Comparison of an Energy-based and a Momentum-based Agglomeration Model within an Euler-Lagrange LES Approach

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Universität der Bundeswehr Hamburg

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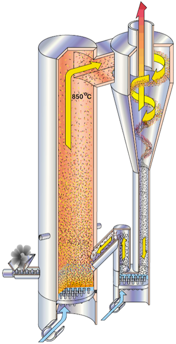
Halle (Saale), Germany

PfS

Turbulent Particle-Laden Flows

- Industrial applications
- Medical technology
- Natural phenomena



Fluidized bed

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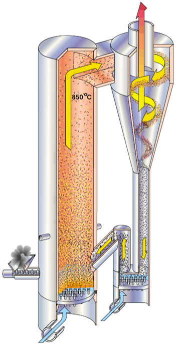

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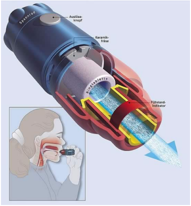

Inhalation spray

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- Medical technology
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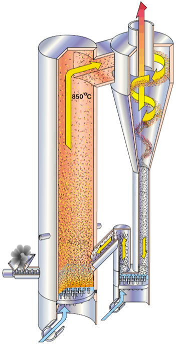

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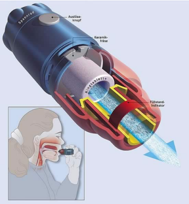
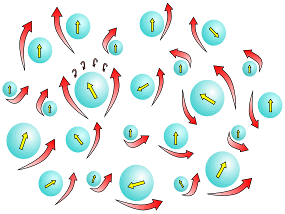


Inhalation spray

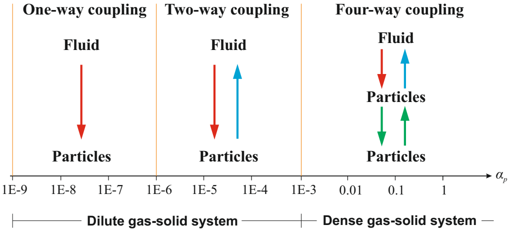
Dust storm

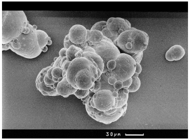
Complex Flow Dynamics

- Gas-particle interaction
- Particle-gas interaction (feedback)
- Particle-particle collision
- Agglomeration of cohesive particles



Turbulent particle-laden flow





Real agglomerate

(Sommerfeld, MVT Website)

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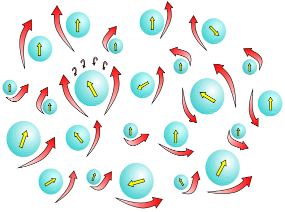

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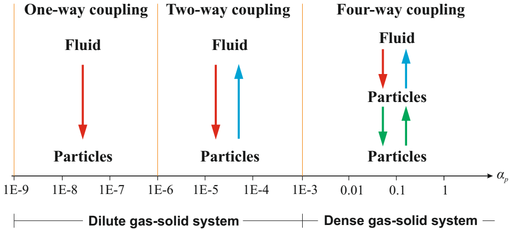

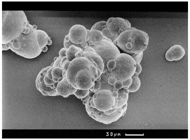

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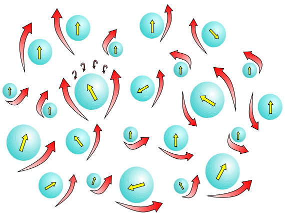

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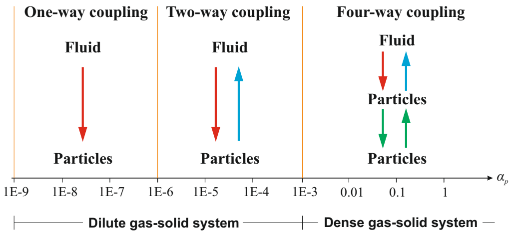

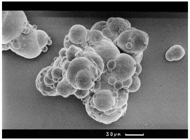

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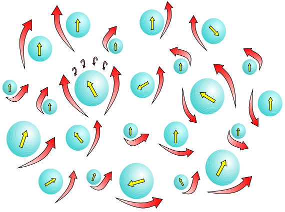

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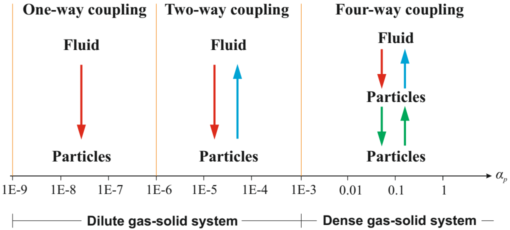
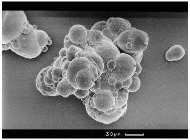




