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Pharmaceutical Multiphase Reactors
CHE.782

Design of Multiphase Flow Processes
669.266

3
Theory-General Background on Closure Models and Spatial Filtering

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A part of this teaching material has been prepared for NanoSim (http://sintef.no/NanoSim/

Theory CPPPO – Coarse-graining

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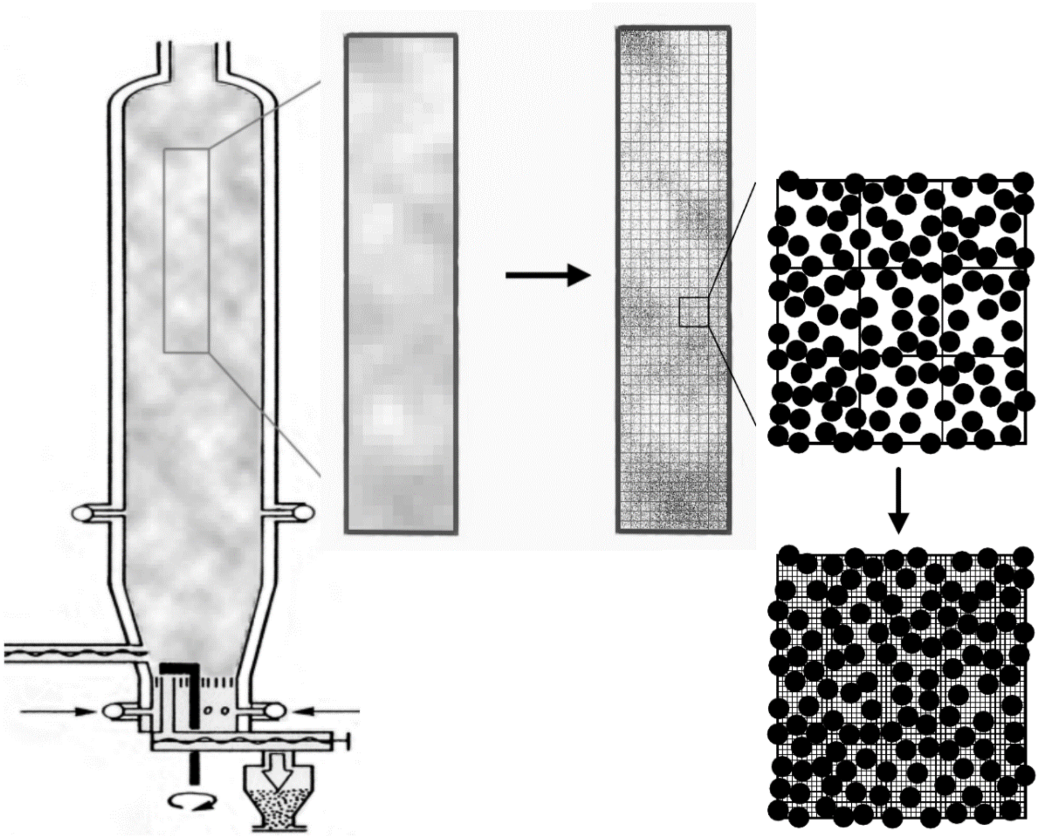


To solve the transport equations on (affordable) coarse grids we need to take into account transport phenomena occurring at sub-grid scales by mean of closure models («**material relations**»[1])

Closure models can be derived by **filtering «resolved» simulations**

Van Der Hoef et al. 2006, Multiscale modeling of Gas-Fluidized beds, Advances in chemical engineering.

[1]https://ec.europa.eu/research/industrial_technologies/pdf/review_of_materials_modelling_iv.pdf

Favre average

- Used when filtering multiphase transport equations (A.Favre,1992)
- Favre variables are mass-weighted variables. A Favre averaged variable is defined as:

$$\widetilde{\psi} = \frac{\overline{\rho\psi}}{\overline{\rho}}$$

In the case of an incompressible multiphase flow:

$$\widetilde{\psi}_p(\mathbf{x}, t) = \frac{\int K(\mathbf{x} - \mathbf{z}, t - t')\phi_p(\mathbf{z}, t')\psi_p(\mathbf{z}, t')d\mathbf{z}dt'}{\int K(\mathbf{x} - \mathbf{z}, t - t')\phi_p(\mathbf{z}, t')d\mathbf{z}dt'}$$

Where the subscript *p* indicates a phase variable and ϕ_p is the phase volume fraction.

