Review of Numerical Methods for Multiphase Flow

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Content of the Lecture

- Classification of multiphase flows
- Classification of numerical methods for multiphase flows.
  - Particle-resolved direct numerical simulations
  - Interface tracking method for bubbly flows
  - Lattice-Boltzmann method (particle resolved)
  - Direct numerical simulations with point-particles
  - Approaches with turbulence modelling (point-particles)
    - Euler/Euler (two fluid) approach
    - Euler/Lagrange approach
- Summary/Conclusions
Multiphase flows may be encountered in various forms:

- Transient two-phase flows

- Separated two-phase flows

- Dispersed two-phase flows

The two-fluid concept is suitable, but requires methods for handling the interface (e.g., Tracking, VOF, ............)
Examples of separated multiphase flows:

- Slug flow
- Churn flow

*Slug flow in oil-water-gas pipe flow*
Dispersed two-phase flow systems and important technical and industrial applications.

<table>
<thead>
<tr>
<th>Continuous/Dispersed Phase</th>
<th>Industrial/Technical Application</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gas-solid flows</td>
<td>pneumatic conveying, particle separation in cyclones and filters, fluidised beds, coal combustion</td>
</tr>
<tr>
<td>Liquid-solid flows</td>
<td>hydraulic conveying, liquid-solid separation, particle dispersion in stirred vessels</td>
</tr>
<tr>
<td>Gas-droplet flows</td>
<td>spray drying, spray cooling, spray painting, spray scrubbers, spray combustion</td>
</tr>
<tr>
<td>Liquid-droplet flows</td>
<td>mixing of immiscible liquids, liquid-liquid extraction</td>
</tr>
<tr>
<td>Liquid-gas flows</td>
<td>bubble columns, aeration of swage water, flotation</td>
</tr>
</tbody>
</table>

Moreover, numerous examples of multiphase flows may be found in industry, such as: liquid-gas-solids reactors or spray scrubbers (droplets and particles dispersed in a gas flow)
Examples of dispersed gas-solid flows:

- **Dilute two-phase flow**
  - aerodynamic transport

- **Dense two-phase flow**
  - particle-particle interaction

Gas-Solid Flow; Euler/Lagrangian Calculation
(Helland et al. 2000)
Estimation of the interaction between particles based on the inter-particle spacing for a regular cubic arrangement:

\[
\frac{L}{D_p} = \left( \frac{\pi}{6 \alpha_p} \right)^{1/3}
\]

\[\alpha_{p,\text{max}} = 0.524\]

Regimes of dispersed two-phase flows:

Example:
- gas-solids flow:
  \(\eta = 1.0\)
  \(\alpha_p = 5 \cdot 10^{-4}\)
  \(\rho_p = 2500 \text{ kg/m}^3\)
  \(\rho_F = 1.18 \text{ kg/m}^3\)
  \(L/D_p = 10.15\)
Dispersed multiphase flows are characterised by the following properties of the particle phase.

**Integral values for characterising two-phase flows:**
- volume fraction of the dispersed phase
- mass fraction, porosity

**Characteristics of the particles:**
- size distribution
- particle shape, porosity
- surface and surface structure

**Particle motion in fluids:**
- velocity distribution of particles
- fluctuating velocity of particles
Classification of Multiphase Flows

- **Volume fraction of the particle phase and porosity:**
  \[ \alpha_p = \frac{\sum_i N_i V_{p_i}}{V} \]
  \[ \varepsilon = 1 - \alpha_p \]

- **Effective density of both phases (or bulk density):**
  \[ \rho_p^b = c_p = \alpha_p \rho_p \]
  \[ \rho_F^b = (1 - \alpha_p) \rho_F \]

- **Mixture density:**
  \[ \rho_m = \rho_F^b + \rho_p^b = (1 - \alpha_p) \rho_F + \alpha_p \rho_p \]

- **Number concentration (particles per unit volume):**
  \[ n_p = \frac{N_p}{V} \]