Real agglomerate

(Sommerfeld, MVT Website)

Motivation

- Relevance of turbulent particle-laden flows to processes employed in a wide range of applications
- Advanced understanding of the complex flow behavior in the context of particle dispersion and agglomeration
- Flexibility and cheapness of the numerical simulations in comparison with experiments
- Advanced predictive technique for describing fluid motion, Large–Eddy Simulation, coupled with a deterministic collision model
- Extension of our in-house code $\mathcal{LESOCC}$ to include particle agglomeration

Objectives

- **Modeling**
  - Particle agglomeration
  - Kinetics of the resulting agglomerate
  - Structure of the agglomerate
- **Implementation**
  - CFD-code $\mathcal{LESOCC}$
  - Testing based on simple test cases
- **Validation**
  - Laminar shear flow
  - Turbulent channel flow

CONTINUOUS PHASE

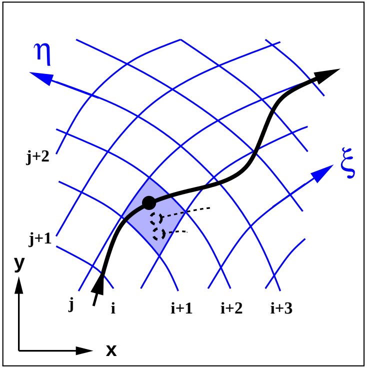
- **LESOCC** (**L**arge **E**ddy **S**imulation **O**n **C**urvilinear **C**oordinates)
- **Navier–Stokes solver** (incompressible fluid)
- **3D Finite volume method**
  - ☞ Curvilinear body–fitted coordinate system
  - ☞ Non–staggered (cell–centered) grid arrangement
  - ☞ Block–structured grids
- **Spatial discretization**
  - ☞ Viscous fluxes: central differences $O(\Delta x^2)$
  - ☞ Convective fluxes: five different schemes, central diff. $O(\Delta x^2)$
- **Temporal discretization**
  - ☞ Predictor step (momentum eqns.): low–storage Runge–Kutta scheme, $O(\Delta t^2)$
  - ☞ Corrector step (pressure–correction equation): SIP solver (ILU)
- **Pressure–velocity coupling:** Momentum interpolation of Rhie & Chow
- **Various subgrid-scale and wall models**
- **High–performance computing techniques:** Vectorized & parallelized

DISPERSED PHASE

Dispersed Phase

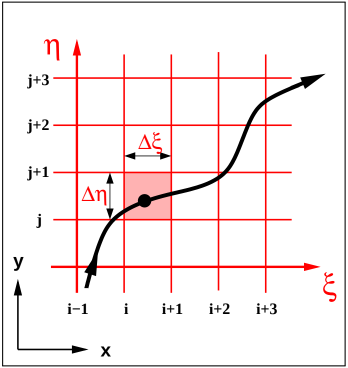
- **Modeling assumptions**
  - Lagrangian frame of reference for the dispersed phase
  - High density ratio $\rho_p/\rho_f \gg 1$
  - Drag, gravity, buoyancy and lift forces
  - High volume fraction: Two– and four–way coupling
- **Newton's second law**
  - $\dfrac{d\boldsymbol{u}_p}{dt} = \dfrac{\boldsymbol{u}_f - \boldsymbol{u}_p}{\tau_p/\alpha} + \boldsymbol{g}\left(1 - \dfrac{\rho_f}{\rho_p}\right) + \dfrac{F_L}{m_p}$
  - $\dfrac{d\boldsymbol{\omega}_p}{dt} = -\dfrac{10}{3\,\tau_p}\boldsymbol{\Omega}_{rel}$ with $\boldsymbol{\Omega}_{rel} = \dfrac{1}{2}\nabla \times \boldsymbol{u}_f - \boldsymbol{\omega}_p$
  - $\dfrac{d\boldsymbol{x}_p}{dt} = \boldsymbol{u}_p$

Physical Space



- Curvilinear grid
- Point location not trivial
- Time-consuming local and global search algorithms

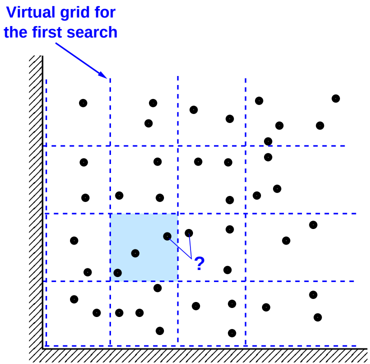
Computational Space



- Orthonormal grid
- Point location trivial
- No search of particle's new position required

