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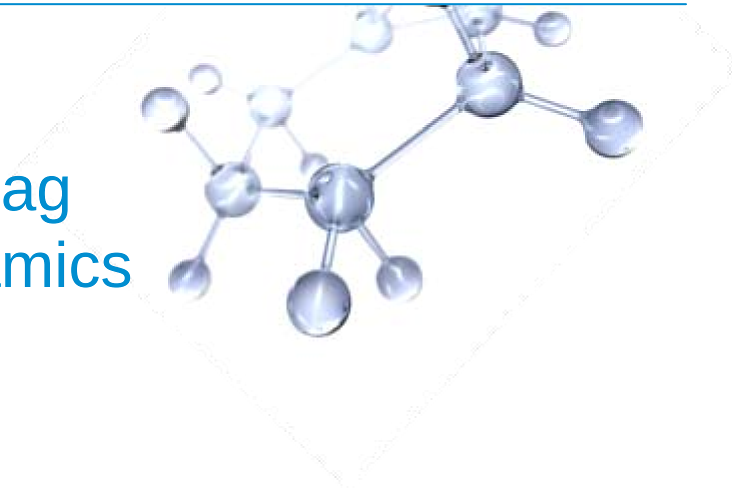

Application of Coarse Grained Drag Law in Computational Fluid Dynamics Simulations of Fluidized Beds

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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.

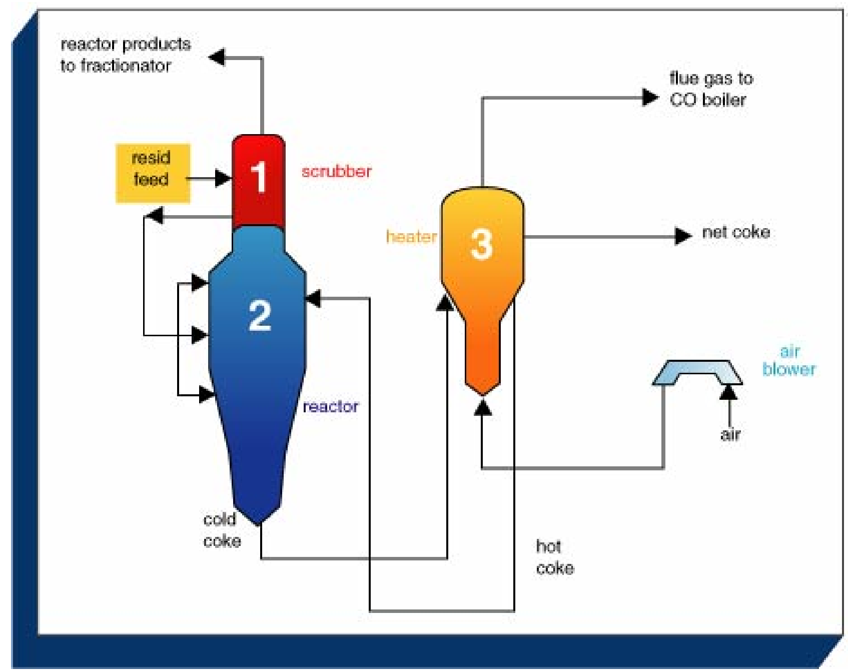
- Validated CFD models can increase confidence in scale-up of commercial fluid bed systems by providing a physical basis to bridge scale gap

