Efficient simulation of heated gas-solids flows

CCSI™ Carbon Capture Simulation Initiative

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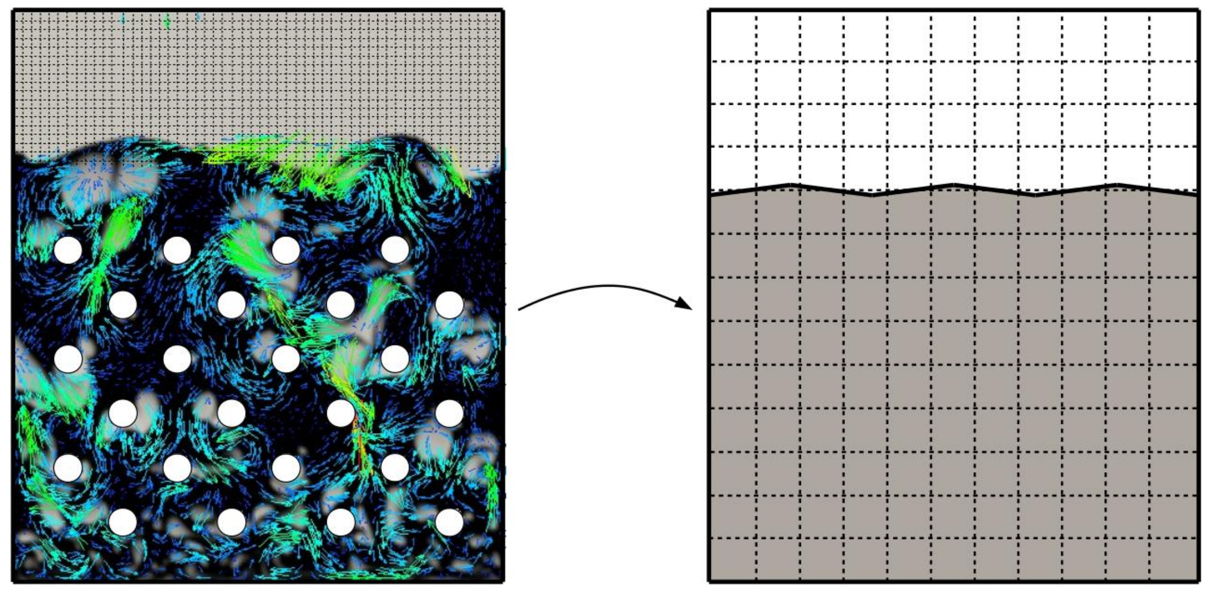
1. Introduction

Modeling gas-solid flows typically requires very fine computational grids, making it impractical for full scale applications. To overcome these issues, we use coarse-grid simulations with sub-grid filtering models[1,2] to approximate the unresolved physics. This research extends these methods by developing a model for heated gas-solid flows with immersed heat transfer cylinders.