Particle Tracking: C–Space vs. P–Space

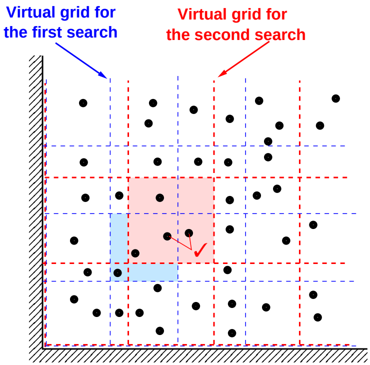
Particle-Particle Collision Detection



Likely collision partners in virtual cells

(First Search)

Particle-Particle Collision Detection



Likely collision partners in virtual cells

(Second Search)

- Only particles in a virtual cell are checked for collisions
- Second search to find closest particles in neighboring cells
- Reduction of computational effort from $\mathcal{O}(N_p^2)$ to $\mathcal{O}(N_p)$

Hard-Sphere Model

- Spherical rigid particles
- Particle deformation neglected
- Friction obeys Coulomb's law

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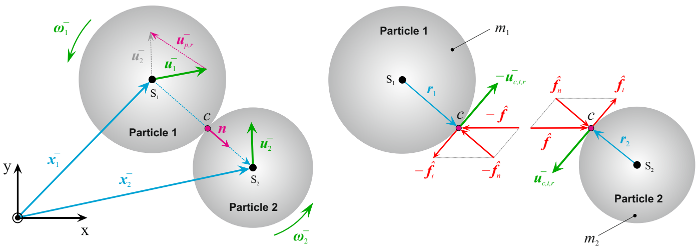
Particle-Particle Collision



Collision is possible

$(u_2 - u_1) \cdot n < 0$

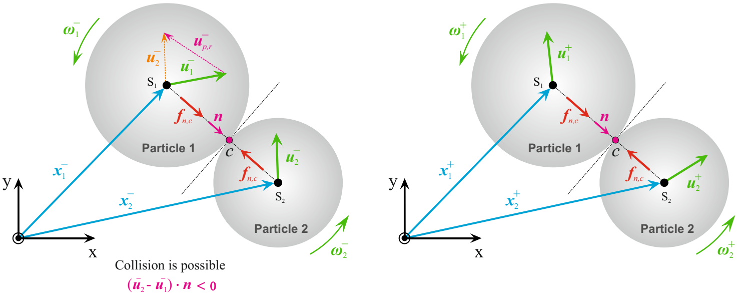
Particle Agglomeration

- **Modeling assumptions**
  - Hard-sphere model
  - Dry, electrostatically neutral particles
  - Van-der-Waals force
  - Spherical agglomerates
- **Agglomeration models**
  - Momentum-based agglomeration model
  - Energy-based agglomeration model

MOMENTUM-BASED AGGLOMERATION MODEL (MAM)

Normal component of the total impulse

$$\hat{\boldsymbol{f}}_n = \underbrace{\hat{\boldsymbol{f}}_{n,a}}_{\text{Repulsive Impulse}} + \underbrace{\hat{\boldsymbol{f}}_{n,c}}_{\text{Cohesive Impulse}}$$



[1] **Breuer, M., Almohammed, N.**: *Modeling and simulation of particle agglomeration in turbulent flows using a hard–sphere model with deterministic collision detection and enhanced structure models*, Int. J. of Multiphase Flow **73**, 171–206, (2015).

Collision Type

- **No-slip condition**

$$\left|\boldsymbol{u}_{c,t}^{-}\right| \leq \frac{7}{2}\,\frac{\mu_{st,w}}{1+e_{t,w}}\,\left(\hat{f}_{n,a}+\hat{f}_{n,c}\right)$$

$\rightarrow$ Cohesive impulse enhances the friction at the contact point

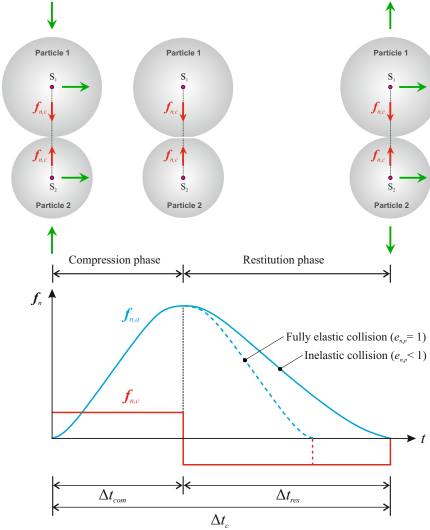
- **Sticking collision**

  Collision partners stick to each other

- **Sliding collision**

  Collision partners slide over each other

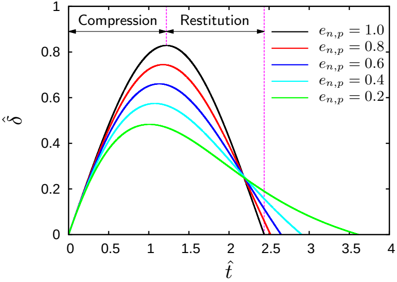
Modeling of the Cohesive impulse



$$\hat{f}^*_{n,c} = \underbrace{\frac{1}{\hat{m}} \int f_{n,c}\, dt}_{\text{Compression}} + \underbrace{\frac{1}{\hat{m}} \int f_{n,c}\, dt}_{\text{Restitution}}$$

