Multiphase flow dynamics
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Outline

- Classification of multi-phase flows

- Modeling approaches
  - Homogeneous flow model
  - Lagrangian particle tracking
    - General description
    - Methods for dense suspensions (DPM, MP-PIC)
  - Eulerian-Eulerian two-fluid models
  - Algebraic slip mixture model
  - Other approaches

- Example: Eulerian-Eulerian modeling of dense gas-solid flow
Multiphase flows can be classified according to

- **the combination of phases:**
  - gas-solid (fluidized beds, conveying, combustors, etc.)
  - gas-liquid (sprays, nuclear reactors)
  - liquid-solid (crystallisers, sedimentation, fiber suspensions)
  - liquid-liquid (oil-water separation)
  - gas-liquid-solid (catalytic cracking)
  - etc.

- **The volume (or mass) fraction of the dispersed phase**
  - dilute (relaxation time $t_p <$ collision time $t_c$)
  - dense

\[ t_p = \frac{\rho_p d_p^2}{18 \mu_f} \quad (\text{Re}_p < 1) \]
\[ t_p = \frac{4 \rho_p d_p}{3 \rho_f C_D u_{fp}} \quad (\text{Re}_p > 1) \]

- **The type of distribution of the dispersed phase**
  - homogeneous
  - heterogeneous (e.g. clusters, sprays, flocks)

- **The geometry of the phase interfaces**
  - separated flows
  - mixed flows
  - dispersed flows
• Multiphase flows can be treated as single phase flows when
  • the amount of the dispersed phase(s) is very small
  • the carrier phase is not affected
  • the dispersed phase(s) are of no interest

• In special cases single phase flow can be treated as multiphase flow, e.g.
  • in mixing of fluid streams of different temperature and/or concentration
  • in the description of the different scales of turbulence

• A computational phase in multiphase CFD is not same as a phase in the physical sense
  • computational phase represents a mass moving at a ‘single’ velocity

### TYPES OF PHASE INTERACTION

**One-way coupling:**
Fluid flow affects particles/dispersed phase

**Two-way coupling:**
Above + dispersed particles modify fluid flow

**Four-way coupling:**
Above + particle-particle interaction
Multiphase flow and turbulence

- multiphase flows are typically by nature 'turbulent' (phase interfaces distort the flow field which leads to fluctuations in velocities and other properties)

- dispersed phase modifies carrier phase turbulence
  - big particles enhance turbulence
  - small particles damp turbulence
  - carrier phase turbulence becomes unisotropic

- carrier phase turbulence enhances dispersion and clustering of the dispersed phase

- in dense suspensions the turbulent fluctuations in the different phases are strongly coupled and often of a different character than in single-phase flows

Approach 1: Homogeneous flow model

- Simplest multiphase CFD model

- Assumes that dispersed phase travels at the same velocity as the carrier phase

- Mixture momentum equation

- Mixture continuity equation

- Phase continuity equations: transport of dispersed phase through ‘diffusion’

- Fast; describes well particle size and other distributions

- Describes well effects of turbulence on mixing of the dispersed phase
Approach 2: Particle tracking methods

- also called Lagrangian approach
- utilizes the equation of motion of a single particle
- initially used for dilute suspensions (one-way and two-way coupling)
- natural description for mixtures of particles with different properties
- usable for steady state simulation only in cases with distinct inlets (e.g. sprays, burners)
- can be used for dense suspensions if collisions are accounted for (the so-called micro-scale models; complicated and slow)

Equation of motion

according to Maxey & Riley (Phys. Fluids, 26:883-889, 1983)
Note: modified from the older BBO-equation

\[
m_p \frac{d\mathbf{v}_p}{dt} = (m_p - m_f) \mathbf{g} + m_f \frac{d\mathbf{v}_f}{dt} - \frac{m_f}{2} \frac{d}{dt} \left( \mathbf{v}_p - \mathbf{v}_f - \frac{r_p^2}{10} \nabla^2 \mathbf{v}_f \right) \\
- 6\pi r_p \mu_f \left( \mathbf{v}_p - \mathbf{v}_f - \frac{r_p^2}{6} \nabla^2 \mathbf{v}_f \right) - 6r_p^2 \sqrt{\pi} \mu_f \rho_f \int_{t_0}^{t} \frac{d}{d\tau} \left( \mathbf{v}_p - \mathbf{v}_f - \frac{r_p^2}{6} \nabla^2 \mathbf{v}_f \right) \frac{1}{\sqrt{t-\tau}} d\tau
\]

Forces acting on the particle: gravity + added mass + viscous drag + Basset history effects
Validity of Maxey & Riley equation

- For laminar flow (and mean field of turbulent flow)

\[ \frac{r_p}{L} \ll 1, \quad \frac{r_p W}{v_f} \ll 1, \quad \frac{r_p^2 U}{v_f L} \ll 1 \]

\( L \) is characteristic length scale, \( W \) characteristic relative velocity, \( U/L \) the scale of fluid velocity gradient for undisturbed flow.

- For turbulent flow

\[ \frac{r_p}{\eta_k} \ll 1, \quad \frac{r_p W}{v_f} \ll 1, \quad \frac{r_p^2 v_k}{v_f \eta_k} \ll 1 \]

\( \eta_k \) and \( v_k \) are the Kolmogorov microscales of length and velocity:

\[ \eta_k = \left( \frac{v^3}{\varepsilon} \right)^{1/4} \]

\[ v_k = (v_f \varepsilon)^{1/4} \]

\( \varepsilon \) is the dissipation rate of turbulent kinetic energy

Equation of motion in Stokes regime \((Re_p<1)\)

Usually simplified:

\[ m_p \frac{dv_p}{dt} = (m_p - m_f)g - 6\pi r_p u_f (v_p - v_f) \]

For rapidly accelerating or oscillating flows this approximation can be poor.

