Drag force for spherical and cylindrical particles at different packed bed porosities and wide range of Reynolds number

R. Brahem¹, D. Ferré¹, J. Ouari¹, K. Hammouti ², A. Wachs³

¹ Chemical Engineering Departement - IFP Energies Nouvelles - France
² Fluid Mechanics Department - IFP Energies Nouvelles - France
³Department of Chemical Engineering - Department of Mathematics
University of British Columbia - Canada
Outline

- Industriel & scientific contexts
- Numerical methods and simulated systems
- Results & discussion
- Conclusions & perspectives
Hydrodynamics of G/S/L reactors

- G/S, L/S and L/G/S reactors: fixed, fluidised, ebullated, transported beds …
- Example: catalytic hydro-conversion of heavy oils in ebullated G/L/S bed
  - Exothermic reactions, high contaminant contents, rapid coke deposition
  - Ebullated bed: perfectly stirred reactor (good control of exothermicity) by retro-mixing of liquid and catalyst, constant pressure drop (no plugging)
  - Enhancing mass and heat transfers: use of different catalyst shapes → Impact on hydrodynamics only evaluated through experimental measurements of overall parameters

Further understanding of shape effect is needed (through both experimental and numerical studies)
Particulate flows modelling: multi-scale approaches

- **Different interactions:** fluid-particles and particles-particles interactions
- **Multiscale approaches:** characterisation at small scales and propagation of information to large scales (closure laws)

![Diagram showing different flow regimes and coupling](image)

*Li et al. 2004*

*Crowe et al. 2012*

*Van der Hoef et al. 2006*
Fluid particles interaction: drag modelling

Different approaches proposed in literature:

\[ \mathbf{F}_d = \beta (\mathbf{u}_f - \mathbf{u}_s) \]

- Fully theoretical (ex. cells models) (Zick & Homsy (1982); Happel (1958); Reed & Anderson (1980))

- Semi-theoretical:
  - “pseudo fluid” approaches: implicit consideration of the surrounding particles through an effective fluid (effective density and viscosity) (Zuber (1964); Barnea & Mizrahi (1973))
  - Analogy with pipe flow: pressure drop expressed as the sum of viscous and inertial contributions (Ergun (1952))

- Fully empirical: based on Richardson & Zaki (1954) observation

\[ \frac{U}{U_t} = \varepsilon_f^n \]
Fluid particles interaction: drag modelling

- Different approaches proposed in literature:

\[ \overrightarrow{F_d} = \beta (\overrightarrow{u_f} - \overrightarrow{u_s}) \]

- Fully theoretical (ex. cells models) (Zick & Homsy (1982); Happel (1958); Reed & Anderson (1980))
  - Limited success for high Re numbers (De Felice (1995))

- Semi-theoretical:
  - “pseudo fluid” approaches: implicit consideration of the surrounding particles through an effective fluid (effective density and viscosity) (Zuber (1964); Barnea & Mizrahi (1973))
  - Experimental results on binary systems (Grbavčić et al. (1992)): agreement only for high ratio between mean particle diameters

- Fully empirical: based on Richardson & Zaki (1954) observation
  \[ \frac{U}{U_t} = \varepsilon^n_f \]
Fluid particles interaction : drag modelling

**Pipe flow analogy**
- Tow extreme regimes: viscous (Blake-Kozny equation) and inertial regimes (Burke-Plummer equation)
- Ergun (1952): combination of viscous and inertial terms (experimental fitting for the constants)
- Improvements proposed:
  - Gibilaro (1986)
  - Hill et al. (2001)
  - Beetstra et al. (2007)

**Empirical approach**
- Most used Wen & Yu (1966): the most used
- Improvements proposed:
  - Rowe (1987)
  - Khan and Richardson (1989)

**Particle shape effect**: little studied in concentrated systems (Levec & Nemec, 2005)
Numerical methods

- Direct numerical simulations (DNS)
  - Particles’ dynamics: Grains3D, Discrete Element Method (DEM) solver
    - Newton’s equations (momentum and moment balances) and contact force (using soft sphere model)
  - Fluid flow: PeliGRIFF, Distributed Lagrange Multiplier/ Fictitious Domain (DLM/FD) solver
    - Momentum and continuity balances using fixed Cartesian mesh (the constraint on particle surfaces handled by DLM method)


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Methodology

- Single particle (2-6 processors & ~24h)
  - Cylindrical particle R=L/d =5
  - Different Re numbers and orientations toward flow direction

Objective: comparison to literature correlations and identification of reliable expression → injection in a Wen & Yu like form

\[ C_D = \frac{F_{D,x}}{\frac{1}{2} \rho_f U_f^2 S_{proj}} \]
Methodology

- **Concentrated systems**
  - 1\(^{st}\) way: fluidized bed at different Re with sufficiently long simulation time (for statistics)
    - 100 particles and bi-periodic side boundaries for 20 s:
      - ~200 millions cells for on 256 processors
    - ~4months !!!
  - 2\(^{nd}\) way: fixed bed at different solid volume fractions and different Re numbers
    - Fixed tri-periodic systems with limited number of particles:
      - ~11 millions cells on 32 to 64 processors (between 24h and 72h)
    - Small systems and important effect of the bed microstructure
      - Microstructure effect: 3 simulations for each operational condition
Numerical model: fixed bed simulations