$$\hat{f}^*_{n,c} = -\frac{1}{\hat{m}} f_{n,c} \, \Delta t^*_c$$

with: $\Delta t^*_c = \Delta t_{res} - \Delta t_{com}$



Agglomeration Conditions [1]

- **Limiting impulse**

$$\hat{f}_{l,n} = \hat{\boldsymbol{f}}_l \cdot \boldsymbol{n} = -(\boldsymbol{u}_2^- - \boldsymbol{u}_1^-) \cdot \boldsymbol{n}$$

$$\hat{f}_{l,t} = \hat{\boldsymbol{f}}_l \cdot \boldsymbol{t} = -(\boldsymbol{u}_2^- - \boldsymbol{u}_1^-) \cdot \boldsymbol{t}$$

- **Sticking collision** → One condition

$$\hat{f}_{l,n} > \hat{f}_{n,a} + \hat{f}^*_{n,c} \Rightarrow -\hat{f}^*_{n,c} > -e_{n,p} (\boldsymbol{u}_2^- - \boldsymbol{u}_1^-) \cdot \boldsymbol{n}$$

- **Sliding collision** → Two conditions

$$\hat{f}_{l,n} > \hat{f}_{n,a} + \hat{f}^*_{n,c} \quad \& \quad \left|\hat{f}_{l,t}\right| < \left|\hat{f}_t\right|$$

$|\hat{f}_t|$ has to be large enough to stop the particle from further sliding.

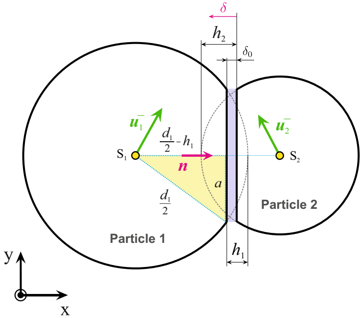
ENERGY-BASED

AGGLOMERATION MODEL

(EAM)

Energy-based Agglomeration Model [2]

- First proposed by Hiller (1981)
- Applied by Sommerfeld and Ho (2002), Ho (2004)
  - Head-on frictionless collision
  - $\Delta E_{\text{vdW}} \geq E^{+}_{kin,r}$
- Extended by Alletto (2014)
  - Inclusion of rotation and friction
  - $\Delta E_{\text{vdW}} \geq E^{+}_{kin,r} + E^{+}_{rot} - E_{rot,ag}$
  - Rebound in either the normal or the tangential direction
- Improved by Almohammed and Breuer [2]

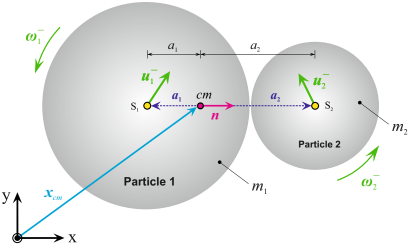


[2] **Almohammed, N., Breuer, M.**: *Modeling and simulation of agglomeration in turbulent particle-laden flows: A comparison between energy-based and momentum-based agglomeration models*, Powder Technology, submitted, (2015).

- **Position and velocity**

$$\boldsymbol{x}_{ag}^{+} = \frac{m_1 \boldsymbol{x}_1^{-} + m_2 \boldsymbol{x}_2^{-}}{m_1 + m_2}$$

$$\boldsymbol{u}_{ag}^{+} = \frac{m_1 \boldsymbol{u}_1^{-} + m_2 \boldsymbol{u}_2^{-}}{m_1 + m_2}$$



- **Angular momentum**

$$\boldsymbol{L}_{ag} = I_1\,\boldsymbol{\omega}_1^{-} + I_2\,\boldsymbol{\omega}_2^{-} + \frac{\hat{m}}{2}(d_1 + d_2)\,\boldsymbol{n} \times (\boldsymbol{u}_2^{-} - \boldsymbol{u}_1^{-})$$