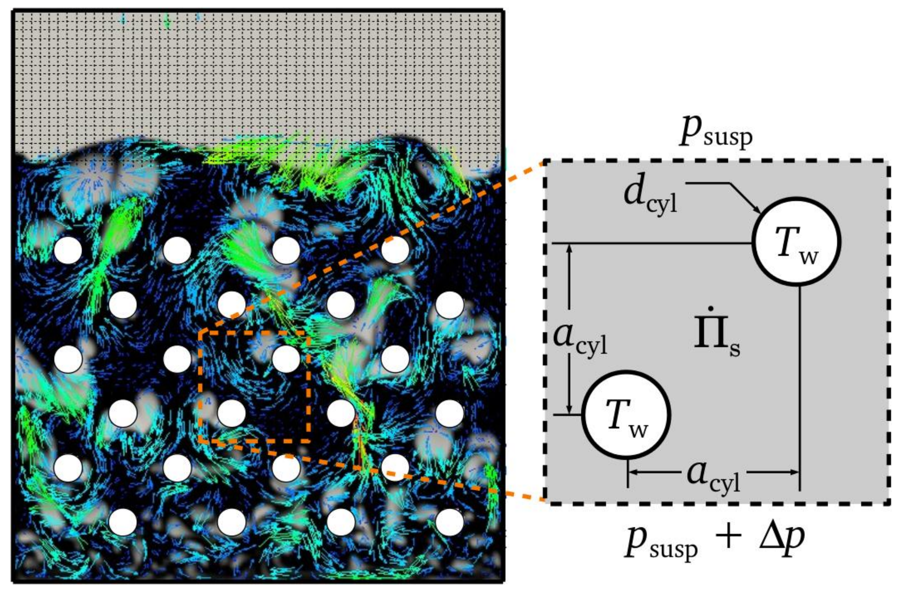
2. Filtering Methods

Sub-grid filtering is based on Large Eddy Simulations[3] for turbulence modeling, where many fine-grid simulations are averaged to constitute the closure models. The general filtering procedure follows:

1. Construct unit-cell domain from the full domain.
2. Select model parameters (i.e., model predictors).
3. Design and run simulation campaign, varying input parameters over their respective ranges.
4. Filter results by averaging quantities of interests.
5. Analyze filtered data using regression to constitute closure model(s) based on predictors.

3. Problem Description

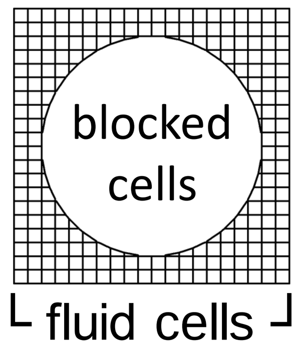
System is a bubbling fluidized bed with immersed heat transfer cylinders (45° staggered configuration) and solids with an exothermic reaction heat source $\dot{\Pi}_s$.



Model Parameters include solids-fraction ϕ_s; solids-velocities u_s, v_s; cylinder diameter D_{cyl} and spacing a_{cyl}, while the quantity of interest is the cylinder-suspension heat transfer coefficient h_{cgs}.

4. Numerical Methods

Simulations were run using the open-source finite-volume CFD code Multiphase Flow with Interphase eXchanges (MFIX)[4] using the Eulerian-Eulerian two-fluid model, where both phases are treated as interpenetrating continua. Modeling the curvature of the cylinders is accomplished through the cut-cell method[5] where the cells are truncated to conform closely to the geometry.



5. Filtering Model

The cylinder-suspension heat transfer rate Q_{cgs} is calculated by summing the energy conservation equations for the gas and solids phases and integrating over the domain volume:

$$\partial_t(\phi_g \rho_g C_{p,g} T_g) + \nabla \cdot (\phi_g \rho_g C_{p,g} \mathbf{v}_g T_g) = \nabla \cdot (\phi_g k_g \nabla T_g) + H_{gs}$$

$$+\ \partial_t(\phi_s \rho_s C_{p,s} T_s) + \nabla \cdot (\phi_s \rho_s C_{p,s} \mathbf{v}_s T_s) = \nabla \cdot (\phi_s k_s \nabla T_s) - H_{gs} + \dot{\Pi}_s$$

