Particle-Particle Collision Model for Dispersed Gas-Particle Flows: Implementation and Validation

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Outline

• Introduction – modelling of dispersed gas-solid flows
• Stochastic particle-particle collision model – overview
• Algorithm of the collision model
• Validation of the collision model
  – Test case description
  – Comparison with experimental results
• Summary and advisable extensions
Modelling of highly loaded dispersed gas-particle flows

- Two common techniques for dispersed gas-solid flows:
  - Euler-Euler
  - Euler-Lagrange

- Euler-Lagrange model is suitable only for dilute flows
  - two-way coupling

- For highly loaded gas-solid flows, four-way coupling is essential
  - interaction gas ↔ particle
  - momentum transfer between particles → collisions
  - realisation by the presented model
Stochastic particle-particle collision model

- Sequential trajectory calculation
- Presence of neighbouring particles is taken into account
- Creation of a **virtual** collision partner according to local statistical mean particle properties
- Calculation of a collision probability
- Random process decides whether or not a collision takes place
- If it occurs the collision is calculated deterministically

- Enormous computational effort by simultaneous tracing of all particles is avoided
- Collision model is of iterative nature
Requirements for applicability

- High mass loading
- moderate volumetric concentration (<~ 20%)
- Only binary collisions
  - inter-particle distance $\gg$ particle diameter
  - aerodynamic forces dominate
  - not suitable for fluidised beds
  - $\rho_P \gg \rho_{\text{Gas}}$
- Spherical particles

Stochastic particle-particle collision model, requisites
Algorithm of the collision model (1)

- **Navier-Stokes solver**
- **Lagrange solver**
  - **next trajectory**
  - **current trajectory**

- **all trajectories calculated?**
  - yes
  - no
    - **current trajectory complete?**
      - yes
      - no

- **averaging procedure**
  - yes
  - no

- **Collision model subroutine, User FORTRAN**
Algorithm of the collision model (2)

- instantaneous velocity $P_2$
- collision frequency
- collision probability
- local time step
- collision?
  - yes
  - sliding
  - non-sliding
- new velocities
- old velocities

Collision model subroutine, User FORTRAN
- position $P_2$
- deterministic calculation of collision

Stochastic particle-particle collision model, algorithm
Algorithm of the collision model (3)

Navier-Stokes solver → Lagrange solver →

- instantaneous velocity P2
- collision frequency
- collision probability
- local time step
- collision?
  - yes
  - no → old vel’s

Collision model subroutine, User FORTRAN

- position P2
- deterministic calculation of collision
  - yes
  - no → sliding
  - non-sliding

- yes
  → all trajectories calc.ed?
  - yes
  - no → current trajectory complete?
  - yes
  - no → averaging procedure
Instantaneous velocity of the virtual particle P2

- Velocity of P2 comprises:
  - a mean part from the local average values
  - a fluctuating part including a correlation term between the two particles due to Sommerfeld [3,4] and a random term

\[ v'_{2,i} = R(St_t) \, v'_{1,i} + \sigma_{P,i} \sqrt{1 - R(St_t)^2} \xi \]

  - correlation function is determined by LES of a homogeneous isotropic turbulence field

\[ R(St_t) = \exp \left( -0.55 \, St_t^{0.4} \right) \]

- Angular velocity of the particle is calculated the same way
  - no correlation between particles
Collision frequency, probability and time step

- Collision frequency depends on:
  - particle number density \( n_p \)
  - diameters of real and fictitious particle
  - instantaneous velocities of both particles

\[
f_c = \frac{\pi}{4} \left( d_{P1} + d_{P2} \right)^2 |\vec{v}_1 - \vec{v}_2| \, n_P
\]

- Collision probability → function of collision frequency and time step

\[
P_c = 1 - \exp(-f_c \Delta t)
\]

  - decision by means of a uniformly distributed random number

- Lagrangian time step → limited for stability and accuracy reasons

\[
\Delta t \leq 0.05 \frac{1}{f_c}
\]
Position of the collision partner

- Stochastic determination
- Probability equally distributed over cross section

Deterministic calculation of the collision

- Distinction between sliding and non-sliding collision
- Determination of transferred momentum
Implementation in ANSYS CFX

• User Fortran subroutine in FORTRAN 77
• Link to the CFX solver by an interface provided by ANSYS
• Four-way coupling is made available for gas-solid flows
• The model is contained in the next version of CFX (11, Beta-status)