- **Angular velocity**

$$\boldsymbol{L}_{ag} = [I_{ag}]\,\boldsymbol{\omega}_{ag} \quad ; \quad [I_{ag}] = \begin{pmatrix} I_{xx} & I_{xy} & I_{xz} \\ I_{yx} & I_{yy} & I_{yz} \\ I_{zx} & I_{zy} & I_{zz} \end{pmatrix}$$

Agglomerate Structure Models [1]

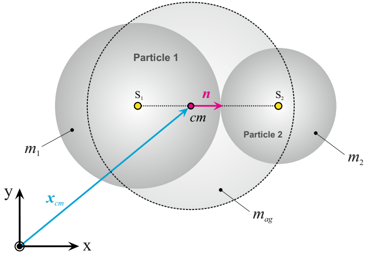
1. **Volume-equivalent Sphere Model (VSM)**
2. Inertia-equivalent Sphere Model (ISM)
3. Closely-packed Sphere Model (CSM)

$$\boldsymbol{\omega}_{ag} = \frac{\boldsymbol{L}_{ag}}{I_{ag}}$$

$$I_{ag} = \frac{1}{10}\, m_{ag}\, d_{ag}^2$$

$$m_{ag} = m_1 + m_2$$

$$d_{ag} = \sqrt[3]{d_1^3 + d_2^3}$$



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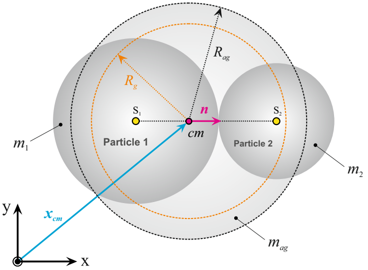
$$\boldsymbol{\omega}_{ag} = \frac{\boldsymbol{L}_{ag}}{I_{ag}} \quad ; \quad I_{ag} = \frac{1}{10}\, m_{ag}\, d_{ag}^2$$

$$\frac{2}{3} m_{ag} R_g^2 = \frac{2}{5} m_{ag} R_{ag}^2$$

$$d_{ag} = \sqrt{20/3}\, R_g \quad ;$$

$$\rho_{ag} = \frac{\rho_1\, d_1^3 + \rho_2\, d_2^3}{d_{ag}^3} \neq \rho_1$$



Structure Models [1]

1. Volume-equivalent Sphere Model (VSM)
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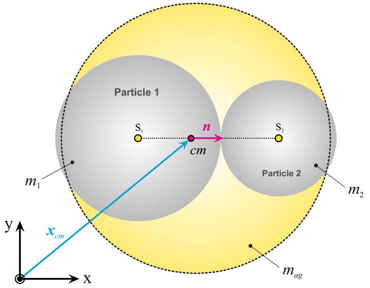
3. **Closely-packed Sphere Model (CSM)**

$$\boldsymbol{\omega}_{ag} = \frac{\boldsymbol{L}_{ag}}{I_{ag}} \quad ; \quad I_{ag} = \frac{1}{10}\, m_{ag}\, d_{ag}^2$$

$$\rho_{ag} = f_{pack}\, \rho_o \quad \text{with:} \quad 0 < f_{pack} < 1$$

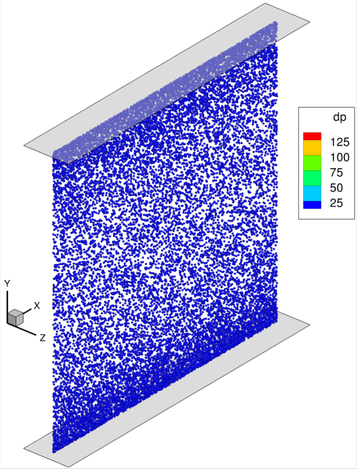
$$f_{pack} = \frac{V_{sphere}}{V_{cube}}$$

$$d_{ag} = \left(\frac{\rho_1\, d_1^3 + \rho_2\, d_2^3}{\rho_{ag}} \right)^{1/3}$$



2D Laminar Shear Flow [3]

- Constant shear rate $\dot{\gamma} = 71\ \mathrm{s}^{-1}$
- $2\delta \times 2\delta \times \delta$ ($\delta = 0.0195$ m)
- $64 \times 64 \times 10$ grid points
- Periodic boundary conditions in x- and z-direction
- No-slip condition on the wall
- $20,140$ primary particles with $d_p = 25\,\mu$m



[3] **Balakin, B., Kosinski, P., Hoffmann, A. C.**: *The collision efficiency in a shear flow*, Chemical Engineering Science **68**, 305–312, (2012).