- 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

ExxonMobil FLUID COKING Conversion Technology



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

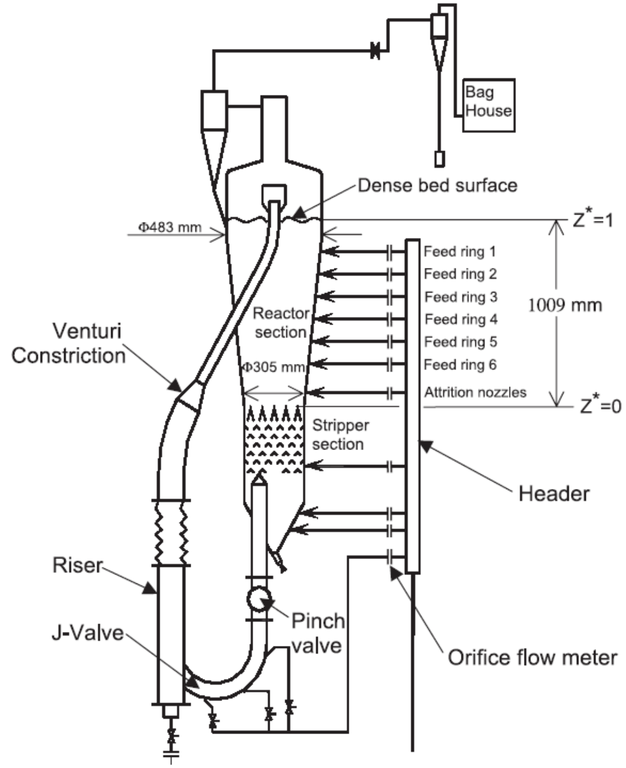


Fig. 1. Schematic of UBC pressurized fully cylindrical cold model of Syncrude Cokers.

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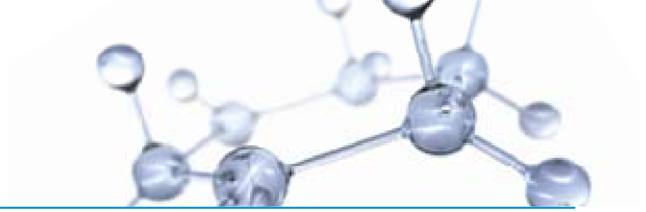
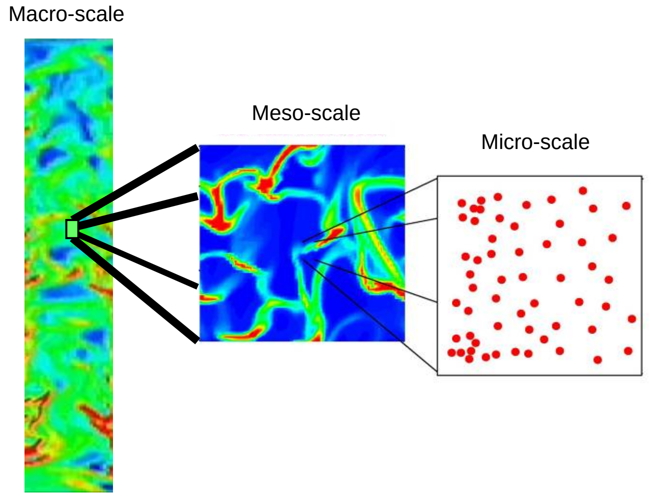
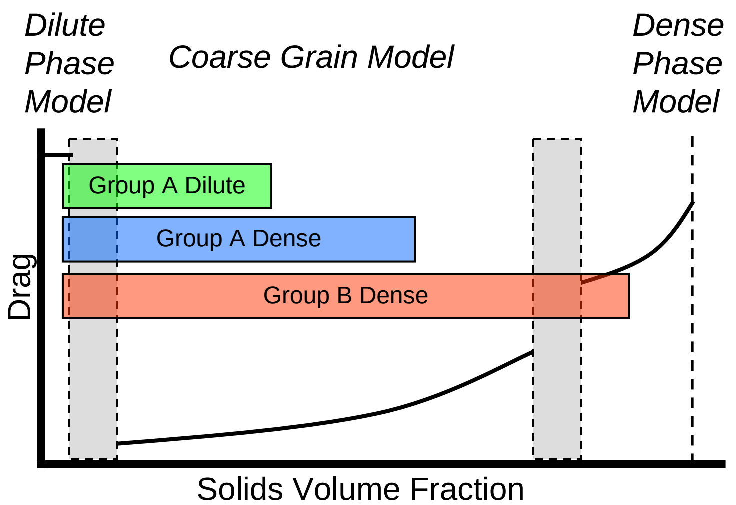
Gas-solids drag model using coarse-graining methodology



