Application of Coarse Grained Drag Law in Computational Fluid Dynamics Simulations of Fluidized Beds

Alvin Chen, Timothy Healy, Nicholas Jones

April 22 – 23, 2009

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Motivation

• Multiphase (gas-liquid-solids) systems integral to many refining processes
  • Fluid catalytic cracking – transfer lines, feed zone, termination, riser, regenerator
  • FLUID COKING™ / FLEXICOKING™ – transfer lines, reactor, heater
  • Distillation – pipestill feed zones, chimney trays

• **Goal:** Improve understanding of multiphase physics to enable step improvements in process technologies

• The traditional approach to scale-up has been to extrapolate from scaled down cold-flow models (typically 1/10th to 1/20th scale) to commercial scale, hot units.

• Validated CFD models can increase confidence in scale-up of commercial fluid bed systems by providing a physical basis to bridge scale gap.

• Simulation of multi-phase systems requires augmentation of current CFD methods
  • Techniques to adequately capture physics while keeping simulation size tractable
  • Appropriate model validation with experimental or commercial operating data
Fluidized solids process example: FLUID COKING process

- **FLUID COKING** is a process for upgrading resid to lighter liquid products
  - Utilizes several process vessels: 1) scrubber 2) reactor 3) burner

- Liquid feed is injected into a fluidized bed of coke particles

- Liquid feed coats particles and then begins to thermally crack forming lighter products which in turn vaporize to fluidize coke particles
  - Proper fluidization allows for the reactor to operate isothermally

- Pressure balance required to circulate coke particles between vessels

- Heat balance required to supply energy for endothermic reactions
  - Heat for cracking process supplied by hot coke circulated from the burner vessel
Modeling efforts enable technology step change in gas-solids applications

- Develop CFD models to account for the hydrodynamics of gas-solids fluidized beds for simulation of commercial scale
  - Liquid and gas injection models
  - Chemical kinetics
  - Coarse-grained gas-solids drag representation

- Validate gas-solids drag model with cold-flow data
  - Scaled down fluid coker test unit from Song et al.
    - Air and FCC particle system
    - Axial pressure drop data
    - Axial and radial voidage profiles
    - Axial and radial solids velocity profiles
  - Use of jet penetration models to account for air injection from nozzles
  - Set CFD outlet boundary pressure to adjust fluidized bed height

Fig. 1. Schematic of UBC pressurized fully cylindrical cold model of Syncrude Cokers.

Taken from Song et al., Powder Tech, 147 (2004) 126-136
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Gas-solids drag model using coarse-graining methodology

- Need to understand gas-solids dynamics at different length scales
  - Micro-scale for particle collisions
  - Meso-scale for clustering behavior of particles
  - Macro-scale for gross bed hydrodynamics
- Desire to study macro-scale interactions and avoid the need to resolve interactions at smaller scales
  - Grid resolution as small as 10 particle diameters required to fully resolve meso-scale dynamics
- Coarse-graining approach provides a technique for modeling the gas-solids interactions at the subgrid scale
  - Meso-scale dynamics are modeled using scaling relationships
  - Effective drag is varied with solids volume fraction and grid resolution
- Coarse-graining allows simulation of commercial scale fluidized beds with large computational cell sizes
Components of CFD model for scaled down cold-flow unit

- **Computational domain**
  - Stripper internals
  - Solids inlet and outlet transfer lines
  - Cyclone inlets and diplegs returning solids

- **Two-fluid model for a single mean particle size**
  - FCC particles $d_p = 99$ microns, $\rho_p = 1700$ kg/m$^3$

- **Vapor jets from scaled down feed nozzles and attritors**
  - ~100 vapor jets in service
  - Jets not fully resolved due to disparity in length scales
  - Jets accounted for as local momentum and mass sources
  - Jet penetration guided by Merry’s correlation
    \[ \frac{L}{d_0} = 4.5 \left( \frac{\rho_v u_0^2}{(1 - \varepsilon) \rho_p g d_p} \right)^{0.4} \left( \frac{\rho_g}{\rho_p} \right)^{0.2} \left( \frac{d_p}{d_0} \right)^{0.2} \]

- **Additional vapor sources used to represent stripper steam spargers and fluidization steam near the solids outlet**
CFD provides insight into internal dynamics

- Rich dynamic behavior apparent when studying instantaneous snap shots
- Time averages generated from instantaneous profiles mimic experimental measurements
- Well known core-annular flow structure captured by time averaged CFD result
- CFD predictions in quantitative agreement with experimental measurements

Fig. 3. Axial time-mean pressure gradient profiles in reactor section. Base conditions, \( U_L = 0.74 \text{ m/s}, U_g = 0.25 \text{ m/s}, G_e = 18.6 \text{ kg/m}^2 \text{ s}\).

Taken from Song et al., *Powder Tech*, 147 (2004) 126-136

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CFD predicted solids profiles match experiments

- Voidage profiles match very well with experimental measurements below $Z^* = 0.6$
- Discrepancy near top of bed ($Z^* > 0.6$) consistent with difference in bed level

Fig. 6. Voidage distribution in reactor section. Base conditions, $U_i = 0.74$ m/s, $U_r = 0.25$ m/s, $G_w = 18.6$ kg/m$^2$.s. Feed jet penetration calculated from Eq. (2).

Taken from Song et al., Powder Tech, 147 (2004) 126-136
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Location of core/annular boundary predicted by CFD

- Agreement between CFD predictions of average velocity profiles and experiment is excellent below $Z^* = 0.6$
- Discrepancy near top of bed ($Z^* > 0.6$) consistent with difference in bed level

Fig. 9. Overall distribution of time-average vertical velocity component in reactor section. Base conditions, $U_f=0.74$ m/s, $U_s=0.25$ m/s, $G_{sf}=18.6$ kg/m²s. Feed jet penetration calculated from Eq. (2).

Taken from Song et al., *Powder Tech*, 147 (2004) 126-136
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Conclusions

• Coarse-graining methodology is able to adequately represent sub-grid dynamics and effective gas-solids drag occurring on the subgrid scale
  • Technique enables the use of relatively coarse mesh to relieve computational resource demands for commercial scale simulations

• Good agreement between CFD predictions and experimental data
  • Local voidage and solids vertical velocity match well throughout dense bed
  • Able to predict the time-averaged zero solids vertical velocity surface
  • Good agreement with bed pressure drop and axial bed density profiles

• Separation of coupled physics (e.g. gas-solids drag from reaction and liquid injection) is a useful approach to model validation

• CFD models have been successfully applied to numerous applications within ExxonMobil including FCC, FLUID COKING / FLEXICOKING, Gas-to-Liquids, and Distillation