Zeroth Moment of Particle Size Distribution

$$M_0(t) = \frac{M_0(0)}{1 + 0.5\,\beta K M_0(t) t}$$

1. **Theoretical Model**
2. Numerical Results

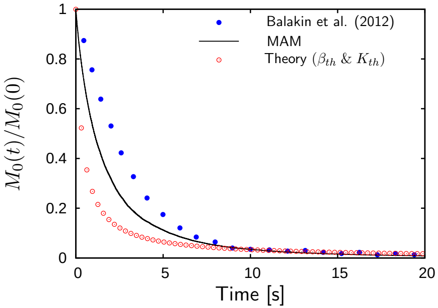
- **Agglomeration rate**

$$\beta = \beta_{th}^{*} = f(\bar{\lambda}) \left(\frac{8\,H}{36\pi\mu\dot{\gamma}d_0^3} \right)^{0.18}$$

- **Collision frequency**

$$K^{**} = \frac{\dot{\gamma}}{\pi} \left(V_1^{1/3} + V_2^{1/3} \right)^3$$

$$K_{th} = 4/3\,\dot{\gamma}\,(d_0)^3$$



(van de Ven and Mason, 1977)*

(Saffman and Turner, 1956) **

Zeroth Moment of Particle Size Distribution

$$M_0(t) = \frac{M_0(0)}{1 + 0.5\,\beta K M_0(t) t}$$

1. Theoretical Model
2. **Numerical Results**

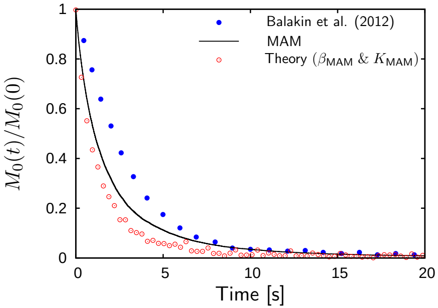
- **Agglomeration rate**

$$\beta = \beta_{\mathsf{MAM}}$$

- **Collision frequency**

$$K^{**} = \frac{\dot{\gamma}}{\pi}\left(V_1^{1/3} + V_2^{1/3}\right)^3$$

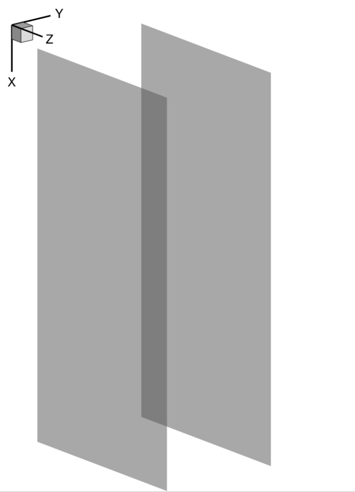
$$K_{\mathsf{MAM}} = \frac{\dot{\gamma}}{\pi N_{col}} \sum_{i=1}^{N_{col}} \left(V_{1,i}^{1/3} + V_{2,i}^{1/3}\right)^3$$



(Saffman and Turner, 1956) **

3D Turbulent Channel Flow [1,2]

- Re = 11,900 ($Re_\tau = 644$)
- $2\pi\delta \times 2\delta \times \pi\delta$ ($\delta = 0.02$ m)
- $128 \times 128 \times 128$ grid points
- Periodic boundary conditions in x- and z-direction
- No-slip condition on the wall
- 6×10^6 primary particles with $d_p = 4$ and $12\,\mu$m
- Elastic particle-particle and particle-wall collisions with friction
- Smooth and rough walls



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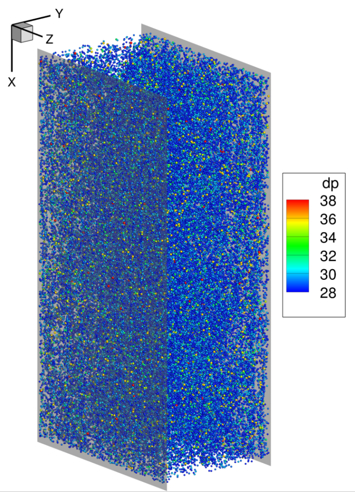
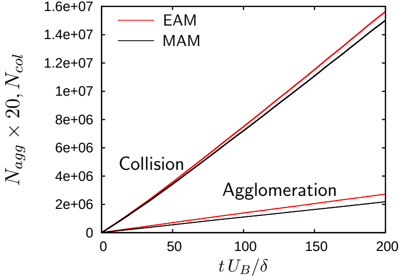
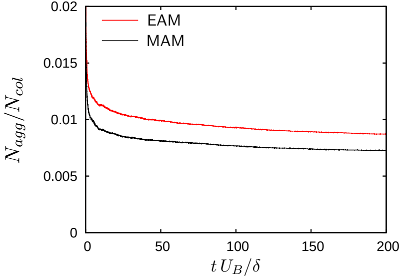
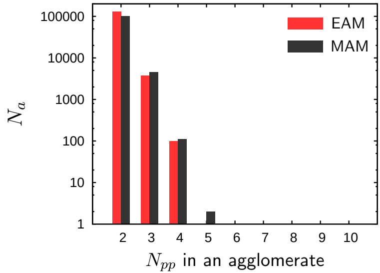