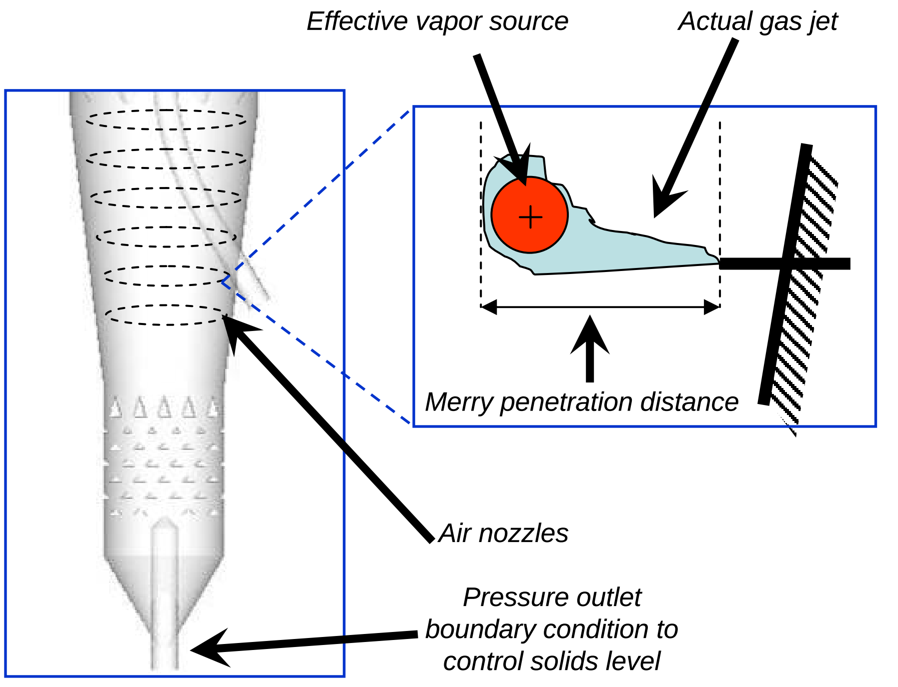
- Need to understand gas-solids dynamics at different length scales
  - Micro-scale for particle collisions
  - Meso-scale for clustering behavior of particles
  - ***Macro-scale for gross bed hydrodynamics***
- Desire to study macro-scale interactions and avoid the need to resolve interactions at smaller 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
  - Igci, et al., *AIChE Journal*, **54** (2008) 1431-1448
  - 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, ρ_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
    - $$\frac{L}{d_0} + 4.5 = 5.25\left(\frac{\rho_0 u_0^2}{(1-\varepsilon)\rho_p g d_p}\right)^{0.4}\left(\frac{\rho_g}{\rho_p}\right)^{0.2}\left(\frac{d_p}{d_0}\right)^{0.2}$$
- Additional vapor sources used to represent stripper steam spargers and fluidization steam near the solids outlet