- **Mass loading of particles (generally only for gas-solid flows):**
  \[ \eta = \frac{\dot{m}_p}{\dot{m}_F} = \frac{\alpha_p \rho_p U_p}{(1 - \alpha_p) \rho_F U_F} \]
Particle methods:
Numerical calculation of the behaviour of bulk solids with and without flow:
- Molecular dynamics (MD)
- Granular dynamics (GD)
- Discrete element methods (DEM)

Full direct numerical simulation (DNS):
Resolution of particle contour and flow around the particle:
- contour-adapted grid
- Interface tracking
- Volume of Fluid (VOF)
- Lattice Boltzmann (LBM)

Discharge of bulk solids from a silo

Prof. D.D. Joseph
Direct numerical simulations (DNS) and large eddy simulations (LES):
- Point-particle assumption
- for turbulence studies

Homogeneous isotropic turbulence

Numerical methods for dispersed multiphase flows (RANS-type methods):
- Reynolds-averaged conservation equations with turbulence model, point-particle assumption:
  - Mixture models
  - Euler/Euler (two-fluid) approach
  - Population balance method
  - Euler/Lagrange approach
Application of different numerical approaches:

- Taylor-bubble with VOF
- Point-particle-DNS for turbulent flow
- RANS-calculation for technical systems

Increasing modelling requirements
The volume-of-fluid method (VOF): 

The interface is being reconstructed based on the solution of a transport equation for the volume fraction.

\[ \frac{\partial f}{\partial t} + \bar{u} \cdot \nabla f = 0 \]
Influence of shear flow on bubble migration calculated by a VOF approach (Tomiyama et al. 1993)

\[
Eo = \frac{g (\rho_f - \rho_g) D_b^2}{\sigma}
\]

\[
Mo = \frac{g \mu_f^4 (\rho_f - \rho_g)}{\rho_f^2 \sigma^3}
\]

Determination of lift forces

\( Eo = 1, \; Mo = 10^{-3} \)

\( Eo = 10, \; Mo = 10^{-3} \)
Flow around nearly spherical and large non-spherical bubbles simulated by VOF (Bothe et al. 2007)

\[
E_{O_h} = \frac{g (\rho_f - \rho_g) D_h^2}{\sigma}
\]

Tomiyama correlation

\[
C_A = \begin{cases} 
\min \left(0.288 \cdot \tan h \left(0.121 \text{Re}_B\right)\right), & \text{für: } E_{O_h} < 4 \\
f \left(E_{O_h}\right), & \text{für: } 4 \leq E_{O_h}
\end{cases}
\]

\[
f \left(E_{O_h}\right) = 0.00105 \, E_{O_h}^3 - 0.0159 \, E_{O_h}^2 - 0.0204 \, E_{O_h} + 0.474
\]
Interface resolved direct numerical simulations allow a detailed analysis of the atomisation process.

Numerical grid: $128 \times 128 \times 896$
Mesh size: 2.36 $\mu$m

Numerical grid: $256 \times 256 \times 2048$
Mesh size: 1.17 $\mu$m

BERLEMONT 2008
Level Set/Ghost Fluid Method
Interface Tracking Approach

- Direct numerical simulations of the bubble motion using an interface tracking approach (Prof. Tryggvason).
- Time-dependent solution of the three-dimensional, Navier-Stokes equations.

\[
\frac{\partial \rho \vec{u}}{\partial t} + \nabla \cdot (\rho \vec{u} \vec{u}) = -\nabla p + \left(\rho - \rho_0\right) \vec{g} + \nabla \cdot \mu \left(\nabla \vec{u} + (\nabla \vec{u})^T\right) + \int_{F} F_s \delta(\vec{x} - \vec{x}_f) \, da
\]

- Surface tension

- The surface tension force is calculated from the curvature of the interface.

- Incompressible gas- and liquid-phase:

\[
\nabla \vec{u} = 0
\]

- Equation of state for the density and the viscosity:

\[
\frac{\partial \rho}{\partial t} + \vec{u} \cdot \nabla \rho = 0 \\
\frac{\partial \mu}{\partial t} + \vec{u} \cdot \nabla \mu = 0
\]
* Rectangular grid for the flow domain.
* Interface grid to mark the position of the interface.
* The interface is resolved within 2-3 meshes of the grid resolving the flow domain.