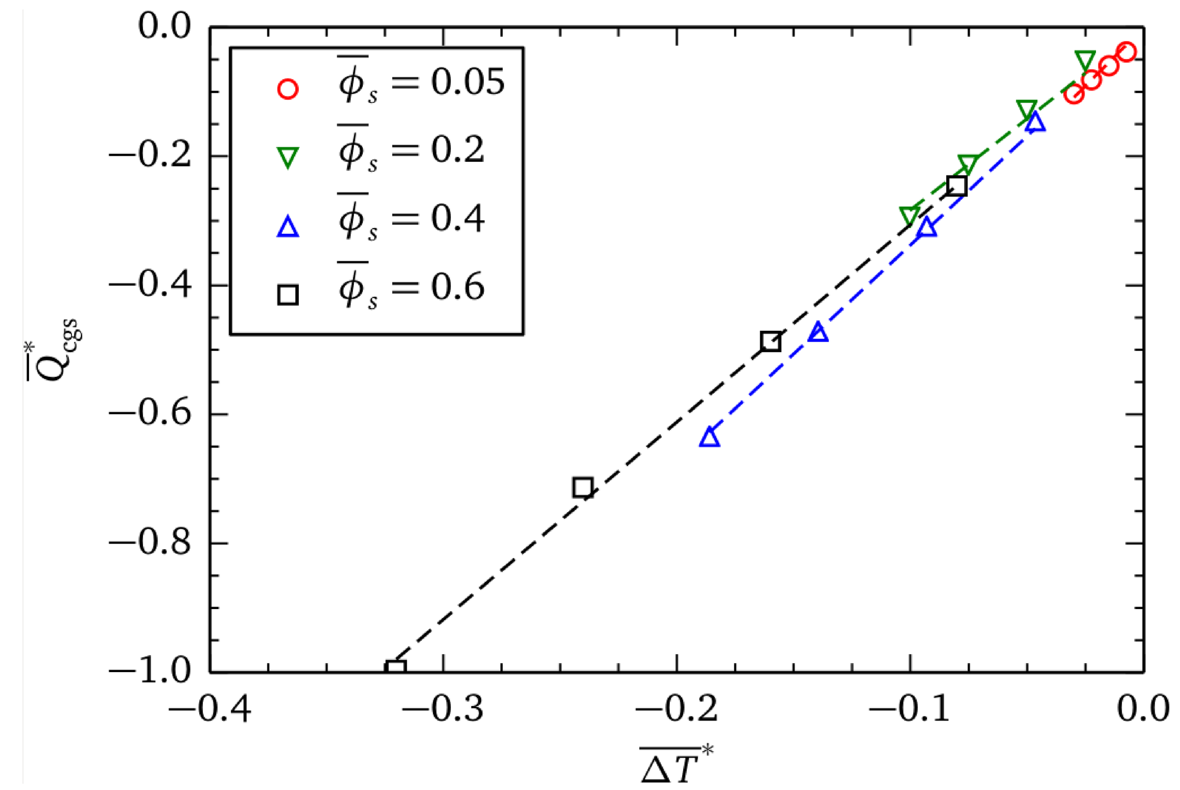
$$\bar{Q}_{cgs} = \frac{1}{V} \int_V \left[\partial_t(\phi_g \rho_g C_{p,g} T_g + \phi_s \rho_s C_{p,s} T_s) - \dot{\Pi}_s\right] dV$$

Based on heat transfer theory, we propose a model that is linearly dependent on the temperature difference between the suspension and cylinders, $\Delta\tilde{T}$:

$$\bar{Q}_{cgs} = \bar{h}_{cgs} \Delta\tilde{T}.$$

6. Results

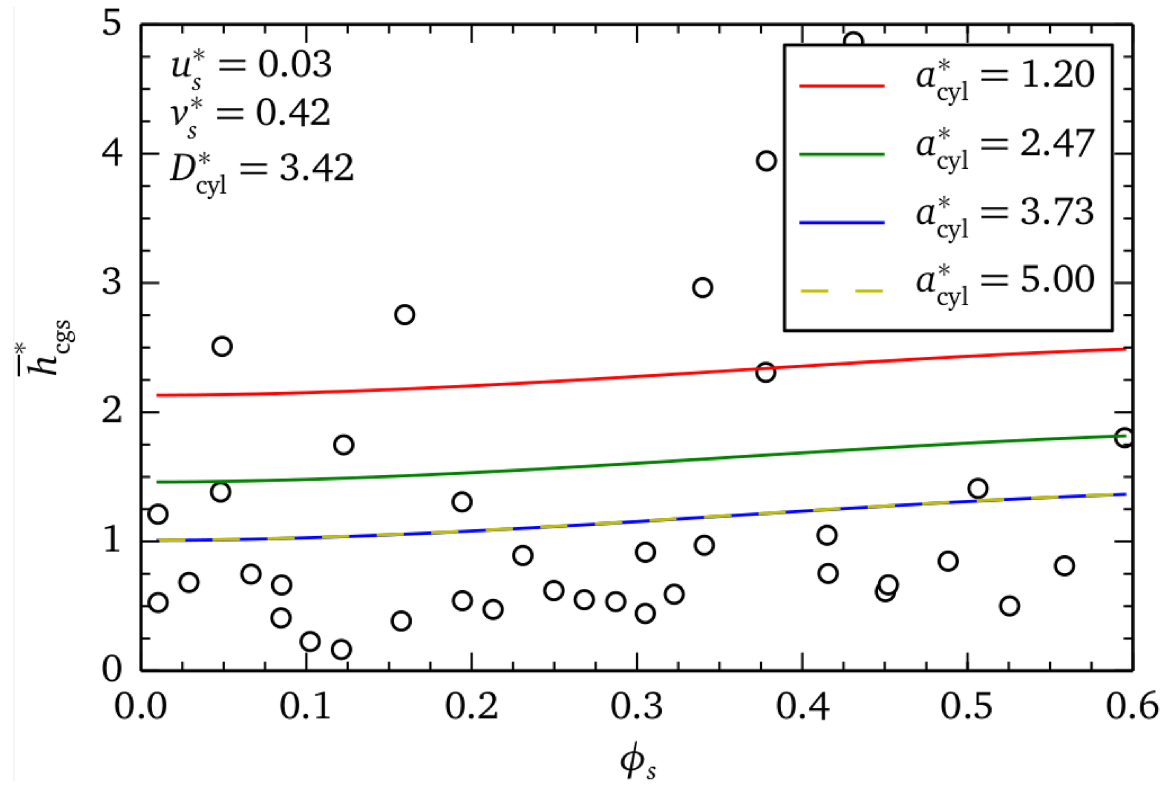
An initial campaign of 16 simulations (factorial design) was used to confirm the proposed linear model.