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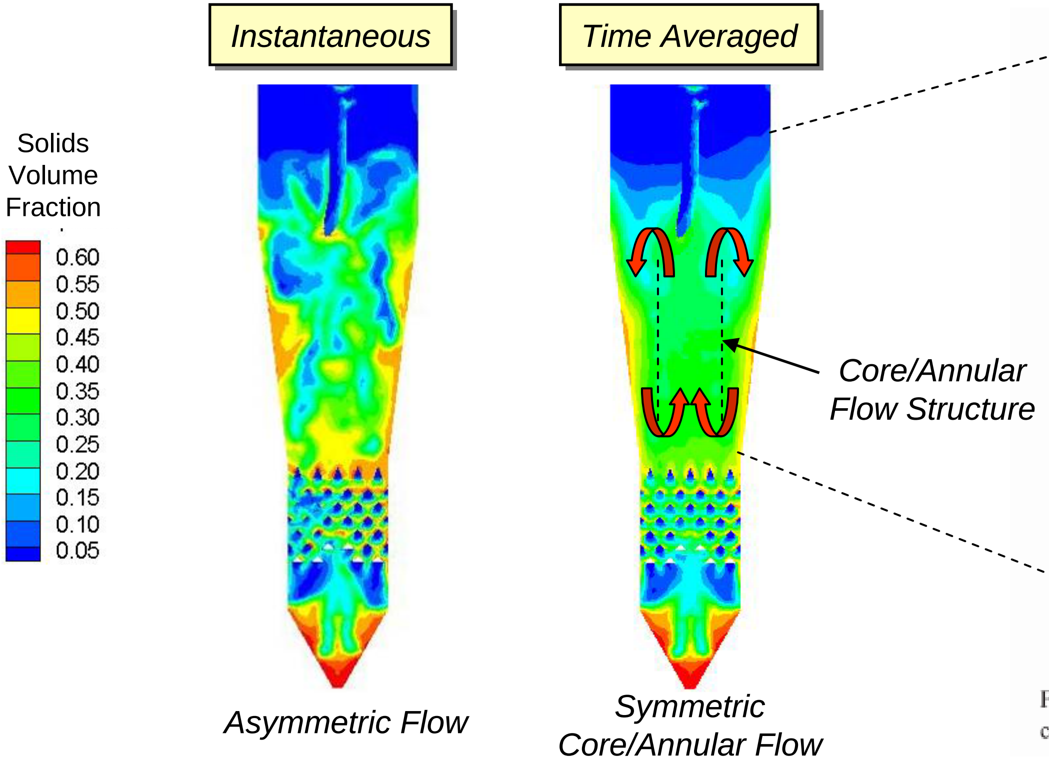
CFD provides insight into internal dynamics



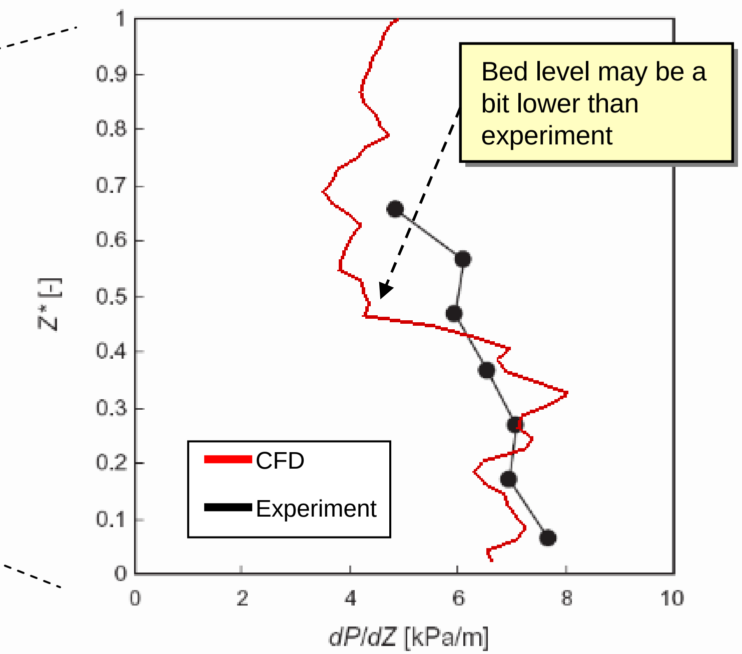


Fig. 3. Axial time-mean pressure gradient profiles in reactor section. Base conditions, U_f=0.74 m/s, U_s=0.25 m/s, G_{sf}=18.6 kg/m^2 s.