**Density ratio:**

\[
\frac{\rho_f}{\rho_b} = 20
\]

**Spatial Discretisation:**
2nd-order central differences

**Time Discretisation:**
2nd-order explicit method

**Periodic boundary conditions at the cube faces**

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Binary mixture of bubbles, instantaneous distribution, case 1, Simulation for 29 small and 29 large bubbles ($\alpha = 6\%$).

- Volume ratio: 2
- Diameter ratio: 1.26

Ga = 600, 1200
Eo = 0.63, 1.0

\[ \text{Ga} = \frac{(\rho_f - \rho_g) \rho_f g D_b^3}{\mu_r^2} \]

\[ \text{Eo} = \frac{g (\rho_f - \rho_g) D_b^2}{\sigma} \]
Binary mixture case 2 (Göz and Sommerfeld 2004):

- Volume Ratio: 8
- Diameter Ratio: 2
- $\alpha = 6\%$: 40 small, 5 large
- $\alpha = 12\%$: 64 small, 8 large
- $Ga = 900, 7200$
- $Eo = 1, 4$
Direct numerical simulations of bubble motion in a cube by accounting for interface deformation.

Behaviour of bi-disperse bubble systems (case 2)

- $\alpha = 2\%$: 28 small, 4 large
- $\alpha = 6\%$: 40 small, 5 large
Turbulent kinetic energy for case 1 and 2:

- temporal development
- turbulent kinetic energy in dependence of gas hold-up
Bubble Reynolds number in dependence of gas hold-up:

**Case 1**

\[ \text{Re}_d = \frac{\rho_f D_b U_b}{\mu_f} \left(1 - \alpha_b \right) \]
Trajectories of non-spherical bubbles obtained by interface tracking method (Hua et al. 2007)
Lattice Boltzmann Method 1

- Lattice-Boltzmann method is based on the simulation of discrete fluid elements in order to predict the macroscopic flow system.
- The LBM is very robust and suitable for complex geometries.
- The basic variable of the Boltzmann statistics is the distribution function $f(x, v, t)$ which declares the number of fluid elements having the velocity $v$ at the location $x$ and time $t$:
- Macroscopic properties are related to the moments of the probability function:

$$m = \int \int f(x, v, t) \, d^3x \, d^3v$$

$$\rho(x, t) = \int f \, d^3v$$

$$\rho(x, t) \, u(x, t) = \int v \, f \, d^3v$$
Lattice Boltzmann Method 2

- Boltzmann equation (rate of change due to transport and collision) with single relaxation approach (Bhatnagar Gross Krook (BGK) equation):

\[
\left( \frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla \right) f(x, \mathbf{v}, t) = -\frac{1}{\tau} \left( f(x, \mathbf{v}, t) - f^{(0)}(x, \mathbf{v}, t) \right)
\]

\( \tau = 0.515 \)

- The Lattice Boltzmann equation (post collision distribution) arises from the discretisation of the BGK equation in time, space and velocity:

\[
f^{\sigma i}_t(x + v^{\sigma i} \Delta t, t + \Delta t) - f^{\sigma i}_t(x, t) = -\frac{\Delta t}{\tau} \left( f^{\sigma i}_t(x, t) - f^{(0)}^{\sigma i}(x, t) \right)
\]

Propagation term

Collision term

- Macroscopic properties, discretised:

\[
\rho(x, t) = \sum_\sigma \sum_i f^{\sigma i}_t(x, t)
\]

\[
\rho(x, t) u(x, t) = \sum_\sigma \sum_i v^{\sigma i}_t f^{\sigma i}_t(x, t)
\]

\( v^{\sigma i}_t = \frac{\Delta x^{\sigma i}}{\Delta t} \)
Lattice Boltzmann Method 3

- Discrete velocity vectors of the D3Q19 model:

- Three-dimensional
- Spatial discretisation by regular grid (voxels)
- 19 discrete velocity directions
- Sequential solution:
  - Propagation step
  - Collision step

Velocity vectors in the different directions:

\[
\mathbf{v}_{\sigma i} = \left\{ \begin{array}{ll}
(0,0,0), & \sigma = 0, \quad i = 1 \\
(\pm 1,0,0)c, (0,\pm 1,0)c, (0,0,\pm 1)c & \sigma = 1, \quad i = 1 \ldots 6 \\
(\pm 1,\pm 1,0)c, (\pm 1,0,\pm 1)c, (2,\pm 1,\pm 1)c, & \sigma = 2, \quad i = 1 \ldots 12 
\end{array} \right.
\]

Lattice constant

\[
c = \frac{\Delta x}{\Delta t}
\]

\[
v_{\sigma i} = \frac{\Delta x_{\sigma i}}{\Delta t}
\]
Lattice Boltzmann Method 4

- Discrete equilibrium distribution function (Maxwellian distribution for Kn << 1):

\[
f^{(0)}_{\sigma i}(x, t) = \omega_\sigma \left( 1 + \frac{3v_{\sigma i} \cdot u(x, t)}{c^2} + \frac{9(v_{\sigma i} \cdot u(x, t))^2}{2c^4} - \frac{3u^2(x, t)}{2c^2} \right)
\]

- Pressure (equation of state):

\[
p(x, t) = \rho(x, t) \cdot c_s^2
\]

\[
c_s = \frac{c}{\sqrt{3}}
\]

- From a series expansion around the equilibrium distribution (Chapman-Enskog-Expansion) the dependence of the viscosity on the relaxation parameter (e.g. \( \tau = 0.515 \) follows:

\[
\nu = \frac{kT}{mT} \left( \tau - \frac{\Delta t}{2} \right) \quad \Rightarrow \quad \nu = \frac{1}{6} c^2 (2\tau - \Delta t)
\]
Standard wall boundary condition:

Curved wall boundary condition:

Local grid refinement:

Forces over a particle are obtained from a momentum balance (reflection of the fluid elements)

6 Cells per Agent Particle
Validation: Particle Sitting on a Wall under Shear Flow

**Moving Wall**

INLET  

OUTLET  

Non-Slip

Resolution: 40 grid cells of the finest mesh

**Domain Size**

- \( x/D = 18, y/D = 18, z/D = 18 \)
- Three refinement regions

**Re_S = 0.02**

\[
\text{Re}_S = \frac{\rho \, D_P \, G}{\mu}
\]

\( CD \) vs. \( \text{Re}_S \)

\( z / D \) vs. \( x/D = 18, y/D = 12 \)

- **Saffman**
- **Leighton & Acrivos**
- sim. Derksen & Larsen
- sim. Zeng et al.
- correlation Zeng et al.
- present LBM

Resolution: 40 grid cells of the finest mesh
Lattice-Boltzmann simulations are performed for a carrier particle (100 µm) randomly covered with the drug particles (3, 5 or 10 µm); Cui et al. 2014:

The particle cluster is centrally fixed in a cubic domain

Re < 100: X = 7.8·D_{carrier}; Y = Z = 6.5·D_{carrier}
Re > 100: X = 10.4·D_{carrier}; Y = Z = 9.1·D_{carrier}

Determination of fluid forces on the drug particles for flow conditions obtained by RANS calculations
Flow Structure at Different Re

Present simulations

Re = 16

Re = 32

Re = 100

Re = 200

Measurement of Taneda

Re = 17.9

Re = 37.7

Re = 104

Re = 202
- Total force on all the fine particles in dependence of position angle for four different random distributions (colored dots) and resulting polynomial fitting curve (Re = 100, coverage degree 50 %, \( \frac{D_{\text{fine}}}{D_{\text{carrier}}} = 5/100 \)).