In comparison with MAM, EAM predicts:

- Higher N_{col} and N_{agg}
- Higher agglomeration rate
- Greater N_a of two-particle agglomerates

Comparison of Agglomeration Models

Submodels (SMs)

- **Two-way Coupling**

  Feedback effect of the particles on the continuous phase

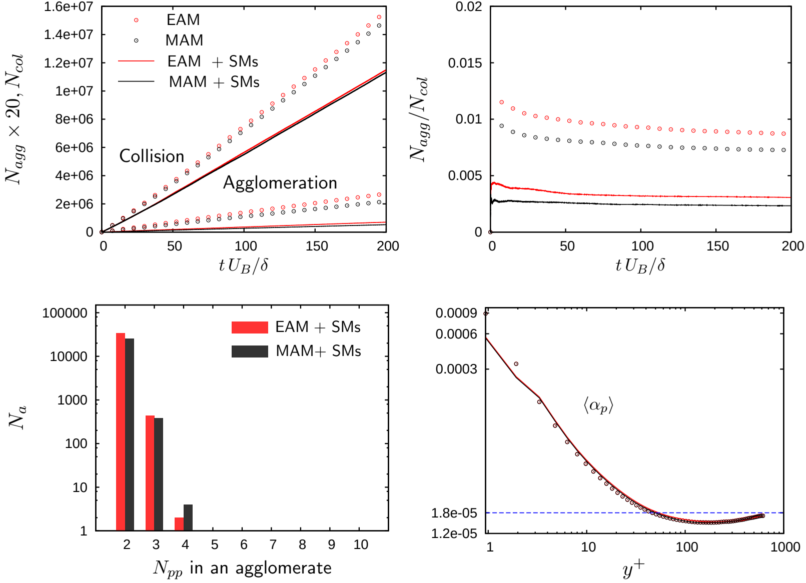
$$f_i^{PSIC} = -\sum_{k=1}^{N_p} \frac{F_{D,i}}{\Delta Vol} = -\sum_{k=1}^{N_p} \frac{3\,\mu_f\,\pi\,d_p\,\alpha\,(u_{f,i}-u_{p,i})}{\Delta Vol}$$

- **Lift forces**
  - Saffman force
  - Magnus force
- **Subgrid-scale model for the particles**

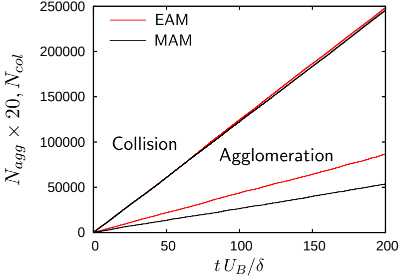
  Effect of the unresolved scales within LES on particle motion

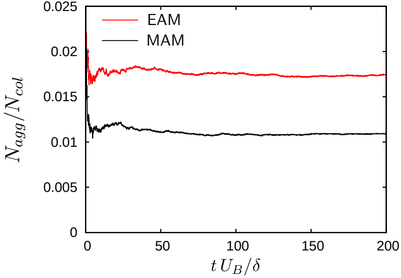
$$\boldsymbol{u}_f = \overline{\boldsymbol{u}}_f + \boldsymbol{u}'_f \qquad \text{with} \quad \boldsymbol{u}'_f = \sqrt{\frac{2}{3} k_{SGS}}\, \boldsymbol{\xi}$$

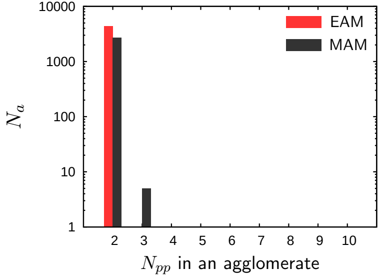
$$k_{SGS} = \frac{1}{2}\left(\overline{\boldsymbol{u}}_f - \overline{\overline{\boldsymbol{u}}}_f\right)^2$$



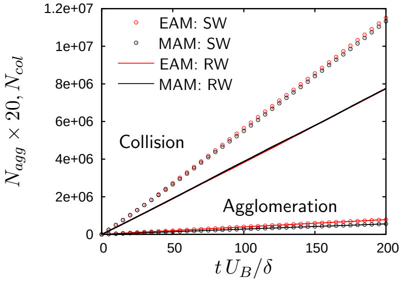
Comparison of Agglomeration Models with Submodels

