum exchange rate and was not able to capture the fluidization process; the Gidspow model predicts larger bubble size compared to the Syamlal-O'Brien model
- Direct numerical simulation is able to derive closure laws to be used in MFIX
- A new drag model has been developed and implemented in MFIX. The new drag model produces better results based on the comparisons with experimental data
- Drag model can also have a large impact on flow heat transfer in fludized beds
- Future work will focus on the development of an improved heat transfer model

LIST OF PAPERS PUBLISHED, STUDENTS SUPPORTED UNDER THIS GRANT

- **Archival journal publications:**
  - Feng, Z-G., Ponton, M. E. C., Michaelides, E. E., and Mao, S. (2014). "Using the Direct Numerical Simulation to Compute the Slip Boundary Condition of the Solid Phase in Two-Fluid Model Simulations." *Powder Technology.* j.powtec.2014.01.020
  - Feng, Z.G. (2014), "Direct Numerical Simulation of Forced Convective Heat Transfer from a Heated Rotating Sphere in Laminar Flows," ASME *J. of Heat Transfer, " Journal of Heat Transfer*. doi:10.1115/1.4026307
  - Feng, Z-G and Musong, S. (2014), "Direct Numerical Simulation of Heat and Mass Transfer of Spheres in a Fluidized Bed," *Powder Technology*. http://dx.doi.org/10.1016/j.powtec.2014.04.019.
  - Musong, S. and Feng, Z-G (2014), "Mixed Convective Heat Transfer from a Heated Sphere at an Arbitrary Incident Flow Angle in Laminar Flows," Int. J. Heat and Mass Transfer, vol. 78, pp. 34-44.
  - Feng, Z-G, Alatawi, E. S., Roig, A., and Sarikaya, C.(2015), "A resolved Eulerian-Lagrangian simulation of fluidization of 1204 heated spheres in a bed with heat transfer." ASME Journal of Fluid Engineering, in print.
- **6 conference proceeding papers**

- **Student involved in the project**
  - Miguel Cortina, Yifei Duan, Samuel Musong (PhD candidates)
  - Adams Roig, Kody Smajstrla, Cenk Sarikaya, Steven Cooks (master students)
  - Silvia Murguia, Carlos Mendez, Joshua Moran (Undergraduate students)

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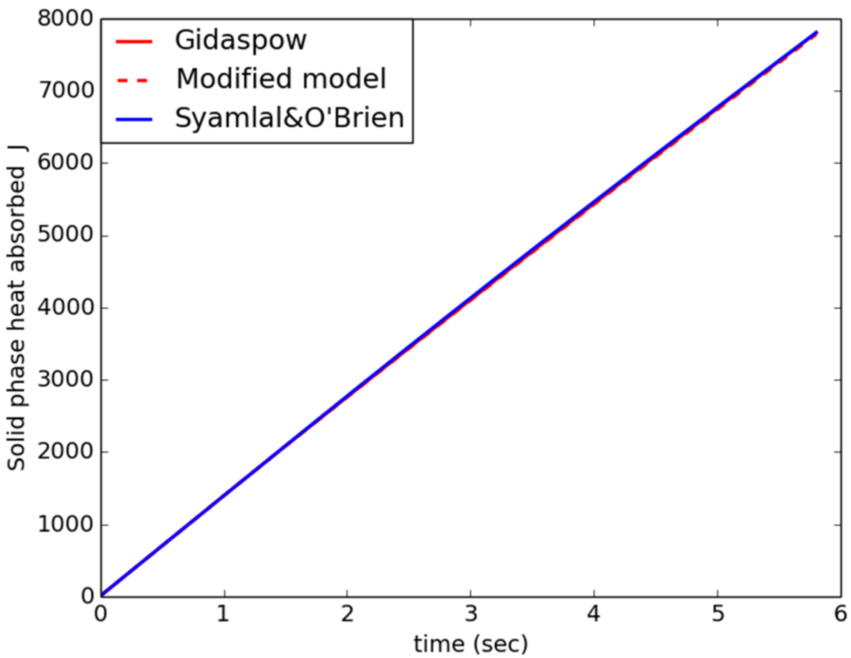
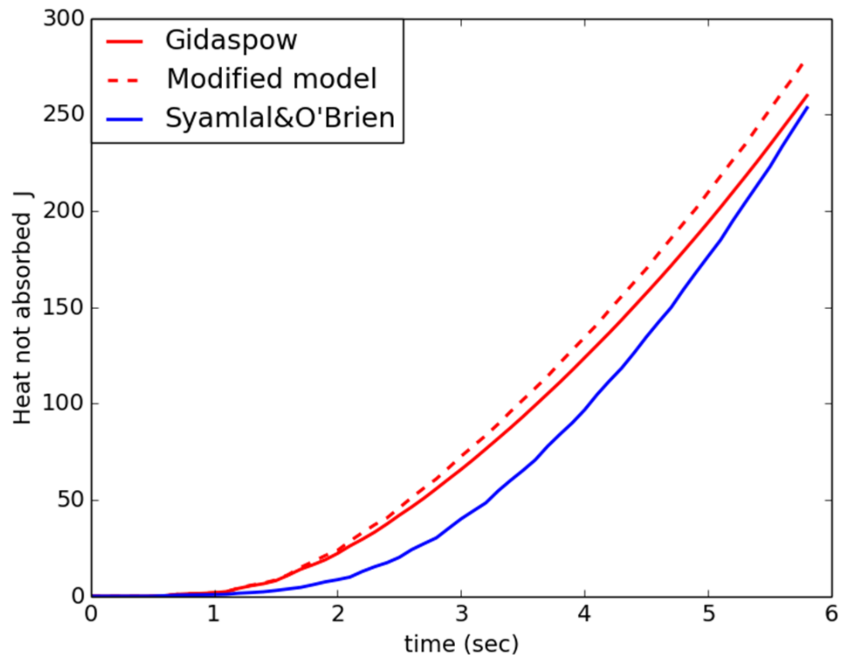
Thank you