![Graph showing the force on drug particles depending on position angle with data points and polynomial fit.](image)
Different Reynolds Number

- Fitting curves for the normal force on fine particles as a function of position angle for different Reynolds numbers (coverage degree 50 %, \(D_{\text{fine}}/D_{\text{carrier}} = 5/100\))

\[ F_{\text{vdW}} \approx 35 \text{ nN} \]

Fitting curve:
- \(Re = 70\)
- \(Re = 140\)
- \(Re = 200\)

Direct lift-off is not likely to occur, hence detachment occurs by sliding or rolling.
Flow Resistance of Agglomerates

Resistance coefficients for different agglomerates (Dietzel & So 2013):

<table>
<thead>
<tr>
<th>Agglomerate type</th>
<th>Aerodynamic coefficient [-]</th>
</tr>
</thead>
<tbody>
<tr>
<td>L_30</td>
<td>160</td>
</tr>
<tr>
<td>C_30</td>
<td>100</td>
</tr>
<tr>
<td>VES</td>
<td>80</td>
</tr>
</tbody>
</table>

- agglomerates with identical volume equivalent diameter
- 30 primary particles
- 50 grids per volume equivalent size
- porosity of convex hull (dendrite: 0.78, compact: 0.57)
- Reynolds number of agglomerate: 0.3

Drag and lift coefficient $c_d$, $c_l$:

- Sphere
- Agg_O1
- Agg_O2
- Agg_O3
- Agg_O4

Graph showing the distribution of drag and lift coefficients for different agglomerates.
Direct numerical simulations (DNS) for dispersed turbulent two-phase flows by considering the particles as point-particles and using a Lagrangian approach to simulate the dispersed phase (all real particles).

- The grid needs to resolve all turbulence structures (i.e. Kolmogorov scale).
- The calculations are limited to smaller flow Reynolds numbers.
- The particles need to be smaller than the grid size and smaller than the Kolmogorov scale.
- The equation of motion needs to be solved by accounting for all relevant particle forces (generally Stokes flow).
- DNS has been applied mainly to basic turbulence research, in order to analyse the particle behaviour in turbulent flows and to derive closure relations or modelling approaches.
Direct Numerical Simulation (DNS): ⇒ time-dependent solution of the three-dimensional conservation equations by resolving the smallest turbulent scales.

⇒ Continuity equation: \[
\frac{\partial \rho}{\partial t} + \frac{\partial (\rho \, u_i)}{\partial x_i} = 0
\]

⇒ Momentum equations: \[
\frac{\partial (\rho \, u_i)}{\partial t} + \frac{\partial (\rho \, u_j \, u_i)}{\partial x_j} = -\frac{\partial p}{\partial x_i} - \frac{\partial \tau_{ij}}{\partial x_j} + S_{p,u_i} + \rho \, g_i
\]

⇒ Stress tensor: \[
\tau_{ij} = -\mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) + \frac{2}{3} \mu \frac{\partial u_j}{\partial x_j} \delta_{ij}
\]

⇒ Kronecker symbol: \[
\delta_{ij} = \begin{cases} 
1 & \text{if } i = j \\
0 & \text{if } i \neq j
\end{cases}
\]

Particle source terms are obtained from all fluid dynamic forces acting on all particles in a control volume.
Direct numerical simulations (96^3) on turbulence modification by particles in isotropic turbulence (Bovin et al. 1998):

Re_λ = 62
L_f = 0.02 m
T_E / τ_K = 10
(τ_{12}^F / τ_K)_φ=0 = 1.26, 4.49, 11.38

Turbulent kinetic energy

Particle dissipation

Dissipation rate

St
Analysis of particle preferential accumulation in homogeneous isotropic turbulence (Scott and Shrimpton 2007):

- Domain size: $64^3$
  - Enstropy
  - Velocity field

$St = 0.25$

$St = 4.0$
The numerical calculation of industrial flow processes is generally based on the Reynolds-averaged Navier-Stokes (RANS) equations.