Current limitation

• No particle rotational motion
• Simplified particle-wall collision treatment
• If this aspect is improved in future → inter-particle collision model will account for angular velocities
Validation by experiment of Fohanno & Oesterlé [6]

- Experiment was arranged exactly for this purpose
- Enforced crossing of trajectories
- Flow induced by gravitation
- Glass particles, $d_P = 3$ mm
- $\rho_P = 2500$ kg/m³
- Collision effects dominate
Comparison of particle trajectories:

Particle trajectories without / with collision model
Comparison of particle number density (with collision model):

- Small mass flow rate, $\alpha = 6.5 \cdot 10^{-4}$
  - 3 measuring planes
  - Particle streak velocimetry (2D optical method)

- Large mass flow rate, $\alpha = 1.9 \cdot 10^{-3}$

Particle number density at small / large particle mass flow rate
Grid refinement study and Lagrangian time step

• Coarse grid: 10500 elements, 30000 trajectories
• Fine grid: 620000 elements, 480000 trajectories
• Lagrangian time step depends on grid refinement
• Accuracy of variable fields is improved

• For equally good statistic → number of trajectories quadratic in number of elements
Measurement error and concentration profiles

- Estimated measuring error:
  - 10-13% for mean values
  - 15-20% for standard deviations
- Particle concentration profiles from measurement & simulation:
  - for small and large mass flow rate
  - main source of error: inaccurate particle-wall treatment

Comparison of results: experiment and simulation – concentration profiles
Particle axial mean velocity profiles

- Reason for deviations:
  - Favourable downward flow of air in the simulation → reduction of drag and faster downstream of particles
  - Inadequate particle-wall collision treatment

Comparison of results: axial mean velocity profiles of particles

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Particle velocity standard deviation in transverse direction

- Deviation in plane A not allegeable by inaccurate particle-wall collision treatment
  - intense air turbulence or
  - non-uniform particle supply → explanation but improbable
    → likely caused by measurement errors
- Differences in planes B and C → lower trajectory crossing point
- Fluctuations decrease with increasing mass flow rate

Comparison of results: velocity standard deviation in transverse direction
Particle absolute velocity in plane of visualisation

- Almost no decrease of absolute velocity in simulation
- Noticeable decline in experiments
  - 3D effects of inter-particle collisions
  - dissipation effects due to inelastic collisions
  - conversion of translational in rotational energy (most probable)
  - dependent on collision frequency

Comparison of results: absolute velocity in plane of visualisation
Scatter plot of particle velocity fluctuations (exp.)

- Plane A: 2 types of trajectories:
  - vertically falling: → 2\textsuperscript{nd} quadrant
  - oblique rebounding from wall: → 4\textsuperscript{th} quadrant
- Panes B & C: 3 types of trajectories, symmetry:
  - vertically falling: → centre
  - rebounding from both walls: → off-centre
- Plane C: considerable scatter
  - homogenisation of particle flow due to collisions

Experimental results: particle velocity fluctuations, small mass flow rate
Scatter plot of particle velocity fluctuations (exp. & sim.)

Comparison of results: scatter plots of particle velocity fluctuations

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Summary and advisable extensions (1)

• Application of a collision model for highly loaded dispersed gas-particle flows is indispensable
• Qualitatively correct prediction of
  – particle velocity profiles
  – homogenisation of the particle flow
  – attenuation of velocity fluctuations
  – influence of the mass flow rate
• Deviations due to
  – insufficiently accurate particle-wall collision modelling
  – no particle rotation
  – no rotation induced lift force (Magnus-effect)
  – no shear induced lift force (Saffman-force)
Summary and advisable extensions (2)

- Comparison with simulations by Pachler [7] of the same experiment including particle rotation shows a slight improvement of the results.


- In flows dominated by particle-wall collisions, particle rotation should be included, as the 3 other validation cases accomplished suggest.

- Providing of detailed results in scope of engineering accuracy.

- Distinct advancement without enhancing the effort considerably.
Stochastic particle-particle collision model

- Model was derived by Oesterlé & Petitjean [1,2]
- Extension to consideration of correlated particle motions by Sommerfeld [3,4]
- Detailed formulation by Frank [5]

Further test cases

- Test case 2: Vertical pipe flow by Tsuji et al. [8]
- Test case 3: Rectangular particle laden jet flow by Sommerfeld [9]
- Test case 4: Swirling particle laden flow by Zhou et al. [10]


Further test cases for validation

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