Importance of closure laws to heat transfer

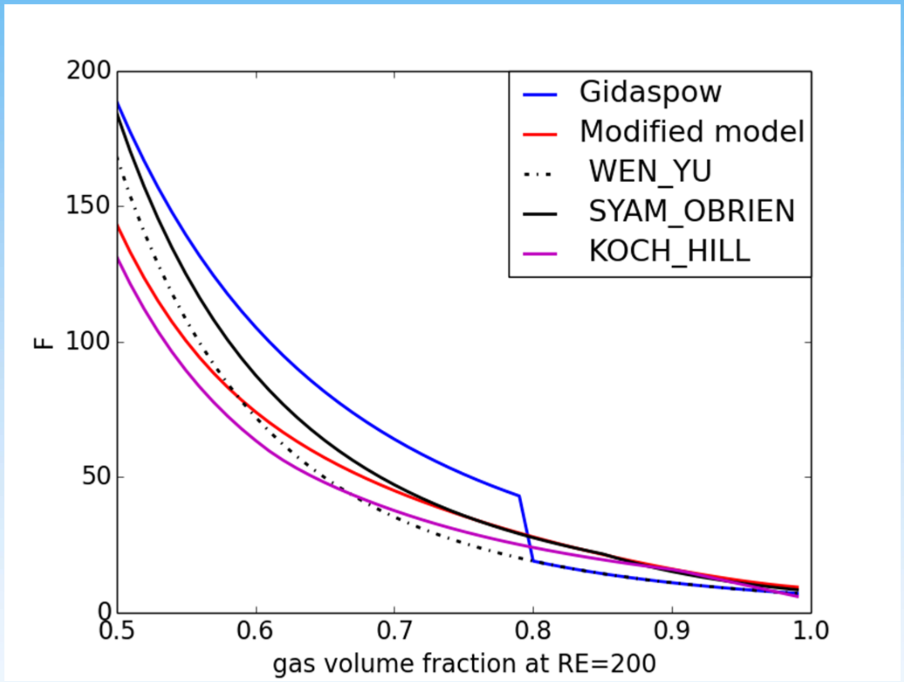


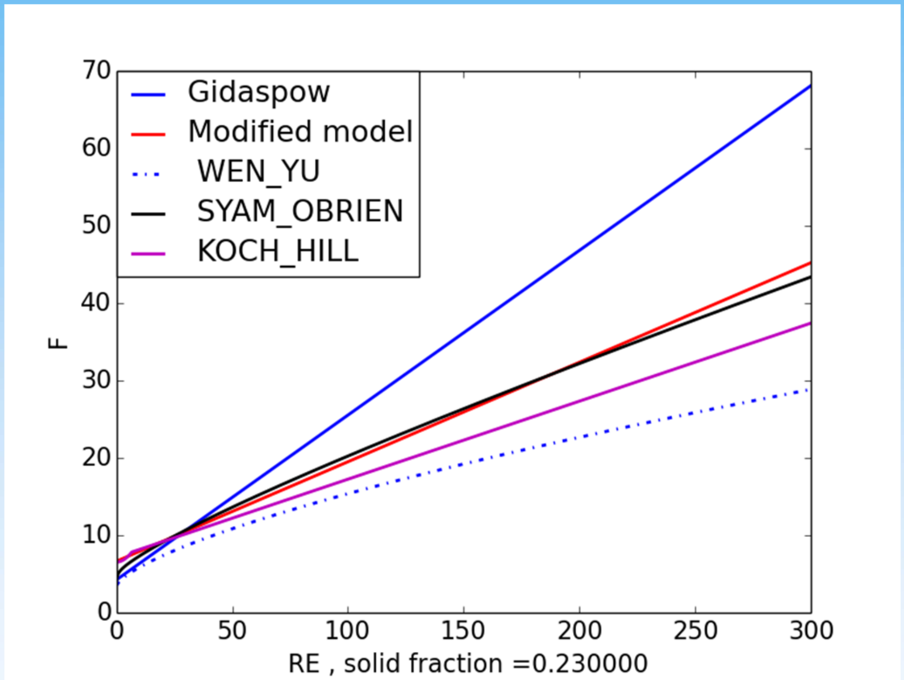


Total heat absorbed and not absorbed for solid phase in 6s after injection

Despite the temperature distribution, before system reaching a thermodynamic balance, especially