Turbulence modelling (e.g. $k-\varepsilon$ turbulence model, Reynolds-stress model)

Approaches for dispersed multiphase flows:
Modelling Strategy

- With reduced complexity of the numerical method used, the modelling (closure) requirements are increasing:

  Particle resolved simulations (full DNS) → RANS methods with point particles

  **Increased modelling**

- **Modelling approach:**

  - **Modelling of micro-physical phenomena:**
    - non-spherical particles
    - particle-wall collisions
    - droplet coalescence
    - bubble break-up

  - Experimental studies

  - Direct numerical simulations

- **The resulting analytical and/or empirical models have to be implemented and validated based on detailed experiments.**
Two-Fluid Approach 1

Euler/Euler approach (two-fluid approach)

- Both (multiple) phases are treated as interpenetrating continua.
- The properties of the dispersed phase have to be averaged for the control volumes ($D_p << \Delta x$).
- Similar sets of conservation equations are obtained for both phases, allowing for identical solution algorithms.
- Requires considerable modelling work to describe the relevant micro-physics (closure of the conservation equations):
  - Interaction between the phases
  - Turbulent dispersion of particles (fluid-particle correlation)
  - Wall collisions of particles (wall roughness effect)
- The consideration of size distributions requires the solution of several sets of conservation equations (for each phase).
- Numerical diffusion at particle phase boundaries may result in errors.
- This approach is especially suitable for high volume fractions of the dispersed phase.
- The two-fluid approach might be also coupled to a population balance.
Classification of multi-fluid models:

**Mixture Models**

- **Drift flux model:**
  - The slip between the phases is calculated by analytical correlations

- **Homogeneous model:**
  - All phases share the same velocity field (no slip)

**Complete Multi-Fluid Model**

- **Reduced turbulence model:**
  - Turbulence model only for the continuous phase
  - The fluctuation energy of the dispersed phase is related to the fluid turbulence by appropriate correlations

- **Multiphase turbulence model:**
  - For each phase conservation equations are solved for the turbulence properties including coupling
The averaging of the conservation equations for a multiphase flow results in the following set of equations (Simonin 2000):

**Continuity equations:**

\[
\frac{\partial}{\partial t} (\alpha_f \rho_f) + \frac{\partial}{\partial x_i} (\alpha_f \rho_f U_i) = 0
\]

\[
\frac{\partial}{\partial t} (\alpha_n \rho_n) + \frac{\partial}{\partial x_i} (\alpha_n \rho_n U_{n,i}) = C(m_n)
\]

Mass transfer due to collision/coalescence

**Momentum equation continuous phase:**

\[
\alpha_f \rho_f \frac{\partial U_{f,i}}{\partial t} + \alpha_f \rho_f \frac{\partial U_{f,j}}{\partial x_j} = - \frac{\partial P}{\partial x_i} + \mu \frac{\partial^2 U_{f,i}}{\partial x_j x_j} - \alpha_f \rho_f \frac{\partial}{\partial x_j}(u'_{f,i} u'_{f,j}) - \sum_{N} \alpha_n \rho_n \frac{F_{Pi}}{m_n}
\]
Momentum equation dispersed phase:

\[
\alpha_n \rho_n \frac{\partial U_{n,i}}{\partial t} + \alpha_n \rho_n U_{n,j} \frac{\partial U_{n,i}}{\partial x_j} = -\rho_n \frac{\partial P}{\partial x_i} - \frac{\partial}{\partial x_j}\left(\alpha_n \rho_n \overline{u'_{n,i} u'_{n,i}}\right)
\]

\[+ C(m_n u'_{n,i}) + \alpha_n \rho_n g_i + \alpha_n \rho_n \frac{F_{n,i}}{m_n}\]

Momentum transfer due to drag force:

\[
\overline{F_{n,i}} = \frac{18 \mu_f f_D}{\rho_p D_p^2} m_p \left\{ (U_{f,i} - U_{n,i}) + V_{n,i} \right\}
\]

Turbulent dispersion described by drift velocity:

\[
V_{n,i} = -D_{fn,ij} \left[ \frac{1}{\alpha_n} \frac{\partial \alpha_n}{\partial x_j} - \frac{1}{\alpha_f} \frac{\partial \alpha_f}{\partial x_j} \right]
\]
Diffusion coefficient:

\[ D_{fn,ij} = \tau_{fn} \overline{u'_{f,i} u'_{n,j}} \]