- **Generation of tri-periodic and random particle packing**
  - *Grains 3D*: mixing through elastic shocks between particles

- **Fixed bed**:
  - Mean orientation toward flow main direction
  - Histogram of orientations toward the 3 axes

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Numerical model: fixed bed simulations

- Fluid flow simulation: imposing pressure drop
  - 3 different $\varepsilon_s$ (0.3, 0.4 & 0.5) and $4Re$ numbers

- From pressure drop $\Delta P$ to drag force $F_D$ (no wall friction)

$$F_D = -V_p \frac{\varepsilon_f}{(1-\varepsilon_f)} \nabla P$$

- Evidencing shape effect: same simulations carried out with volume equivalent spheres
Single particle results

- Drag coefficient for different $Re$ numbers and orientations

$$C_D = \frac{F_{D,x}}{\frac{1}{2} \rho_f U_f^2 S_{proj}}$$
Single particle results

Drag coefficient for different $Re$ numbers and orientations

$$C_D = \frac{F_{D,x}}{\frac{1}{2} \rho_f U^2 S_{proj}}$$

$S_{eq\_sph}^{\text{projected}}$

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Single particle results

- Comparison to literature correlations

  - Levenspiel & Haider (1989) : using Waddell sphericity
    \[
    C_D = \frac{24}{\text{Re}} \left(1 + A\text{Re}^B\right) + \frac{C}{1 + \frac{D}{\text{Re}}} \]
    \[
    \phi = \frac{S_{\text{sph - eq}}}{S_p}
    \]
    - No orientation indication

  - Tran-Cong et al. (2004) : circularity and different characteristic diameters ratio
    \[
    C_D = \frac{24}{\left(\frac{d_A}{d_n}\text{Re}\right)} \left(1 + \frac{0.15}{c} \left(\frac{d_A}{d_n}\text{Re}\right)^{0.687}\right) + \frac{0.42}{1 + 4.25 \times 10^4 \left(\frac{d_A}{d_n}\text{Re}\right)^{-1.16}}
    \]
    \[
    c = \frac{\pi d_A}{P_p} \quad \frac{d_A}{d_n} = \frac{4 \times A_p}{\pi} \quad \frac{d_n}{V_p} = \frac{3}{\pi}
    \]

    \[
    C_D = \frac{8}{\text{Re} \sqrt{\phi}} + \frac{16}{\text{Re} \sqrt{\phi}} + \frac{3}{\sqrt{\text{Re} \phi}^{3/4}} + 0.42 \times 10^{0.4(-\ln \phi)^{0.2} \frac{1}{\phi_{\perp}}}
    \]
None of the tested correlations is able to predict the orientation effect.

How to take such parameter into account in a concentrated system?
Fixed bed results

- **Drag coefficient results**
  - High dispersion of the results (bed structure dependant)
  - Noticeable difference between the two tested shapes

\[
C_D = \frac{F_D}{\frac{1}{2} \rho_f U_{slip}^2 S_{\text{projected}}^{\text{eq}-\text{sph}}}
\]

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Fixed bed results : Ergun form

- Sum of viscous and inertial contributions
  \[
  \beta = A \frac{\varepsilon_s \mu_f}{\varepsilon_f d_p^2} + B \frac{\varepsilon_s \rho_f |u_f - u_s|}{d_p}
  \]

- Less accurate results of A (very few simulations in viscous regime)
- Variation with solid concentration
- Comparable results with the proposed correlations of Hill et al. (2001) and Beetstra et al. (2007)
Fixed bed results : Wen & Yu form

- Decoupled effects of particle geometry and concentration

\[ \beta = \frac{3}{4} C_{D0} \left( \frac{\varepsilon f \varepsilon_s \rho_f |u_f - u_s|}{d_p} \right) F(\varepsilon_f) \]

- Concentration function using either Schiller & Neumann or Hölzer & Sommerfeld

- Convenient agreement of spheres results to Wen & Yu description

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Comparison to other correlations
Conclusions

- DNS simulations carried out on both single and packed bed systems
- Particle shape impact evidenced on the drag force
- High dispersion in drag results due to microstructure of the bed and lack of comprehensive overall parameter to correlate such structure dependency
- Convenient predictive correlations available for spheres but not for other shapes
Perspectives

- Testing other shapes (cylinders R2.5, trilobes …)
- Impacts of others forces (lift, torque)
- Implementing the following scale (Euler Lagrange: PeliGRIFF DEM/CFD)
- Validation through experimental measurements
- Adapting the results to implementation in multi-Eulerian models

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