for the first several seconds, drag model has little impact on the total heat exchange between solid phase and gas phase.

comparison of different drag models



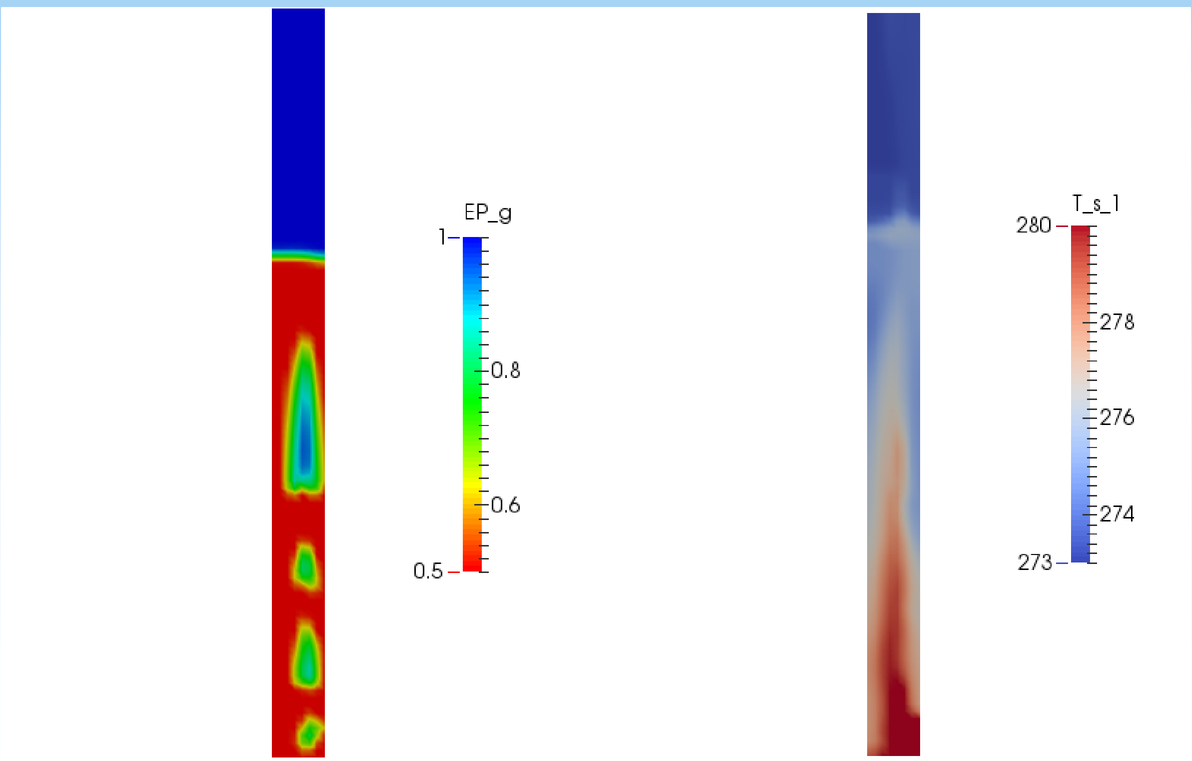


Left: Non-dimensional drag force F along with the gas volume fraction at Reynolds number of 200