Integral time scale of turbulence seen by the particles (Csanady):

\[ \tau_{fn}^l = \frac{T_L}{\sqrt{1 + C_\beta \xi_r^2}} \]

\[ \tau_{fn}^\perp = \frac{T_L}{\sqrt{1 + 4 C_\beta \xi_r^2}} \]

\[ \xi_r = \frac{\Delta \bar{u}}{\sqrt{\frac{2}{3} k}} \]

\[ C_\beta = 0.45 \]

Requires information on turbulent integral time scale
Simple correlations for stationary homogeneous isotropic turbulence:

Fluid-Particle velocity correlation:

\[
\overline{u'_{f,i} u'_{n,j}} = 2 \overline{u'_{f,i} u'_{f,j}} \left\{ \frac{\eta_r}{1 + \eta_r} \right\}
\]

Kinetic energy of particle fluctuating motion:

\[
\overline{u'_{n,i} u'_{n,j}} = \overline{u'_{f,i} u'_{f,j}} \left\{ \frac{\eta_r}{1 + \eta_r} \right\}
\]

In the case of more complex two-phase flows additional transport equations for both properties have to be solved.

Simonin, 1991, 2000
Numerical computation of a bubbling fluidised bed with the two-fluid approach (see Sommerfeld 2013).

- $d_p \sim 140\mu m$
- $\rho_p/\rho_g \sim 11000$
- $U_g \sim 2.5m/s$
- $\Delta x = 30cm$
- $\Delta x = 14cm$
- $\Delta x = 10cm$
- $\Delta x = 3cm$
• The fluid flow is calculated by solving the Reynolds-averaged Navier-Stokes equations (or LES) with an appropriate turbulence model.
• The dispersed phase is simulated by tracking a large number of particles through the flow field (representative particles).
• A statistically reliable determination of the particle phase properties and source terms requires a large number of particles to be tracked.
• This method is a hybrid approach and requires coupling iterations between Eulerian and Lagrangian part.
• The particles are point-particles which have to be considerably smaller then the size of the grids ($D_P << \Delta x$).
• The particle size distribution may be considered with good resolution.
• The relevant micro-processes may be:
  ⇒ Wall collisions of particles
  ⇒ Inter-particle collisions and agglomeration
  ⇒ Droplet/bubble coalescence and break-up
• For high particle concentration the standard approaches may cause considerable convergence problems.
Euler/Lagrange Approach 2

Fluid flow; continuous phase (Sommerfeld 1996; Lain & Sommerfeld 2012):

General form of the conservation equations in connection with the k-ε turbulence model:

\[ \frac{\partial}{\partial t} (\sigma_f \phi) + \frac{\partial}{\partial x_j} (\sigma_f U_j \phi) = \frac{\partial}{\partial x_j} \left( \Gamma \frac{\partial \phi}{\partial x_j} \right) + S_{\phi} + S_{\phi P} \]

\[ \sigma_f = (1 - \alpha_P) \rho \]

effective density

<table>
<thead>
<tr>
<th>( \phi )</th>
<th>( S_{\phi} )</th>
<th>( S_{\phi P} )</th>
<th>( \Gamma_{\phi} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>-</td>
<td>0</td>
<td>-</td>
</tr>
<tr>
<td>( U_i )</td>
<td>( \frac{\partial}{\partial x_j} \left( \Gamma_{U_i} \frac{\partial U_j}{\partial x_i} \right) - \frac{\partial p}{\partial x_i} + \rho g_i )</td>
<td>( S_{U_i, P} )</td>
<td>( \mu + \mu_t )</td>
</tr>
<tr>
<td>( k )</td>
<td>( G_k - \rho \varepsilon )</td>
<td>( S_{k, P} )</td>
<td>( \mu + \frac{\mu_t}{\sigma_k} )</td>
</tr>
<tr>
<td>( \varepsilon )</td>
<td>( \frac{\varepsilon}{k} \left( C_1 G_k - C_2 \rho \varepsilon \right) )</td>
<td>( S_{\varepsilon, P} )</td>
<td>( \mu + \frac{\mu_t}{\sigma_\varepsilon} )</td>
</tr>
</tbody>
</table>

\[ G_k = \mu_t \left( \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) \frac{\partial U_i}{\partial x_j} \]