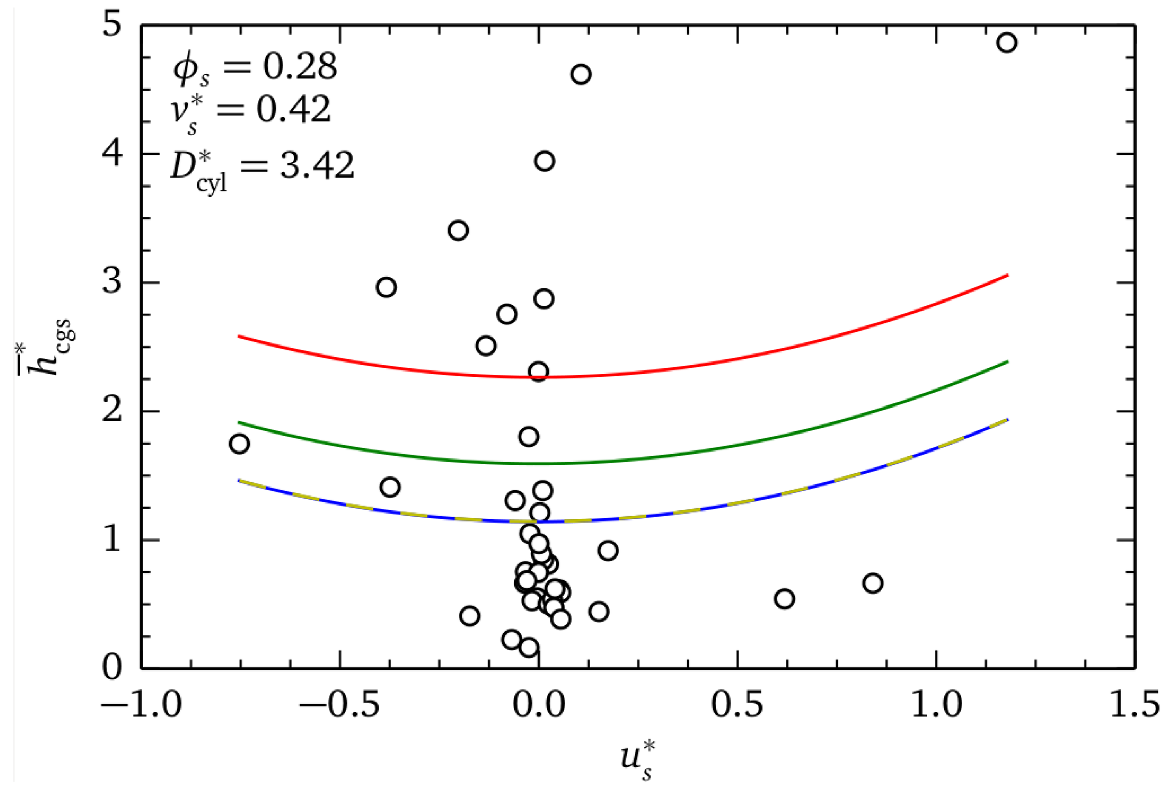


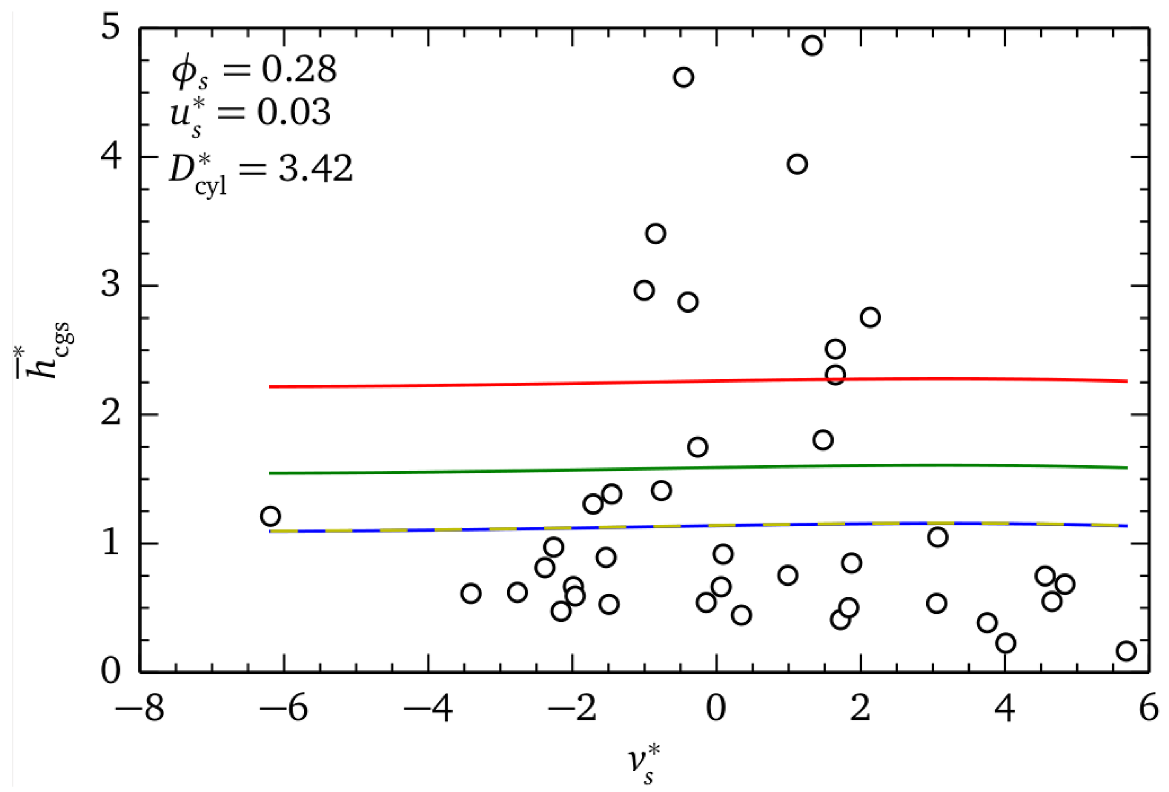
A secondary campaign of 50 simulations (Latin hypercube design) was used to constitute a closure for the effective cylinder-suspension heat transfer coefficient using Gaussian processes and multivariable fractional polynomial regression[6].