Taken from Song et al., *Powder Tech*, **147** (2004) 126-136
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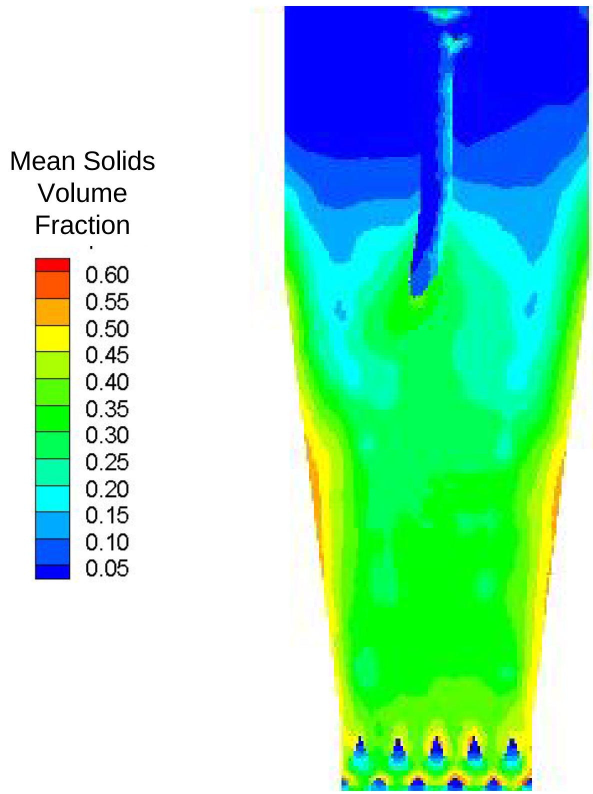
- Rich dynamic behavior apparent when studying instantaneous snap shots
- Time averages generated from instantaneous profiles mimic experimental measurements
- **Well known core-annular flow structure captured by time averaged CFD result**
- **CFD predictions in quantitative agreement with experimental measurements**

CFD predicted solids profiles match experiments



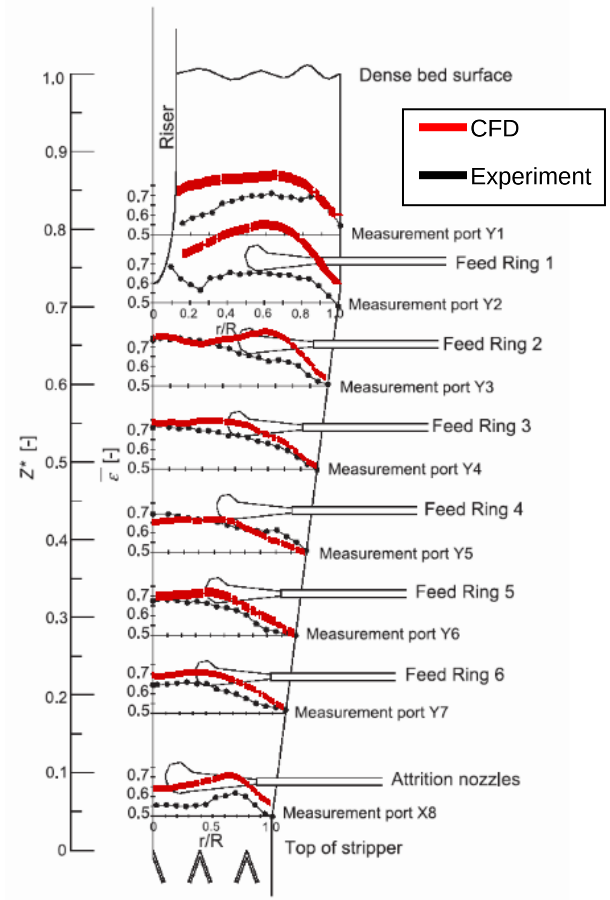


Fig. 6. Voidage distribution in reactor section. Base conditions, U_f=0.74 m/s, U_s=0.25 m/s, G_{sf}=18.6 kg/m^2 s. Feed jet penetration calculated from Eq. (2).