\( \mu_t = C_\mu \rho \frac{k^2}{\varepsilon} \)

constants

\( C_\mu = 0.09 \)
\( C_1 = 1.44 \)
\( C_2 = 1.92 \)
\( \sigma_k = 1.0 \)
\( \sigma_\varepsilon = 1.0 \)

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Dispersed phase: The Lagrangian approach is based on tracking a large number of representative particles through the flow field considering all relevant forces.

\[
\frac{d\vec{x}_p}{dt} = \vec{u}_p
\]

\[
m_p \frac{d\vec{u}_{p,i}}{dt} = \frac{3}{4} \frac{\rho}{\rho_p D_p} m_p C_D \left( u_i - u_{p,i} \right) |\vec{u} - \vec{u}_p| + \frac{\rho_F}{2} \frac{\pi}{4} D_p^2 C_{LS} D_p \left( (\vec{u}_F - \vec{u}_p) \times \vec{\omega}_F \right) + \frac{\rho_F}{2} \frac{\pi}{4} D_p^2 C_{LR} \left| \vec{u}_F - \vec{u}_p \right| \frac{\vec{\Omega} \times (\vec{u}_F - \vec{u}_p)}{|\vec{\Omega}|} + m_p g \left( 1 - \frac{\rho}{\rho_p} \right) + F_i
\]

1. drag force
2. slip-shear lift
3. slip-rotation lift
4. gravity/ buoyancy
5. other forces, e.g. electrostatic

Models elementary processes:
- turbulent dispersion
- particle-rough wall collision
- inter-particle collisions

Rotation:
\[
I_p \frac{d\vec{\omega}_p}{dt} = \frac{\rho_F}{2} \left( \frac{D_p}{2} \right)^5 C_R \left| \vec{\Omega} \right| \cdot \vec{\Omega}
\]
Two-way coupling approach for stationary flows

Under-relaxation of source terms:

\[ S_{\phi P}^{i+1} = (1 - \gamma) S_{\phi P}^i + \gamma S_{\phi P}^{i+1\text{(calculated)}} \]

Under-relaxation of the source terms improves convergence behaviour !!! (Kohnen et al. 1994)

Euler/Lagrange Approach

Eulerian Part
Calculation of the fluid flow without particle phase source terms

Lagrangian Part
Tracking of parcels without inter-particle collisions, Sampling of particle phase properties and source terms

Eulerian Part
Calculation of the fluid flow with particle phase source terms:
- Converged Solution
- Solution with a fixed number of iterations

Lagrangian Part
Tracking of parcels with inter-particle collisions, Sampling of particle phase properties and source terms

Coupling Iterations

Convergence two-way coupling

Output:
Flow field, Particle-phase statistics

Under-relaxation of the source terms improves convergence behaviour !!! (Kohnen et al. 1994)

Under-relaxation of the source terms improves convergence behaviour !!! (Kohnen et al. 1994)

Under-relaxation of the source terms improves convergence behaviour !!! (Kohnen et al. 1994)
Numerical methods for multiphase flows were subdivided into three classes:

- Full DNS methods resolving the particles; or for interfacial systems.
- Methods for dispersed multiphase flows with point particle approximation (DNS, LES and RANS).
- Discrete particle methods (e.g. DPM and DEM) for dense particle systems (with and without flow).

Particle resolved numerical simulations (full DNS) become increasingly important for analysing micro-physical phenomena and providing results for modelling.

Point-particle DNS is mainly used for turbulence studies.

For analysing or optimising processes of technical relevance, RANS approaches are still very important (i.e. Euler/Euler and Euler/Lagrange).

However, the importance of LES is continuously increasing.

The Lagrangian approach has considerable advantages in modelling elementary processes and is preferred for systems with particle size distributions.