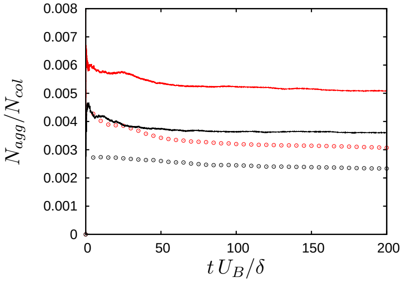


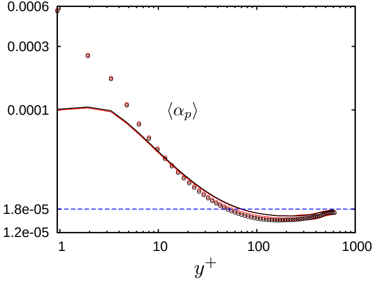




- Similar trends as for large particles
- Higher ΔE_{vdW} and cohesive impulse
- Higher agglomeration rate







- Significant reduction of N_{col}
- Lower volume fraction in the near-wall region
- Higher agglomeration rate by EAM than MAM

1. **Introduction**
2. **Numerical Methodology**
   - Continuous Phase
   - Dispersed Phase
3. **Modeling of Particle Agglomeration**
   - Momentum-based Agglomeration Model
   - Energy-based Agglomeration Model
4. **Model Validation**
   - Shear flow
   - Turbulent Channel Flow
5. **Conclusions and Outlook**

Conclusion

- Improvement of two agglomeration models in the framework of a hard-sphere model
- Proposal of two structure models for an agglomerate
- Successful validation of the MAM in a shear flow
- Application of both agglomeration models in turbulent particle-laden channel flow
- Prediction of similar trends of the physical behavior of the agglomeration process by both agglomeration models
- MAM is superior to EAM due to accurate results and the reduced necessity of empirical parameters

Outlook

- Validation of the agglomeration models with experimental test cases (e.g., shear layer by Ho (2004))
- Comparison with other numerical test cases
- Investigation of the effect of deposition on the walls
- Inclusion of liquid bridge
- Investigation of the effect of deposition on the walls
- Break-up of particles or agglomerates

Thanks for your attention

Acknowledgments

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All kinds of support are gratefully acknowledged.


time for questions

Calculation Procedure [2]

- Collision without considering the van-der-Waals force
- Cohesive impulse introduced based on the van-der-Waals interaction

$$\hat{\boldsymbol{f}}_{ag} = \hat{\boldsymbol{f}}_{ag,n} + \hat{\boldsymbol{f}}_{ag,t}$$

Difference of the van-der-Waals energy

- $\Delta E_{\mathrm{vdW}} = \dfrac{H}{12\,\delta_0^2}\, d_1^2\, d_2^2 \left|\boldsymbol{u}_2^- - \boldsymbol{u}_1^-\right| \left[\dfrac{\rho_1\,\rho_2\left(1 - e_{n,p}^2\right)}{6\,\bar{p}\,(d_1 + d_2)\,(\rho_1\, d_1^3 + \rho_2\, d_2^3)}\right]^{\dfrac{1}{2}}$
- Maximum contact pressure $\bar{p}$ may not be available in the literature.

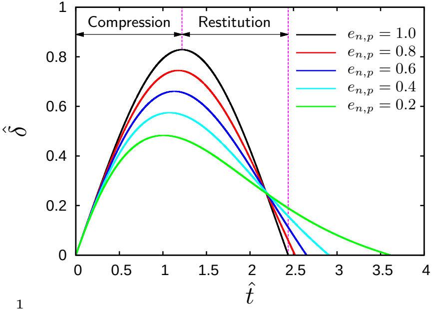
Overlap in the normal direction

$$\frac{d^2\hat{\delta}}{d\hat{t}^2} + 2\,\alpha\,\hat{\delta}^{1/4}\,\frac{d\hat{\delta}}{d\hat{t}} + \hat{\delta}^{3/2} = 0$$

$$\hat{t} = t\left(C^{-1/2} r^{1/2} K/m\right)^{1/2}$$

$$\hat{\delta} = C\,\delta/r$$

with: $C = r\left(\frac{K}{m\,u_n^2}\right)^{2/5}$



Cohesive impulse

$$\hat{f}^*_{n,c} = -0.196\left\{\frac{\hat{m}^{-3}}{\hat{E}^2\,(\boldsymbol{u}_1^- - \boldsymbol{u}_2^-)\cdot\boldsymbol{n}}\right\}^{\frac{1}{5}}\frac{H}{\delta_0^2}\,\hat{r}^{\frac{4}{5}}\,\Delta\hat{t}_{dif}$$