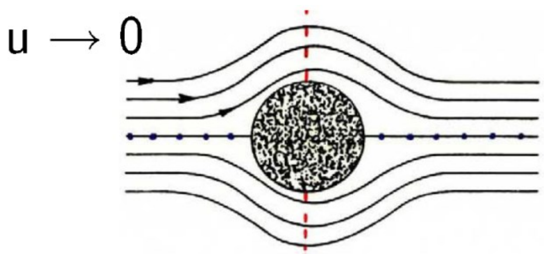
Favre Variance

$$Var(u_i) = \widetilde{u_i u_j} - \widetilde{u_i}\widetilde{u_j}$$

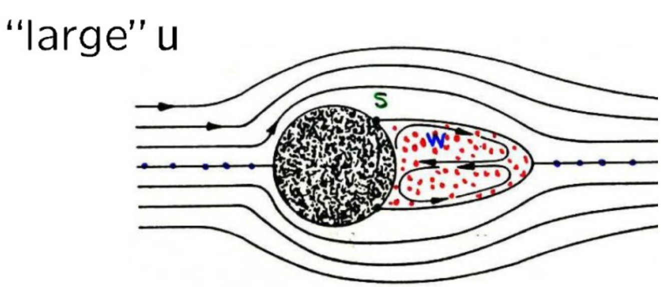
- It equivalent to the **sub-grid** stress tensors and fluxes
- Provides a quantitative measurement for the **dispersion** of the filtered quantity
- Further information can be found in *etc/doc/pdf/Finch_2009_IncrementalCalculationWeightedMeanVariance.pdf* for a complete description of the statistical tools used in CPPPO including running statistics

Approach

1. Typical flow regime laminar. So, take as reference force **Stokes drag force.**



$$F_d = 3\pi\, d_p\, u, \qquad u \;\to 0$$



$$F_d \approx 0.44\, A \frac{1}{2} \pi d_p^2, \qquad u \uparrow\uparrow$$

$$\frac{1}{4} \pi\, d_p^2$$

Approach

2. This yields already the most important **velocity, time, and length scales** that characterize the system behavior

$$u_t = \frac{d_p^{\;2} \rho_p g}{18\, \eta_f}$$

$$\tau_{relax} = \frac{d_p^{\;2} \rho_p}{18\, \eta_f}$$

$$L_{ref} = \frac{u_t^{\;2}}{g}$$

- **All based on Stokes drag force (typically okey for particles with d_p < 50 µm)**
- **Often the Schiller-Naumann drag law is used to better estimate u_t**

$$C_D = C_{D,Stk} f\left(Re_p\right) = \frac{24}{Re_p}\left(1 + 0.15\, Re_p^{\;0.687}\right)$$

$$Re_p = \frac{u\, d_p\, \rho_f}{\eta_f}$$

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Approach

3. Define drag correction factor, and choose u to be the **superficial velocity**

$$F_d = F(\phi)3\pi\mu d_p u, \qquad u \to 0$$

Dimensionless drag force $\longrightarrow$ $F(\phi) = \dfrac{F_d}{3\pi\mu \mathrm{d}_p u}$

4. However, obviously the **true (mean) velocity of the fluid <u>** will be of relevance (analogy to flow through a network of pipes)

$$\langle u \rangle = \frac{u}{1-\phi}$$

5. For the Reynolds number, however, we use the **superficial velocity**

$$Re_p = \frac{|\langle u_{rel} \rangle|(1-\phi) d_p \rho_f}{\eta_f}$$

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Approach

6. Come up with theory of simulation data to fit F(ϕ) at zero Reynolds number

Kim & Russel, 1985

Accurate up to $\phi = 0.1$

$$F(\phi) = (1-\phi)\left[1 + \frac{3}{\sqrt{2}}\phi^{\frac{1}{2}} + \frac{135}{64} ln\phi + 16.456\phi + \ \dots\right]$$