Right: Non-dimensional drag force F along with the Reynolds number at solid fraction of 0.23

Sun heat transfer model at low Re number

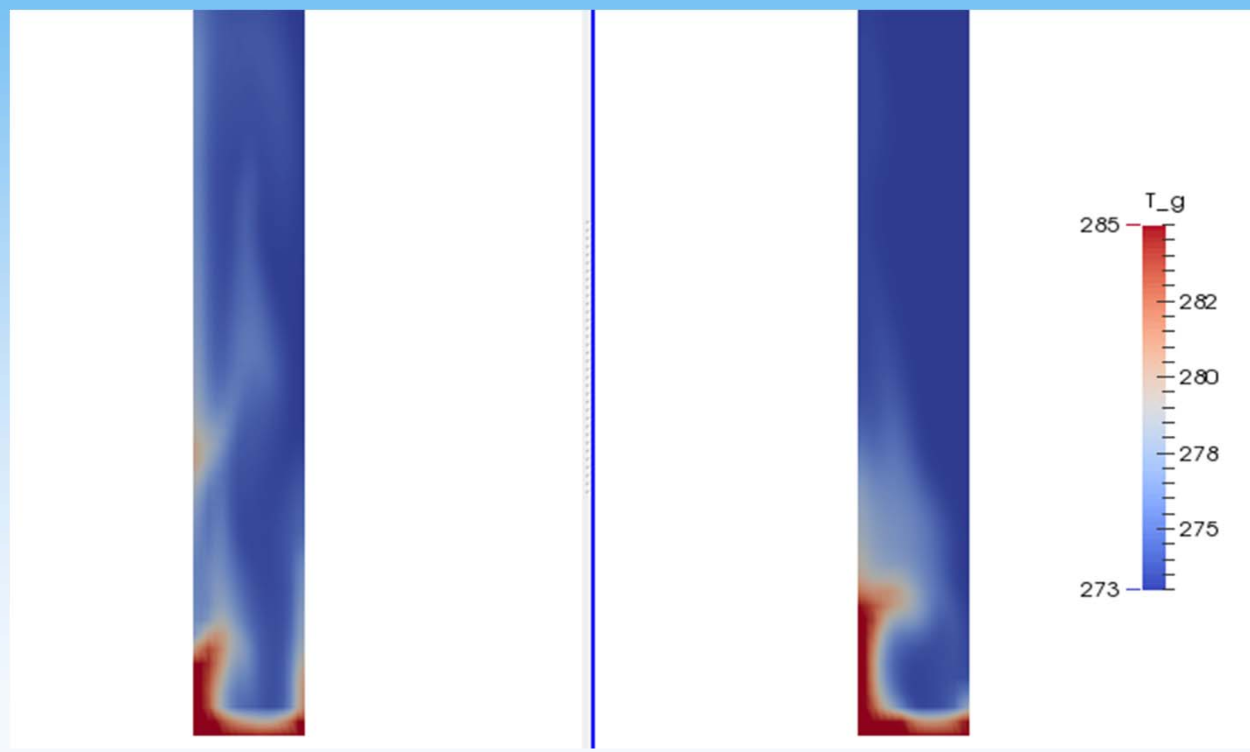
Cylindrical bed is 7cm x 100cm with initial bed height at 50cm. The uniform bottom inlet has a velocity of 61.7cm/s and gas temperature is 1000K. Both the solid phase and the freeboard above are initially at 273K.