Problems can also be expected when density difference between the phases is small.
Drag models

- A large number of empirical correlations exist
- Models that account for particle shape and deformation
- For dilute fluid particle flows, the drag is given by

\[
F = \frac{3}{4} C_D \frac{\rho_f}{d_p} |\mathbf{v}_p - \mathbf{v}_f| (\mathbf{v}_p - \mathbf{v}_f)
\]

Schiller & Naumann correlation

\[
C_D = 0.44 \quad \text{Re}_p > 1000
\]

\[
C_D = \frac{24}{\text{Re}_p} \left[ 1 + 0.15 \text{Re}_p^{0.687} \right] \quad \text{Re}_p \leq 1000
\]

Dispersion of particles

- Eddy interaction model/discrete random walk model: a particle is assumed to interact with an eddy over an interaction time

\[
t_e \approx 0.6 \frac{k}{\varepsilon}
\]

\[
t_c = -t_p \ln \left[ \frac{L_v}{t_p |u_f - u_p|} \right]
\]

- The velocity fluctuation during an eddy is obtained by sampling a normally distributed random function:

\[
u' = f(\sqrt{u'^2}) = f(\sqrt{2k/3})
\]
Numerical methods

One-way coupling

Start

Solution of fluid phase flow field

No

Equation set converged

Yes

Lagrangian tracking of dispersed phase entities

No

Statistics adequate

Yes

End

Two-way coupling

Start

Solution of fluid phase flow field without coupling to dispersed phase

No

Equation set converged

Yes

Lagrangian tracking of dispersed phase entities

No

Statistics adequate

Yes

1

Solution of fluid phase flow field with phase coupling terms

Equation set converged

End

Lagrangian approach, dilute example:

Pulverized coal boiler:
Particle temperature along particle tracks
Lagrangian methods for dense gas-solids flow

- Lagrangian particle tracking methods have been applied e.g. to fluidized beds

- Several approaches that differ
  - in the way a computed particle corresponds to real particles: one particle can present either one or a group of particles
  - in the way particle-particle collisions are treated
    - Discrete Particle Method (DPM):
      - no collisions (used for dilute suspensions)
      - soft-sphere approach (the discrete element method, DEM)
      - hard-sphere approach
    - Dense DPM, CPFD (computation particle fluid dynamic):
      - statistical approach

Lagrangian methods for dense gas-solids flow: soft- and hard-sphere models

- Soft-sphere model of particle-particle collisions:
  - the instantaneous inter-particle contact forces, namely, the normal, damping and sliding forces are computed using equivalent simple mechanical elements, such as springs, dashpots and sliders.
  - a very small time step is required (< 1e-6 s)

- Hard-sphere model of particle-particle collisions:
  - momentum-conserving binary collision
  - interactions between particles pair-wise and instantaneous
  - faster than soft-sphere method due to longer time steps

- Eulerian gas phase

- Lagrangian tracking of parcels of particles
  - Gas-particle and particle-particle interaction forces calculated in the mesh of the gas phase from closures written for Eulerian-Eulerian models for dense gas-particle suspensions (kinetic theory of granular flow, see later in the presentation)

- Also called / similar models:
  - Dense DPM (Dense Discrete Particle Model; Ansys Fluent)
  - CPFD (Computational Particle Fluid Dynamic; Barracuda)

- Description of particle size distribution easy

- Coarse gas phase mesh leads to inaccuracies

Lagrangian simulation, dense example:
Lagrangian approach, summary

- momentum and continuity equation for the carrier phase
- Newton equation for dispersed phase
- good for dilute suspensions, usable also for dense suspensions if collisions are accounted for
- description of dispersion of particles in turbulent flow requires large number of particles
- fast for laminar flow; describes well particle size and other distributions

Approach 3: Eulerian-Eulerian approach

- single phase equations (momentum, continuity) are averaged over time and/or volume and/or a particle assembly (Newton's equation) to obtain multiphase flow equations
- distribution of phases given by volume fraction
- models for phase interaction required
- all phases are described as interpenetrating continua
Volume averaging

Averaging volume

Starting point in volume averaging: Single phase equations + jump conditions

\[
\frac{\partial}{\partial t}(\rho_q) + \nabla \cdot (\rho_q \mathbf{v}_q) = 0
\]

\[
\frac{\partial}{\partial t}(\rho_q \mathbf{v}_q) + \nabla \cdot (\rho_q \mathbf{v}_q \mathbf{v}_q) = -\nabla p_q + \nabla \cdot \mathbf{\tau}_q + \rho_q \mathbf{g}
\]

\[
\rho_q (\mathbf{v}_q - \mathbf{v}_A) \cdot \mathbf{n}_q + \rho_\gamma (\mathbf{v}_\gamma - \mathbf{v}_A) \cdot \mathbf{n}_\gamma = 0
\]

\[
\rho_q \mathbf{v}_q (\mathbf{v}_q - \mathbf{v}_A) \cdot \mathbf{n}_q + \rho_\gamma (\mathbf{v}_\gamma - \mathbf{v}_A) \cdot \mathbf{n}_\gamma = (-p_q \mathbf{I} + \mathbf{\tau}_q) \cdot \mathbf{n}_q + (-p_\gamma \mathbf{I} + \mathbf{\tau}_\gamma) \cdot \mathbf{n}_\gamma - \nabla \cdot \mathbf{\sigma}_{qr} + \frac{2\sigma_{qr}}{|\mathbf{R}_A|} \mathbf{R}_A
\]

\[\mathbf{n}_q\] Unit outward normal vector of phase q

\[\mathbf{v}_A\] Velocity of the interface

\[\mathbf{R}_A\] interface curvature vector

\[\Delta_A = \nabla - \mathbf{R}_A \cdot \nabla\] = surface gradient operator

\[\mathbf{R}_A = \mathbf{R}_A / |\mathbf{R}_A|\]

\[\mathbf{\sigma}_{qr}\] interface surface tension

\[\mathbf{I}\] unit tensor
Averaging

Volume averaging:

\[ \langle \psi_q \rangle = \frac{1}{V} \int_{V_q} \psi_q \, dV \]

Volume average

\[ \widetilde{\psi}_q = \frac{1}{V_q} \int_{V_q} \psi_q \, dV = \frac{1}{\alpha_q} \langle \psi_q \rangle \]

Intrinsic volume average

\[ \overline{\psi}_q = \frac{\int_{V_q} \rho_q \psi_q \, dV}{\int_{V_q} \rho_q \, dV} = \frac{\langle \rho_q \psi_q \rangle}{\alpha_q \rho_q} \]

Mass-weighted (Favre) average

\[ \alpha_q = \frac{V_q}{V} \]

Volume fraction, \( \sum_q \alpha_q = 1 \)