Brinkman, 1947

Diverges for $\phi = 0.667$

$$F(\phi) = (1-\phi)\left[1 + \frac{3}{4}\phi \left(1 - \frac{\sqrt{8}}{\phi} - 3\right)\right]^{-1}$$

Carman-Kozeny, 1937

Does not approach 1 for $\phi \to 0$

$$F(\phi) = 10\frac{\phi}{(1-\phi)^2}$$

Van der Hoef, Beetstra & Kuipers, 2005

$$F(\phi) = \frac{10\phi}{(1-\phi)^2} + (1-\phi)^2\left[1 + \frac{3}{2}\sqrt{1-\phi}\right]$$

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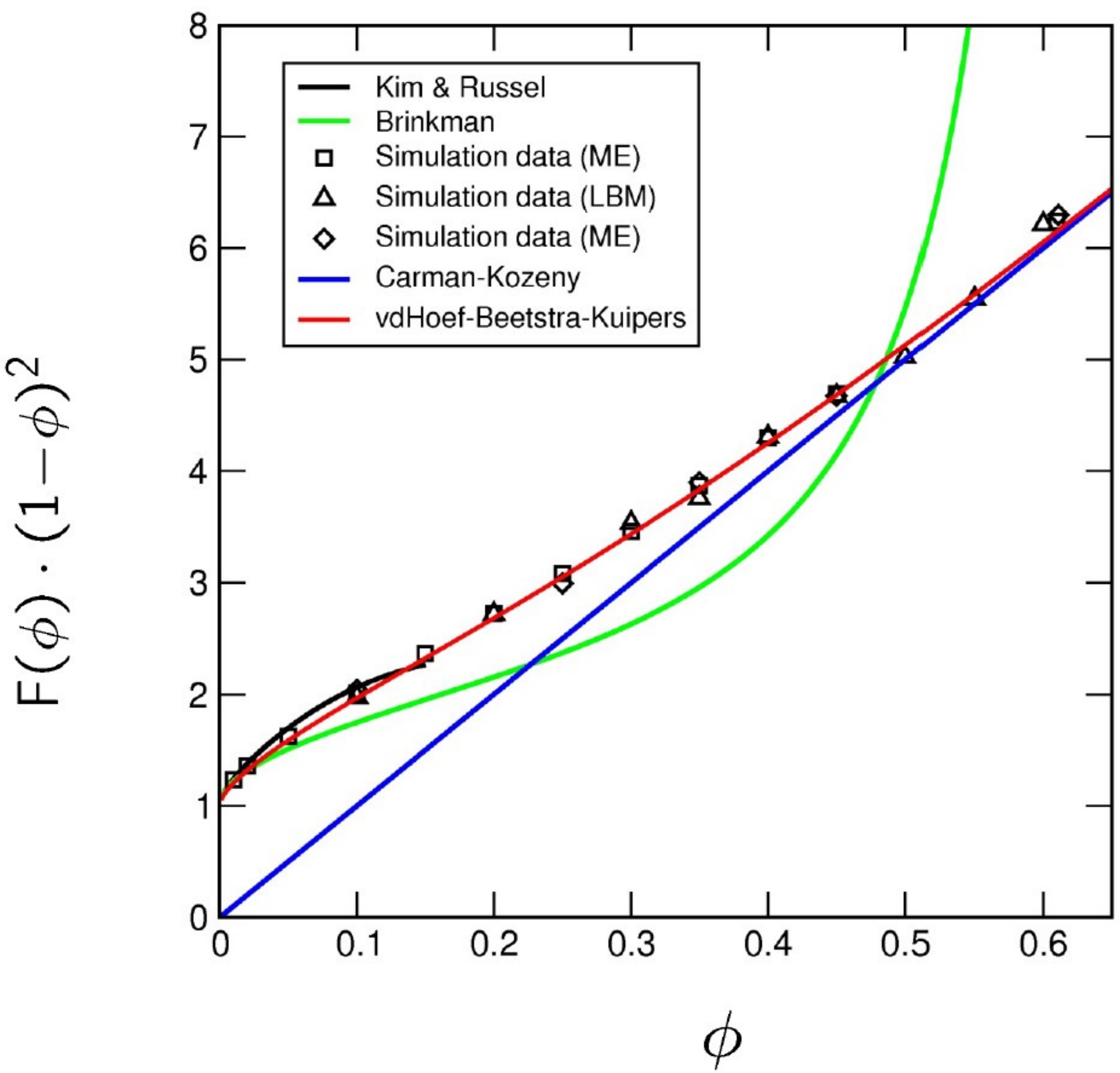
Approach