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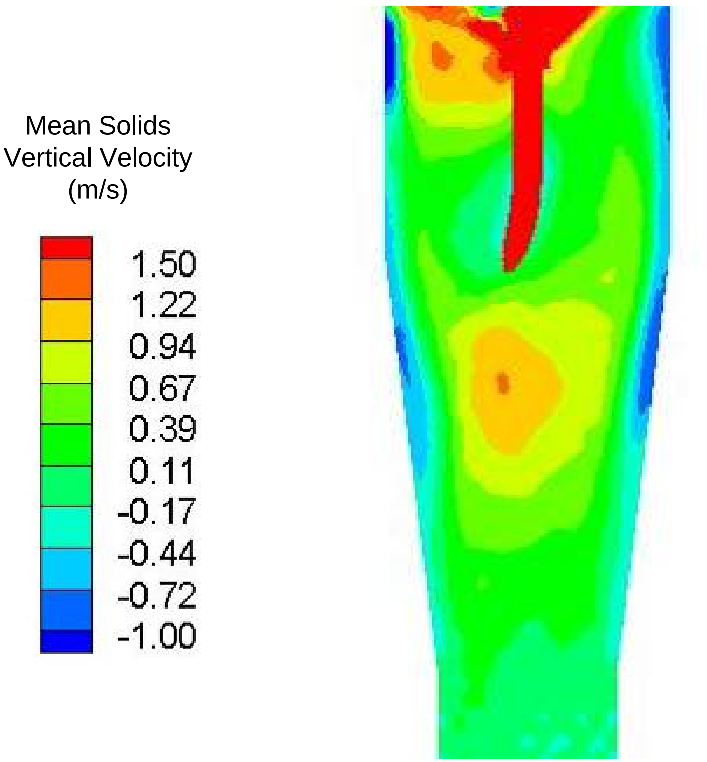
- Voidage profiles match very well with experimental measurements below Z*=0.6
- Discrepancy near top of bed (Z* > 0.6) consistent with difference in bed level

Location of core/annular boundary predicted by CFD



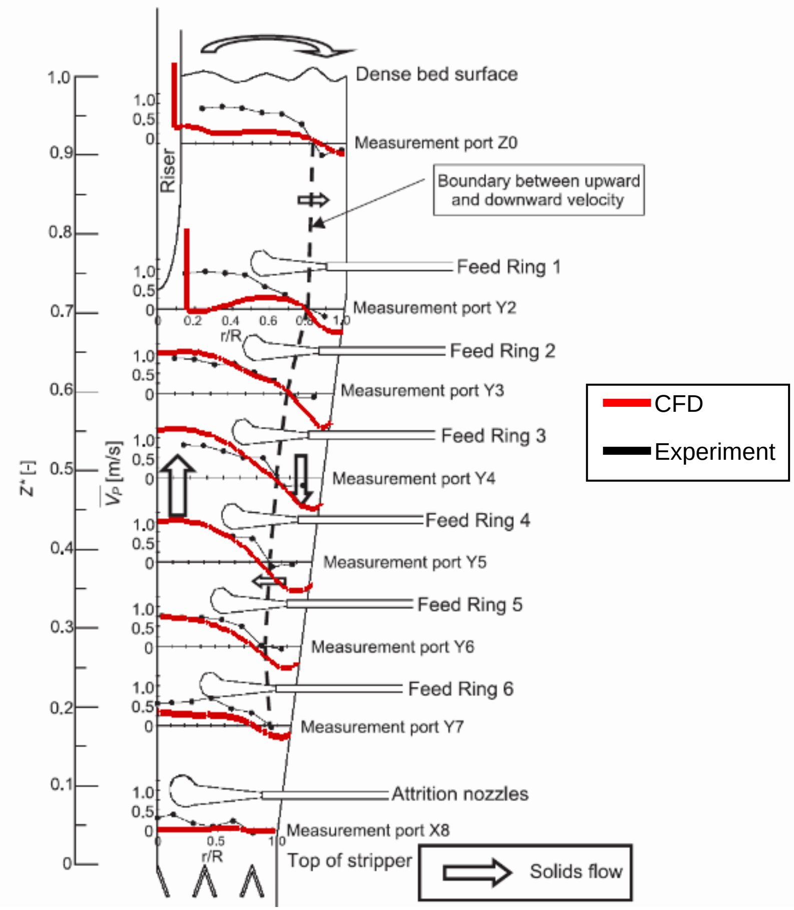


Fig. 9. Overall distribution of time-average vertical velocity component in reactor section. Base conditions, U_f=0.74 m/s, U_s=0.25 m/s, G_{sf}=18.6 kg/m^{2}s. Feed jet penetration calculated from Eq. (2).

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- 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

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