Eulerian-Eulerian balance equations

Continuity:

\[ \frac{\partial}{\partial t} \left( \alpha_q \tilde{\rho}_q \right) + \nabla \cdot \left( \alpha_q \tilde{\rho}_q \bar{v}_q \right) = \Gamma_q \]

Momentum:

\[ \frac{\partial}{\partial t} \left( \alpha_q \tilde{\rho}_q \bar{v}_q \right) + \nabla \cdot \left( \alpha_q \tilde{\rho}_q \bar{v}_q \bar{v}_q \right) \]

\[ = -\nabla \left( \alpha_q \tilde{\rho}_q \right) + \nabla \cdot \left( \tau_q \right) + \alpha_q \tilde{\rho}_q \bar{g} + \mathbf{M}_q + \nabla \cdot \left( \tau_{\delta_q} \right) \]

\( M_q \) is the interaction force.
Turbulent stress term:

$$\left< \tau_{\delta q} \right> = -\left< \alpha_q \rho_q (\mathbf{v}_q - \bar{\mathbf{v}}_q)(\mathbf{v}_q - \bar{\mathbf{v}}_q) \right>$$

Conservation of mass:

$$\sum_q \Gamma_q = 0$$

Surface tension:

$$\sum_q \mathbf{M}_q = -\frac{1}{2V} \sum_q \int_A \left( -\nabla A \sigma_{q\gamma} + \frac{2\sigma_{q\gamma}}{R_A} \right) dA$$

Alternative averaging approaches

- volume averaging
- time averaging
- ensemble averaging
- volume-time averaging
- two-step volume-volume or volume-time averaging (first over the local scale, then over a larger scale)
- three-step averaging
Closures for turbulent stress terms

- No generally accepted turbulence models exist; parameters in any models are probably suspension dependent.

- Several alternatives suggested.

- Mixture turbulence model:
  - Uses mixture properties to calculate viscous stress; applicable for stratified flows and when densities of the phases are of same order.

- Dispersed turbulence model:
  - Appropriate for dilute suspensions.
  - Turbulence quantities of the dispersed phase are obtained using the theory of dispersion of particles by homogeneous turbulence.

- Turbulence model for each phase.

Closures for drag force

- Large number of models exist.

- Drag force is generally written in the form:

\[
M_q = -\frac{3}{4} C_D \frac{\alpha_q \alpha_f \rho_f}{d_q} \left| v_q - v_f \right| \left( v_q - v_f \right)
\]

- Note: in dense flows, \( C_D \) depends on \( \alpha_f \).

- Parameters in drag models should be functions of the averaging scale in inhomogeneous flows!
Description of particle size distribution in the Eulerian-Eulerian method

- Simplest way would be to treat each size class as a separate computational phase (method of classes)
  - Continuity and momentum equation for each size class
  - Computationally slow
  - Numerical difficulties: at least earlier versions than Ansys Fluent 14 produced non-physical results

- Particle size distribution described by methods of moments
  - QMOM (Quadrature Method Of Moments)
  - DQMOM (Direct QMOM)
    - In principle requires solution of momentum equations for velocities of the moments
    - Momentum equations can in some cases be replaced by algebraic equations

Numerical methods for the Eulerian-Eulerian approach

- several algorithms; usually extensions of single phase ones

- e.g. IPSA (Inter Phase Slip Algorithm) performs the following steps in one iteration loop:
  - solve velocities of all phases from momentum equations
  - solve pressure correction equation (which is based on the joint continuity equation)
  - update pressure
  - correct velocities
  - calculate volume fractions from phasic continuity equations
Example: simulated solids volume fractions in a circulating fluidized bed

Two-phase flow

Large particles

'Shree'-phase flow

Small particles

Eulerian-Eulerian models, summary

- momentum and continuity equations for each phase
- several averaging methods used to derive the equations
- best alternative for dense suspensions with large velocity differences/acceleration
- often very slow
- particle size and other distributions difficult to account for
Approach 4: Mixture model

- A local equilibrium between the continuous and dispersed phases, i.e. at every point, the particles move with the terminal slip velocity relative to the continuous phase
  - velocity components for dispersed phases can be calculated from algebraic formulas
  - significantly less equations to be solved

- Also called / similar models:
  - Algebraic slip (mixture) model
  - Diffusion model
  - Suspension model
  - Local-equilibrium model
  - Drift-flux model

Motivation for simplified multiphase models

**Full Eulerian models - problems**

- Numerical problems - long computing times - small time steps
- Difficulties in convergence
- Only a few secondary phases possible
- More difficulties, if mass transfer and chemical reactions are considered

- Simplified models are recommended, if applicable
Detailed derivation of the mixture model (1)

- Starting point: Eulerian model equations
- Continuity equation for phase $k$:
  \[
  \frac{\partial}{\partial t}(\alpha_k \rho_k) + \nabla \cdot (\alpha_k \rho_k \mathbf{u}_k) = \Gamma_k
  \]

- Momentum balance for phase $k$:
  \[
  \frac{\partial}{\partial t}(\alpha_k \rho_k \mathbf{u}_k) + \nabla \cdot (\alpha_k \rho_k \mathbf{u}_k \mathbf{u}_k) = -\alpha_k \nabla p_k + \nabla \cdot \left[ \alpha_k (\mathbf{t}_k + \mathbf{t}_{k}) \right] + \alpha_k \rho_k \mathbf{g} + \mathbf{M}_k
  \]

- Mixture equations are derived by taking a sum over all phases

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Detailed derivation of the mixture model (2)

- Continuity
  \[
  \frac{\partial}{\partial t} \sum_{k=1}^{n} (\alpha_k \rho_k) + \nabla \cdot \sum_{k=1}^{n} (\alpha_k \rho_k \mathbf{u}_k) = \sum_{k=1}^{n} \Gamma_k
  \]

- Define mixture density and velocity as
  \[
  \rho_m = \sum_{k=1}^{n} \alpha_k \rho_k \quad \mathbf{u}_m = \frac{1}{\rho_m} \sum_{k=1}^{n} \alpha_k \rho_k \mathbf{u}_k = \sum_{k=1}^{n} c_k \mathbf{u}_k
  \]