Gas fraction (left) and solid phase temperature (right) at 5s after injection

Importance of closure laws

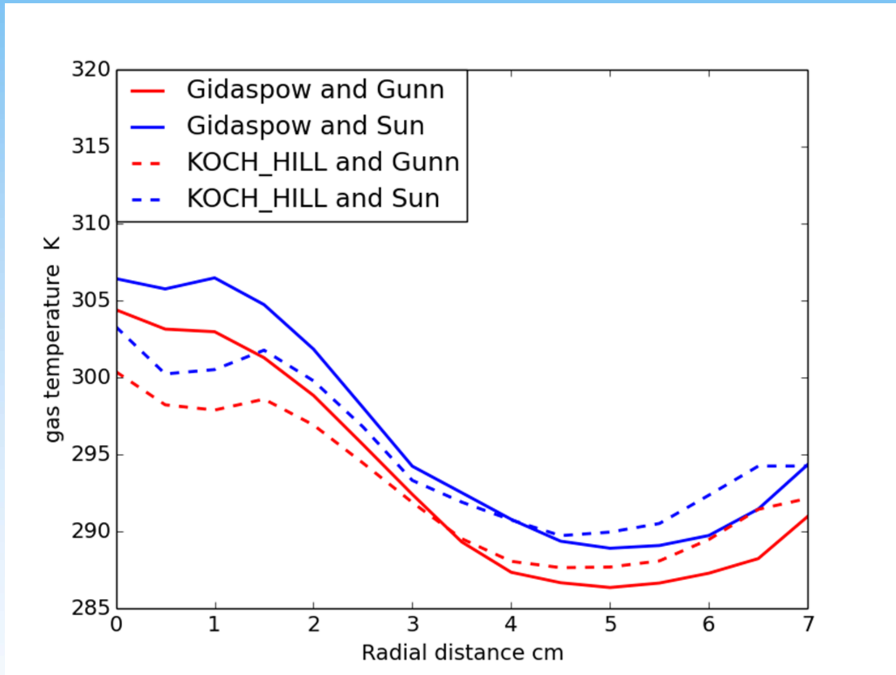
Zoomed view of temperature field of gas phase using two different drag model with Nu correlation given by Sun derived from DNS simulation at low RE number (RE<=100).

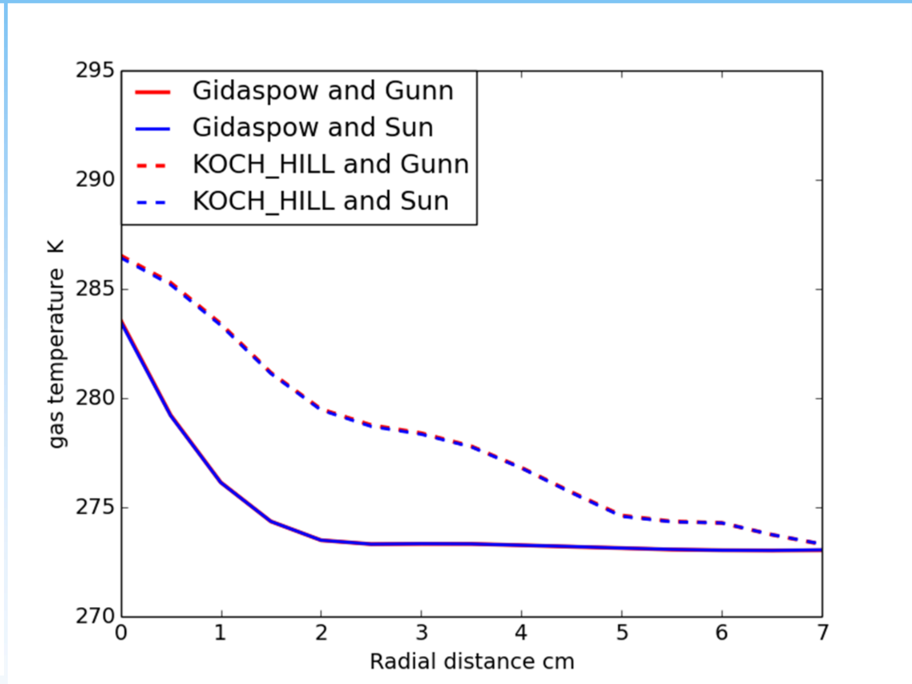


1 second after a simulation of cylindrical fluidized bed with uniform heated bottom inlet (1000K, 61.7cm/s), Gidaspow(left) and Koch&Hill(Right) incorporating Gunn's heat transfer model. Note: only half of the cylindrical bed is shown.

Importance of closure laws

Drag model have an impact on thermodynamics of flow by affecting the flow structure, temperature discrepancies caused by heat transfer model can also be observed in strong interphase heat exchange region.





1 second after a simulation of cylindrical fluidized bed with uniform heated bottom inlet,
gas temperature along radius at 1cm height from bottom(left) and 10cm height (right)