Approach

7. Now, expand to higher Reynolds numbers. A drag model based on experimental data is that of **Ergun**

We model the pressure drop based on a laminar and turbulent contribution

$$-\Delta p = A \frac{\phi^2}{(1-\phi)^3} \frac{\mu u}{d^2} + B \frac{\phi}{(1-\phi)^3} \frac{\rho u^2}{d}$$

Calibrated with experimental data gives: A = 150, B = 1.75

This is known as the **"Ergun Equation"**

We now use the ansatz: $-\Delta p = \frac{\phi}{1-\phi} \frac{18 \mu u}{d^2} F$

…to arrive at the dimensionless form of the Ergun equation: $$\boxed{F(\phi, Re) = 8.33 \frac{\phi}{(1-\phi)^2} + \frac{0.097}{(1-\phi)^2} Re}$$

8. Unfortunately, this relationship does not hold for dilute systems (check the limiting *F*!)

Approach

9. Next attempt: Postulate a law of the form (motivated by Richardson-Zaki experimental data)

$$F(\phi, Re) = F(0, Re)(1-\phi)^{-\beta}$$

Wen & Yu (1966) $\beta = 3.7$

Di Felice (1994) $\beta = 3.7 - 0.65\exp\left[\frac{(1.5-\log(Re))^2}{2}\right]$

10. Recent simulations show, that such a structure is **not accurate enough**. An improved and widely accepted model is:

$$F = \left[F_0(\phi) + G_{0,i}(\phi, Re_{p,i})\right]$$

$$F_0(\phi_p) = \frac{10\,\phi}{(1-\phi)^2} + (1-\phi)^2\left(1+1.5\sqrt{\phi}\right)$$

$$G_{0,i}(\phi, Re_{p,i}) = \frac{0.413 Re_{p,i}}{24\,(1-\phi)^2}\left[\frac{(1-\phi)^{-1} + 3\phi\,(1-\phi) + 8.4 Re_{p,i}^{-0.343}}{1 + 10^{3\phi}\,Re_{p,i}^{-(1+4\phi)/2}}\right]$$

Beetstra et al., 2007

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Summary

1. The drag force on a single particle in a dense flow is modelled with

$$\mathbf{f}_{D,i} = V_{p,i}\ \beta_{p,i}\ \left(\left\langle \mathbf{u}_{f,i} \right\rangle - \mathbf{u}_{p,i}\right)$$

$$\beta_{p,i} = \frac{18\,\eta_f}{d_{p,i}^2}\ (1-\phi)\ F$$

This is the **filtered** (NOT superficial) fluid velocity

2. This is the drag force only. The **pressure gradient force** must be added in addition. In absence of other forces (e.g., gravity), the pressure gradient is

$$\sum_i \mathbf{f}_{D,i} = (1-\phi)\nabla P$$

Outlook

3. We have discussed static particle beds. If individual particles have relative motion, so called "**fluid-mediated particle-particle**" drag forces need to be considered under certain circumstances.

$$\mathbf{f}_{D,i} = -\beta_i \Delta\mathbf{U}_i - \sum_{i \neq j} \beta_{ij} \left(\Delta\mathbf{U}_j - \Delta\mathbf{U}_i \right)$$

4. All we have discussed above is valid for mono-disperse suspensions. **For polydisperse systems, the expressions become significantly more complex**. A good model is that of Beetstra et al. (2007) and **Holloway et al. (2010)**. Essentially, those authors use a dimensionless particle size y_i (the reference being the Sauter diameter) to compute the dimensionless drag force:

$$F^*_{D,i-fixed} = \frac{1}{1-\phi} + \left(F^*_{D,mono} - \frac{1}{1-\phi} \right) \left[a\, y_i + (1-a)\, y_i^{\,2} \right]$$

$$a = 1 - 2.66\phi + 9.096\phi^2 - 11.338\phi^3$$

Impressum & Disclaimer

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