- Resulting equation
  \[
  \frac{\partial \rho_m}{\partial t} + \nabla \cdot (\rho_m \mathbf{u}_m) = 0
  \]

  \[
  \nabla \cdot \sum_k \alpha_k \mathbf{u}_k = \nabla \cdot \sum_k \mathbf{j}_k = \nabla \cdot \mathbf{j}_m = 0
  \]

  If all phases are incompressible

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Detailed derivation of the mixture model (3)

- Momentum balance

\[
\frac{\partial}{\partial t} \sum_{k=1}^{n} \alpha_k \rho_k \mathbf{u}_k + \nabla \cdot \sum_{k=1}^{n} \alpha_k \rho_k \mathbf{u}_k \mathbf{u}_k = -\sum_{k=1}^{n} \alpha_k \nabla p_k + \nabla \cdot \sum_{k=1}^{n} \alpha_k (\mathbf{r}_k + \mathbf{r}_T) + \sum_{k=1}^{n} \alpha_k \rho_k \mathbf{g} + \sum_{k=1}^{n} \mathbf{M}_k
\]

- Diffusion velocity \( \mathbf{u}_{Mk} = \mathbf{u}_k - \mathbf{u}_m \) (not slip velocity!)

- Definitions

\[
\mathbf{r}_m = \sum_{k=1}^{n} \alpha_k \mathbf{r}_k \quad \text{Viscous stress}
\]

\[
\mathbf{r}_{Tm} = -\sum_{k=1}^{n} \alpha_k \rho_k \frac{\mathbf{u}_k \mathbf{u}_k}{\mathbf{F}_k} \quad \text{Turbulent stress}
\]

\[
\mathbf{r}_{Dm} = -\sum_{k=1}^{n} \alpha_k \rho_k \mathbf{u}_{Mk} \mathbf{u}_{Mk} \quad \text{Diffusion stress}
\]

Detailed derivation of the mixture model (4)

- Assumption: all phases share the same pressure, \( p_k = p \)

- Using the definitions of mixture density and velocity and the stresses above, we obtain the resulting momentum balance for the mixture

\[
\frac{\partial}{\partial t} \rho_m \mathbf{u}_m + \nabla \cdot (\rho_m \mathbf{u}_m \mathbf{u}_m) = -\nabla p + \nabla \cdot (\mathbf{r}_m + \mathbf{r}_{Tm}) + \nabla \cdot \mathbf{r}_{Dm} + \rho_m \mathbf{g} + \mathbf{M}_m
\]
Detailed derivation of the mixture model (5)

- Eliminate the phase velocity in the continuity equation for a phase

\[
\frac{\partial}{\partial t} (\alpha_k \rho_k) + \nabla \cdot (\alpha_k \rho_k \mathbf{u}_m) = \Gamma_k - \nabla \cdot (\alpha_k \rho_k \mathbf{u}_{MK})
\]

- Or if phase densities are constants and mass transfer is zero:

\[
\frac{\partial}{\partial t} \alpha_k + \nabla \cdot (\alpha_k \mathbf{u}_m) = -\nabla \cdot (\alpha_k \mathbf{u}_{MK})
\]

which is a balance equation for phase \( k \) volume fraction and includes the effect of slip. Note that this is the same as the intuitive result except for the diffusion velocity instead of slip velocity.

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Detailed derivation of the mixture model (6)

- Relation between the slip velocity and the diffusion velocity

\[
\mathbf{u}_{ck} = \mathbf{u}_k - \mathbf{u}_c \quad \text{slip velocity (c denotes the continuous phase)}
\]

\[
\mathbf{u}_{mk} = \mathbf{u}_k - \mathbf{u}_m = \mathbf{u}_{ck} - \sum_l c_l \mathbf{u}_{cl}
\]

- For only one dispersed phase \( \mathbf{u}_{md} = (1 - c_d) \mathbf{u}_{cd} \)

- Note: so far no additional assumptions or approximations has been made (except the shared pressure, commonly used also in full Eulerian models)

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Slip velocity (1)

- The momentum equation for the dispersed phase is
  \[ \alpha_p \rho_p \frac{\partial \mathbf{u}_p}{\partial t} + \alpha_p \rho_p (\mathbf{u}_p \cdot \nabla) \mathbf{u}_p = -\alpha_p \nabla p + \nabla \cdot \left[ \alpha_p \left( \mathbf{\tau}_p + \mathbf{\tau}_{pT} \right) \right] + \alpha_p \rho_p \mathbf{g} + \mathbf{M}_p \]

- Momentum equation for the mixture (with \( M_m = 0 \))
  \[ \frac{\partial}{\partial t} \rho_m \mathbf{u}_m + \nabla \cdot (\rho_m \mathbf{u}_m \mathbf{u}_m) = -\nabla p + \nabla \cdot (\mathbf{\tau}_m + \mathbf{\tau}_{mT}) + \nabla \cdot \mathbf{\tau}_{Dm} + \rho_m \mathbf{g} \]

- Eliminate pressure gradient and solve for \( \mathbf{M}_p \)
  \[ \mathbf{M}_p = \alpha_p \left[ \rho_p \frac{\partial \mathbf{u}_{Mp}}{\partial t} + (\rho_p - \rho_m) \frac{\partial \mathbf{u}_m}{\partial t} \right] + \alpha_p \left[ \rho_p (\mathbf{u}_p \cdot \nabla) \mathbf{u}_p - \rho_m (\mathbf{u}_m \cdot \nabla) \mathbf{u}_m \right] \]
  \[ -\nabla \cdot \left[ \alpha_p \left( \mathbf{\tau}_p + \mathbf{\tau}_{pT} \right) \right] + \alpha_p \nabla \cdot (\mathbf{\tau}_m + \mathbf{\tau}_{mT} + \mathbf{\tau}_{Dm}) - \alpha_p (\rho_p - \rho_m) \mathbf{g} \]

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Slip velocity (2)

- Now, the following approximations are made:
  - All turbulent terms are omitted for the moment
  - Viscous and diffusion stress terms are small and are neglected
  - The local equilibrium assumption implies
    \[ \frac{\partial \mathbf{u}_{Mp}}{\partial t} \approx 0 \quad (\mathbf{u}_p \cdot \nabla) \mathbf{u}_p \approx (\mathbf{u}_m \cdot \nabla) \mathbf{u}_m \]

- The momentum transfer term is given by
  \[ M_p = \frac{1}{2} \frac{\alpha_p A_p}{V_p} C_D \rho_c |\mathbf{u}_{cp}| \mathbf{u}_{cp} \]
Slip velocity (3)

- Finally:

\[
\frac{1}{2} \rho_c A_p C_D |u_{cp}| u_{cp} = V_p (\rho_p - \rho_m) \left[ (u_m \cdot \nabla) u_m + \frac{\partial u_m}{\partial t} - g \right]
\]

- For small particles (Stokes drag) in gravitational and centrifugal field

\[
u_{cd} = \frac{d_p^2 (\rho_p - \rho_m)}{18 \mu_m} \left[ \frac{u_{m\phi}^2}{r} e_r - g \right]
\]

- This is the slip velocity. The diffusion velocity used in the model equations must be calculated as shown above.