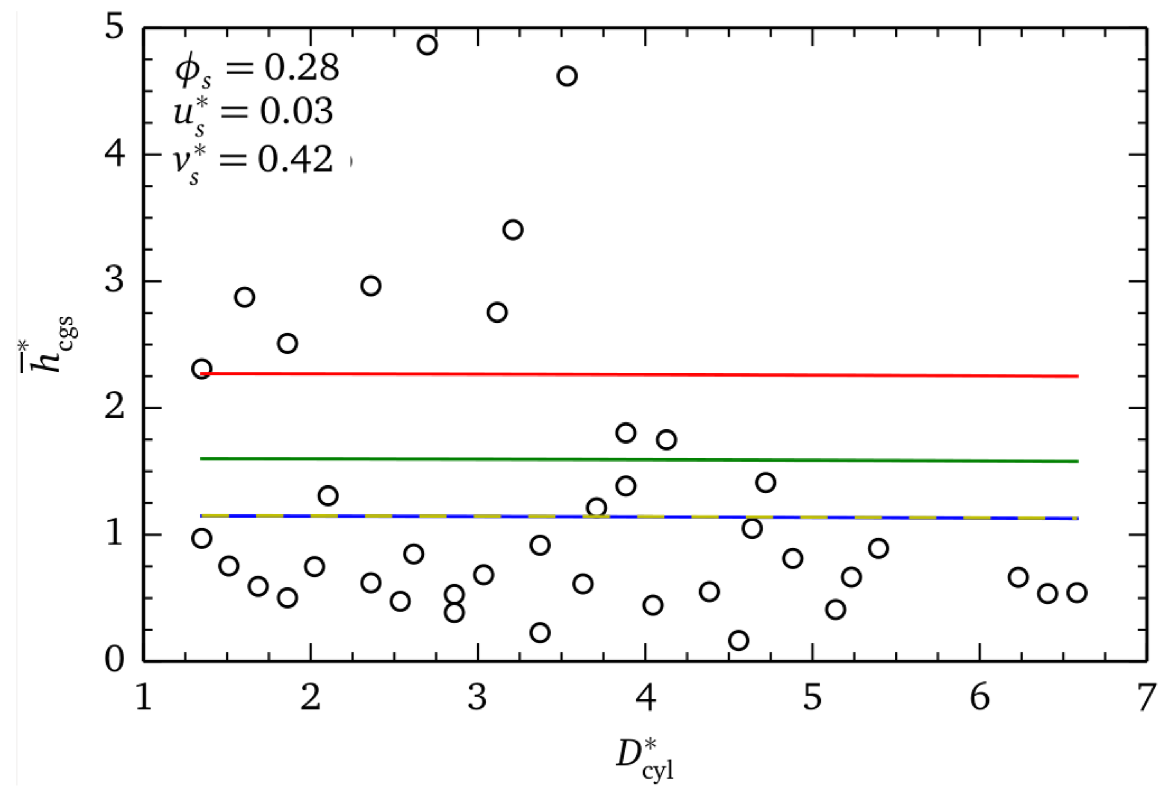
$$\bar{h}_{cgs} = f(\phi_s, u_s, v_s, D_{cyl}, a_{cyl})$$

The plots below show the simulations results (discrete points) and proposed model (solid lines). Asterisks denote dimensionless quantities[6].









7. Conclusions and Future Work

Through sub-grid filtering, we constituted a closure model to approximate the cylinder-suspension heat transfer in coarse-grid simulations of gas-solids flows based on solids-fraction, solids velocities, and cylinder geometry. This work is ongoing and is currently being extended by:

- running a larger, tertiary campaign (factorial design, 625 simulations),
- reformulating the closure models more generally as functions of Reynolds and Prandtl numbers,
- and verifying, validating, and quantifying the uncertainties of the model.

References

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