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Closures for viscous stress in mixture models

Viscous stress: \( \tau_m = \mu_m \left[ \nabla v_m + (\nabla v_m)^T \right] \)

Mixture viscosity (Ishii & Zuver, 1979):

\[
\mu_m = \mu_f \left( 1 - \frac{\alpha_p}{\alpha_{p,max}} \right)^{2.5 \alpha_{p,max} \mu^*}
\]

where \( \alpha_{p,max} \) is the maximum packing and

\[
\mu^* = \frac{\mu_p + 0.4 \mu_f}{\mu_p + \mu_f} \quad \text{for bubbles or drops}
\]

\[
\mu^* = 1 \quad \text{for solid particles}
\]
Treatment of turbulence in mixture models

- in dilute suspensions, mixture turbulent stress is assumed same as carrier phase turbulent stress
- at higher concentrations, modeling required
- turbulence enhances spreading of dispersed phases -> taken into account in continuity equation:

\[
\frac{\partial}{\partial t} (\alpha_p \rho_p) + \nabla \cdot (\alpha_p \rho_p \tilde{v}_m) = \nabla \cdot (D_{mp} \nabla \alpha_p) + \Gamma_p - \nabla \cdot (\alpha_p \rho_p \tilde{v}_{mp})
\]

where \( D_{mq} \) is a dispersion (diffusion) coefficient:

\[
D_{mp} = v_{Tc} \left( 1 + 0.85 \frac{\bar{v}_{cp}^2}{2k/3} \right)
\]

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Turbulent dispersion

- Turbulence is coupled in the mixture model in a straightforward way, because the treatment has a single phase nature. A standard model, e.g. \( k-\epsilon \) model, can be coupled to the mixture equations.
- The turbulent stress and the fluctuating part of \( M_q \) are modeled using a turbulent dispersion (diffusion) coefficient \( D_T \)

\[
u_{mq} \rightarrow u_{mq} + \frac{D_T}{\alpha_q} \nabla \alpha_q
\]

- A suitable model is needed for the dispersion coefficient, for example (Picart et al., 1986)

\[
D_T = v_T \left( 1 + 0.85 \frac{u_{Cd}^2}{2k/3} \right)^{-1/2}
\]

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Mixture model - validity

- The essential approximation is the local equilibrium assumption: the particles are accelerated instantaneously to the terminal velocity.
- Consider again the simplified one-particle equation

\[ m_p \frac{du_p}{dt} = V_p \Delta \rho g - \frac{1}{2} \rho_f A_p C_d u_p^2 \]

- Solution of particle velocity as a function of distance (Stokes regime)
- The characteristic length of acceleration is

\[ l_p = \frac{d_p \rho_p}{18 \mu_f} \]

\[ t_p = \frac{\Delta \rho}{\rho_p} \]

\[ u_t = \frac{\Delta \rho}{\rho_p} \]

If the density ratio is small, the virtual mass and history terms cannot be ignored (both effects increase the response time).
- A suitable requirement for the local equilibrium is \( l_p \ll \) typical system dimension.
Validity range of mixture models, cont.

- Mixture model is usually not suitable for gas-particle flows, because the characteristic length can be large
- Not suitable for clustering flow, where average slip velocity is greater than single particle slip
- Typically used for liquid-solid flows and bubbly liquid-gas flows (not for very big bubbles)

Validating simulations

Solid particles in an agitated vessel

Glass beads of three different sizes in water

Experiments: Barresi and Baldi (1987)

D = 0.390 m, H = 0.464 m
4 baffles (0.039 m)
45° pitched 4-blade turbine
(Dt = 0.130 m, Htb = 0.046 m).
Impeller power number: 1.2

Average mass fraction: 0.5 %

<table>
<thead>
<tr>
<th>dp,exp.(µm)</th>
<th>100-177</th>
<th>208-250</th>
<th>417-500</th>
</tr>
</thead>
<tbody>
<tr>
<td>dp,sim.(µm)</td>
<td>140</td>
<td>230</td>
<td>460</td>
</tr>
<tr>
<td>ρ (kg/m³)</td>
<td>2670</td>
<td>2600</td>
<td>2600</td>
</tr>
<tr>
<td>N (rev/s)</td>
<td>4.83</td>
<td>5.67</td>
<td>6.50</td>
</tr>
</tbody>
</table>
Validating simulations
Solid particles in an agitated vessel

Bubbe drag correlations

\[ C_D = \max \left\{ \min \left[ \frac{24}{\text{Re}_p} \left( 1 + 0.15 \text{Re}_p^{0.687} \right) \frac{72}{\text{Re}_p} \left( 1 + 0.15 \text{Re}_p^{0.687} \right) \frac{8}{3 \text{Eo} + 4} \right] \right\} \]

Tomiyama 1

\[ C_D = \max \left\{ \frac{24}{\text{Re}_p} \left( 1 + 0.15 \text{Re}_p^{0.687} \right) \frac{8}{3 \text{Eo} + 4} \right\} \]

Tomiyama 2

\[ C_D^{\text{ip}} = \begin{cases} \frac{24}{\text{Re}_p} \left( 1 + 0.15 \text{Re}_p^{0.687} \right) & \text{Re}_p < 1000 \\ 0.439 & \text{Re}_p \geq 1000 \end{cases} \]

Ishii-Zuber

\[ E\text{o}=\frac{a(\rho_p - \rho_q)d_p^2}{\sigma} \]
Bubble terminal velocity

In gravitational field

Effect of acceleration

MUSIG-model

- Developed primarily for bubble column applications
  - Bubble motion determined by gravitational acceleration
  - The basic approximation of equal slip velocities of all bubble sizes is fairly good
- In strongly swirling flows (stirred reactors, pumps) the model may not be justified
- Reduces the number of equations to be solved
- Is a two-phase model and has therefore the convergence and stability problems of multiphase CFD
Mixture model example

MUSIG-model (CFX): \( (N+6) \)
- Continuity equation for all phases (N)
- Momentum equation for one bubble phase (average diameter) (6)
- All other bubble classes: same velocity as the class with average diameter
- A large number of bubble classes possible

Mixture models (FLUENT): \( (N+3) \)
- Continuity equation for the mixture and all bubble phases (N)
- Momentum equation for the mixture (3)
- Bubbles: slip velocities from algebraic balance equations
- Numerically well behaved, a large number of bubble classes possible

GAS CAVITIES BEHIND THE BLADES OF THE OUTFKUMPU ROTOR

By Mikko Manninen, VTT
Mixture model summary

- Length scale of particle relaxation must be small compared to the mesh spacing
- Local equilibrium assumption yields the slip velocity
- Transport of the dispersed phase calculated from the phase continuity equation
- Fast; describes well particle size and other distributions
- Describes well effects of turbulence

Other approaches

- VOF (volume of fluid) – method for tracking phase interfaces in separated flows
- Eulerian-Eulerian + Lagrangian
- Eulerian-Eulerian + mixture model
- Mesoscopic simulation methods (e.g. Lattice-Bolzmann method)
- MP-PIC (multi-phase particle in cell; Lagrangian transport of parcels of particles + Eulerian kinetic theory description for solids)
Summary of multiphase CFD:

• Several ways to derive equations

• Simplifications in all models

• Jump conditions at phase interfaces complicated (drag force)

• Multitude of time and length scales -> difficult to choose suitable averaging and simulation scales

• Flows often time-dependent also in macroscopic length scales (e.g. bubbling fluidized beds)

Summary of multiphase CFD, cont.:

• Never fully ‘laminar’

• Turbulence modelling difficult; no general models exist; unisotropy causes problems

• Dense suspensions dominated by particle-particle collisions

• Dilute suspensions dominated by particle-turbulence interaction

• Measurements still necessary for derivation of equation closures and for validation; often not available
Summary of multiphase CFD, cont.:

- Choose the simplest possible model
- Follow the literature
- Compare with measurement data if available
- Results for dilute suspensions already good
- Even dense suspensions can be simulated
- Increasing computer speed will facilitate simulation of more demanding cases in the future

Example of Eulerian-Eulerian modeling: Fluidized beds

- Inhomogeneous flow pattern
- Flow characteristics change as a function of fluidization velocity

Eulerian-Eulerian approach based on KTGF
– background

- Kinetic theory of granular flow (KTGF)

  - A special model developed for dense gas-solid suspensions, see e.g. (Gidaspow D., 1994, Multiphase flow and fluidization: Continuum and kinetic theory descriptions, Academic press, Boston)

  - Theory similar to gas kinetic theory
  - Solid phase equations are derived by ensemble averaging over the single particle velocity distribution function
  - This averaging is done in a local scale assuming locally random distribution of particles

Eulerian-Eulerian approach based on KTGF
– limitations and simplifications

- Because of the randomness assumption, the theory is basically only suitable for transient simulations in fairly fine meshes

- In derivation of the models, only binary collisions between particles are accounted for, and thus KTGF is not valid in dense suspensions, like in bubbling beds

- In practise it is used from packing limit to very dilute conditions

- The theory was originally written for a single particle size
  - Later rigorous extension of the theory to mixtures has been developed

- Here we focus on models for a single particle size
Eulerian-Eulerian approach based on KTGF
– software implementations

- Kinetic theory of granular flow is today found in
  - commercial codes
  - open source codes
  - researchers' and universities own codes

- Alternative closures based on different assumptions have been suggested in the literature

- Here we mainly present models available in the commercial Fluent software

Eulerian-Eulerian approach based on KTGF
– balance equations

Continuity equation for phase q:
\[
\frac{\partial}{\partial t} (\alpha_q \rho_q) + \nabla \cdot (\alpha_q \rho_q \mathbf{v}_q) = 0
\]

Momentum equation for gas phase g:
\[
\frac{\partial}{\partial t} (\alpha_g \rho_g \mathbf{v}_g) + \nabla \cdot (\alpha_g \rho_g \mathbf{v}_g \times \mathbf{v}_g) = -\alpha_g \nabla p + \nabla \cdot (\alpha_g \mathbf{\tau}_g) + \alpha_g \rho_g g + K_{sg} (\mathbf{v}_s - \mathbf{v}_g)
\]

Momentum equation for solid phase s:
\[
\frac{\partial}{\partial t} (\alpha_s \rho_s \mathbf{v}_s) + \nabla \cdot (\alpha_s \rho_s \mathbf{v}_s \times \mathbf{v}_s) = -\alpha_s \nabla p - \nabla p_s + \nabla \cdot (\alpha_s \mathbf{\tau}_s) + \alpha_s \rho_s g + K_{sg} (\mathbf{v}_g - \mathbf{v}_s)
\]
Eulerian-Eulerian approach based on KTGF – balance equation for granular temperature

Granular temperature is defined as an ensemble average

$$\Theta_s = \frac{1}{3} \langle v_s'^2 \rangle$$

where $v_s'$ is the fluctuating solids velocity.

Balance equation for Granular temperature:

$$\frac{3}{2} \left[ \frac{\partial}{\partial t} \left( \alpha_s \rho_s \Theta_s \right) + \nabla \cdot \left( \alpha_s \rho_s v_s \Theta_s \right) \right] = (-p_s I + \tau_s) : \nabla v_s + \nabla \cdot \left( k_{\Theta_s} \nabla \Theta_s \right) - \gamma_{\Theta_s} + \phi_{gs}$$

First term on the right is the generation term, the second term is the diffusion term, the third the dissipation term and the fourth expresses the energy exchange between gas and solids.

Alternatively, the granular temperature is computed from an algebraic equation obtained from the original transport equation by neglecting convection and diffusion terms.

---

Eulerian-Eulerian approach based on KTGF – closures for granular temperature

Radial distribution function related to the probability of collisions (Lun et al):

$$g_{0,ss} = \left[ 1 - \left( \frac{\alpha_s}{\alpha_{s,max}} \right)^3 \right]^{-1}$$

where $\alpha_{s,max}$ expresses the solids volume fraction of a packed bed.

The collisional dissipation of energy can be computed from (Lun et al.)

$$\gamma_{\Theta_s} = \frac{12(1 + e_{ss}^2)g_{0,ss}}{d_s \sqrt{\pi}} \alpha_s^2 \rho_s \Theta_{s}^{3/2}$$

and the energy exchange between gas and solids from (Gidaspow et al.)

$$\phi_{gs} = -3K_{gs} \Theta_s$$
Eulerian-Eulerian approach based on KTGF – closures for granular temperature, continued

The diffusion coefficient is computed, according to Syamlal et al., from

\[
k_{0,s} = \frac{15d_s \rho_s \alpha_s \sqrt{\Theta_s \pi}}{4(41 - 33\eta)} \left[ 1 + \frac{12}{5} \eta^2 (4\eta - 3)\alpha_s g_{0,ss} + \frac{16}{15\pi} (41 - 33\eta)\eta\alpha_s g_{0,ss} \right]
\]

where

\[
\eta = \frac{1}{2} (1 + e_{ss})
\]

Gidaspow suggests instead:

\[
k_{0,s} = \frac{150d_s \rho_s \sqrt{\Theta_s \pi}}{384(1 + e_{ss})g_{0,ss}} \left[ 1 + \frac{6}{5} \alpha_s g_{0,ss} (1 + e_{ss}) \right]^2 + 2d_s \alpha_s^2 \rho_s (1 + e_{ss}) g_{0,ss} \frac{\sqrt{\Theta_s}}{\pi}
\]

Eulerian-Eulerian approach based on KTGF – granular pressure

Lun et al.:

\[
p_s = \alpha_s \rho_s \Theta_s + 2\rho_s (1 + e_{ss})\alpha_s^2 g_{0,ss} \Theta_s
\]

Syamlal & O'Brien:

\[
p_s = 2\rho_s (1 + e_{ss})\alpha_s^2 g_{0,ss} \Theta_s
\]

Ahmadi & Ma:

\[
p_s = \alpha_s \rho_s \Theta_s \left[ (1 + 4\alpha_s g_{0,ss}) + \frac{1}{2} (1 + e_{ss})(1 - e_{ss} + 2\mu_{fric}) \right]
\]
Eulerian-Eulerian approach based on KTGF
– solids shear stress based on KTGF

Phase q stress-strain tensor
\[ \tau_q = \alpha_q \mu_q (\nabla v_q + \nabla v_q^T) + \alpha_q (\lambda_q - \frac{2}{3} \mu_q) \nabla \cdot v_q I \]

Solids shear viscosity is given as a sum of the one predicted by the kinetic theory and a frictional shear viscosity
\[ \mu_s = \mu_{s,ktgf} + \mu_{s,fr} = \mu_{s,ktgf} + \mu_{s,kin} + \mu_{s,fr} \]

The collisional viscosity (Gidaspow et al):
\[ \mu_{s,kin} = \frac{4}{5} \alpha_s \rho_s d_s g_{0,ss} (1 + e_{ss}) \left( \frac{\Theta_s}{\pi} \right)^{\frac{1}{2}} \]

Kinetic viscosity (Syamlal)
\[ \mu_{s,kin} = \frac{\alpha_s \rho_s d_s \sqrt{\Theta_s \pi}}{6(3 - e_s)} \left[ 1 + \frac{2}{5} (1 + e_s) (3e_{ss} - 1) g_{0,ss} \alpha_s \right] \]

The granular bulk viscosity (Lun et al)
\[ \lambda_s = \frac{4}{3} \alpha_s \rho_s d_s g_{0,ss} (1 + e_{ss}) \left( \frac{\Theta_s}{\pi} \right)^{\frac{1}{2}} \]

Eulerian-Eulerian approach based on KTGF
– frictional stress

Johnson and Jackson (1987)
Shear stress:
\[ \tau_s = \tau_{s,ktgf} + \tau_{s,fr} \]
\[ \tau_{fr} = -p_{fr} I + \mu_{s,fr} \left( \nabla v_s + (\nabla v_s)^T \right) \]

Solids pressure:
\[ p_s = p_{ktgf} + p_{fr} \]

Frictional pressure:
\[ p_{fr} = Fr \left( \frac{\alpha_s - \alpha_{s,min}}{\alpha_{s,max} - \alpha_s} \right)^n \]
In FLUENT Fr=0.1 \alpha_s

Frictional viscosity:
\[ \mu_{s,fr} = p_{fr} \sin \phi \]

Schaeffer (1987)
Frictional viscosity:
\[ \mu_{s,fr} = \frac{p_{fr} \sin \phi}{2\sqrt{I_{2D}}} \]
Eulerian-Eulerian approach based on KTGF  
– frictional stress

Syamlal et al. (1993):

**Shear stress:**
\[ \tau_s = \begin{cases} \tau_{s,ktgf} + \tau_{s,ktgf} & \text{if } \alpha_s < \alpha_{s,f,min} \\ \tau_{s,fr} + \tau_{s,fr} & \text{if } \alpha_s \geq \alpha_{s,f,min} \end{cases} \]

**Solids pressure:**
\[ p_s = \begin{cases} p_{s,ktgf} & \text{if } \alpha_s < \alpha_{s,f,min} \\ p_{s,fr} & \text{if } \alpha_s \geq \alpha_{s,f,min} \end{cases} \]

**Frictional pressure:**
\[ p_{s,fr} = \begin{cases} 0 & \text{if } \alpha_s < \alpha_{s,f,min} \\ 10^{25} \alpha_s (\alpha_s - \alpha_{s,f,min})^{10} & \text{if } \alpha_s \geq \alpha_{s,f,min} \end{cases} \]

---

Eulerian-Eulerian approach based on KTGF  
– implementation in the software

- The models are often not implemented as such in numerical solvers.
- Simplifications are introduced in the implementations to improve the numerical stability.
- For example, the radial basis function needs to be restricted close to the packing limit to avoid numerical problems.
- The manuals of commercial codes don’t reveal details of these modifications.
- Sometimes it is possible to track down the actual equations used by a tedious comparison of the values given by the commercial code and different versions of the equations.
Validation of the KTGF model in a 2D CFB
Simulation in a fine mesh (0.625 mm spacing)

Comparison of measured solids volume fraction and velocities with the simulation results at 0.8 m and 1.2 m heights in the 2D CFB at Åbo Akademi. Particle size 0.44 mm and fluidization velocity 3.75 m/s.

Results without drag correction in a coarse mesh

-> the assumption of local homogeneity in the closure equations leads to problems
-> subgrid scale closures required
Modified drag force model used in CFB and turbulent bed simulations

- larger particle size → smaller cluster correction
- finer mesh → smaller correction necessary

Voidage function used at slip velocity 1 m/s. The drag model by Gidaspow et al., recommended in Fluent manuals, is shown for comparison.


Simulations of a 1 m X 7.3 m riser in 2D with macroscopic drag model

Effect of the mesh: the finer the mesh, the finer structures are produced. Average voidage patterns are unaffected.

8000 cells sized 2.5 cm X 3.65 cm
4400, 17600 and 70400 elements

3D simulation of large BFB’s and CFB’s

Relationship between the number of elements and element size:

<table>
<thead>
<tr>
<th>Elements</th>
<th>Element size</th>
</tr>
</thead>
<tbody>
<tr>
<td>20 000</td>
<td>0.85 m³</td>
</tr>
<tr>
<td>100 000</td>
<td>0.5 m³</td>
</tr>
<tr>
<td>1 000 000</td>
<td>0.23 m³</td>
</tr>
<tr>
<td>10 000 000</td>
<td>0.11 m³</td>
</tr>
<tr>
<td>100 000 000</td>
<td>0.05 m³</td>
</tr>
</tbody>
</table>

2D simulation, furnace ‘area’ 30 x 40 m²

<table>
<thead>
<tr>
<th>Elements</th>
<th>Element size</th>
</tr>
</thead>
<tbody>
<tr>
<td>20 000</td>
<td>0.25 m²</td>
</tr>
<tr>
<td>100 000</td>
<td>0.11 m²</td>
</tr>
<tr>
<td>500 000</td>
<td>0.05 m²</td>
</tr>
<tr>
<td>5 000 000</td>
<td>0.015 m²</td>
</tr>
</tbody>
</table>

At least when mesh spacing > 0.5 cm, drag laws need to be adjusted. When mesh spacing > 10 cm, drag laws need further modifications and probably also stress terms need to be modified?!? Macroscopic/steady state/coarse mesh models should be developed!

Macroscopic CFD models

- take into account large control volume size
- are written for steady state
- large fluctuation terms in the equations → equation closure highly demanding
- equation closure requires measurements
- produces reasonable solids distributions
- see e.g.
  - S. Kallio, V. Poikolainen, T. Hyppänen, Report 96-4, Åbo Akademi/Värmetskni
- coarse mesh models (filtered models) similar; meant for transient simulations of large processes
- no generally accepted macroscopic models available today!
Simulation of real fluidization processes
- special features

- Complicated by a multitudinous of particle sizes/types
- Complicated by differences in temperature → energy balance
- Complicated by homogeneous and heterogeneous reactions → species balances necessary
- Laboratory scale processes can be modeled in more details in the transient mode

Additional equations/models required (examples)

- Energy balance equations for each phase
  - Heat capacity for each phase
  - Inter-phase heat transfer models, depend on particle size, temperature, suspension density, velocities etc
  - Reaction enthalpies
  - Radiative heat transfer
  - Conductivity of each phase
- Species balance equations
  - Models for homogeneous and heterogeneous reactions
  - Inter-phase transfer rates
  - Diffusion/dispersion
- Comminution (attrition, fragmentation)
- Solid-solid momentum transfer
Simulation of large industrial processes

- Complicated by a multitudine of particle sizes/types
- Complicated by differences in temperature → energy balance
- Complicated by homogeneous and heterogeneous reactions → species balances necessary
- Complicated by a large size → coarse meshes, long computations
- Simplifications/special approaches necessary

Examples of approaches for large industrial furnaces

- BFB modeling
  - Simplified models for the bed and 1-phase + Lagrangian particles in the freeboard
  - Coarse mesh models
- CFB modeling
  - Empirical bulk solids distribution + balance equations for gas phase, energy, species; fuel mixed using Lagrangian models or dispersion models
  - Full two-phase model (transient (slow!!!) or steady-state (closures being developed and validated e.g. at VTT)
  - Full multi-phase model (slow!!!)
  - Particle-in-cell method (problems with coarse mesh)
Example: steady-state simulation of Chalmers boiler with a time-averaged model

- Gas phase: 5 components
- Solid phase: ash and sand as one Eulerian solid phase
- Coal: particle tracking; drying, devolatilization, combustion; two-way coupled with gas phase
- Solved using rigorous time-averaged equations for steady-state hydrodynamics, with balance equations for Reynolds stresses
- Species balance equations solved for all the components
- Source terms calculated from homogeneous and heterogeneous reactions
- Mixing of enthalpy and chemical components described by dispersion coefficients in energy and species balance equations; dispersion calculated from Reynolds stresses and time scales

Ref.: Taivassalo et al., FBC21, Naples 2012

Example2: steady-state simulation of Chalmers boiler with the time-averaged model (Taivassalo et al., FBC21, Naples 2012)

a) Time-averaged solid volume fraction, b) time-averaged mass-weighted vertical solid velocity, c) typical pathlines for a 1 mm fuel particle coloured by the residence time, d) mole fraction of O₂ and e) the time-averaged gas temperature (°C).
Conclusions on simulation of dense gas-solids flow

- Eulerian-Eulerian is a good approach; MP-PIC is also usable and good for description of particle size distributions

- Cluster formation is characteristic of dense gas-solid flows

- Transient simulations produce correct fluctuation patterns and average distributions, but as such usable only for small geometries

- Industrial processes large, large processes require coarse meshes

- Remember: closure model parameters for transient equations coarse-mesh simulations should be mesh-dependent! No such models available!

- Steady-state models now available at VTT and used for simulation of CFB boiler furnaces