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Analysis of turbulent coagulation in a jet with discretised population balance and DNS

Presentation for the UKCTRF Conference 2021

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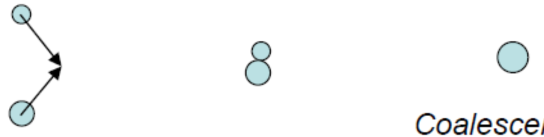
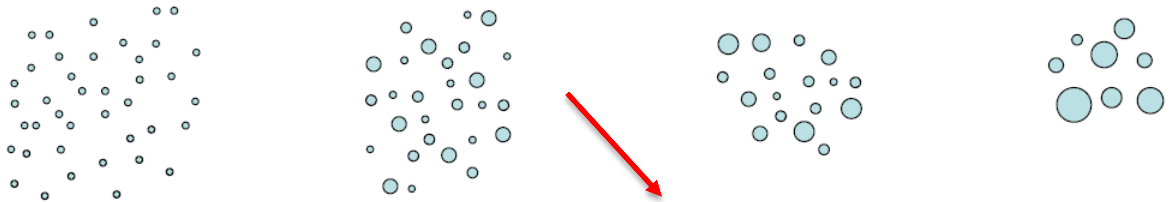
Coagulation

- ***Coagulation*** *is the process where spherical particles collide and form larger particles*
- Coagulation leads to fewer but larger particles ($N\downarrow$, $V_m\uparrow$)



Increasing time (t)



Monodisperse = particles of the same size

Increased polydispersity

Coagulation in turbulent flows

- Coagulation and particle growth are **key processes** in several applications
  - Atmospheric processes
  - Soot formation
  - Flame synthesis of silica S_iO_2 and titania TiO_2 nanoparticles
    - ↳ Coagulation → **dominant** mechanism *(Buesser & Pratsinis2012)*
- In most of the cases, particle coagulation and growth occur in turbulent flows
- Numerical simulations → powerful tool to:
  - Describe such complex phenomena (gain physical insight)
  - Design efficient systems in industrial processes (aerosol chambers)

Buesser, Beat & Pratsinis, Sotiris E2012 Design of nanomaterial synthesis by aerosol processes. Annual review of chemical and biomolecular engineering3, 103–127.

Objective of the study

- Coagulation involves **second-order interactions between particles** of different sizes (akin to **second-order reactions**) and unclosed terms arising from **turbulence-coagulation interaction** (akin to **turbulence-chemistry interaction**)
- Turbulence-coagulation interactions are studied via Direct Numerical Simulations (**DNS**) in a planar jet.
- Reynolds decomposition of the PBE leads to **unknown correlations**. We study the effect of these unknown correlations.
- Understanding of turbulence-coagulation interaction is important for developing accurate models for predicting particle-laden flows

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Governing equations

- **Navier-Stokes equations**

$$\frac{\partial u_j}{\partial x_j} = 0 \quad (1)$$

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{1}{\rho}\frac{\partial p}{\partial x_i} + \frac{\mu}{\rho}\frac{\partial^2 u_i}{\partial x_j \partial x_j} \quad (2)$$

- Incompressible and isothermal flow is considered
- Non-inertial particles (follow pathlines)
- Particles do not affect the properties of the fluid (one way coupling)

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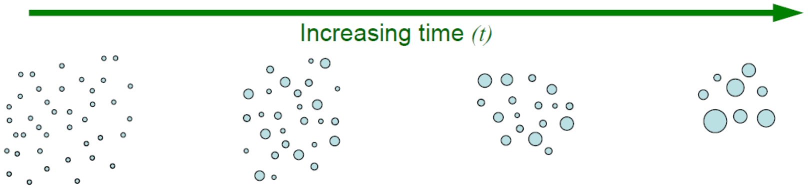
Governing equations



Increased polydispersity

- Concept of Particle Size Distribution (PSD) is introduced

  → number density $n(\boldsymbol{x}, v)$

- **Population Balance Equation** (PBE)

$$\frac{\partial n}{\partial t} + u_j \frac{\partial n}{\partial x_j} = \frac{\partial}{\partial x_j}\left(D_p \frac{\partial n}{\partial x_j}\right) + \frac{1}{2}\int_0^v \beta(w, v-w)n(w)n(v-w)dw - \int_0^\infty \beta(v,w)n(v)n(w)dw \qquad (3)$$

- Coagulation in the *free molecular regime* → $\beta(v, w)$

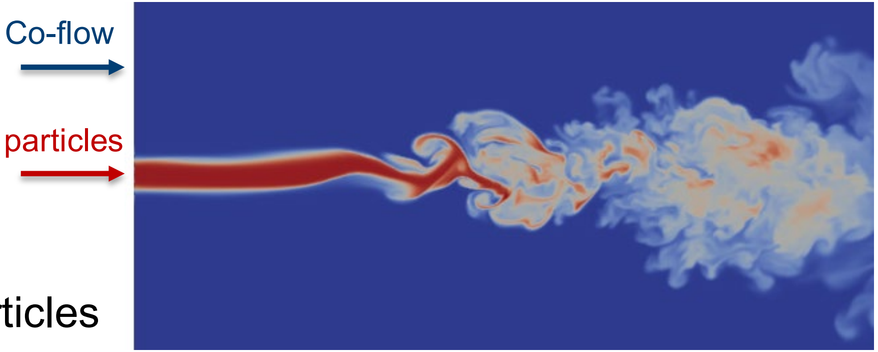
Numerical Method

- An inhouse finite volume CFD solver called "**PANTARHEI**" coupled with an inhouse code for particulate modelling called "**CPMOD**" was employed.
- A discretised (sectional) method was used for PBE *(Liu & Rigopoulos 2019)*
- The PSD is discretised in **35** intervals Δv_i or "bins"
- The PBE is converted into a system of partial integro-differential equations (we solve 35 transport equations with source terms)
- The actual PSD is obtained at each computational cell

Liu, Anxiong & Rigopoulos, Stelios2019 A conservative method for numerical solution of the population balance equation, and application to soot formation. Combustion andFlame205, 506–521.

Simulation Configuration

Evolution of M1



- Direct numerical simulations (DNS) of 3-D spatially developing **planar jet**
- The jet is laden with monodisperse nanoparticles and issues into a particle-free co-flow stream
- $Re = \frac{U_o\, h}{\nu} = \mathbf{3000}$, $\frac{U_\infty}{U_o} = 0.2$, $L_x \times L_y \times L_z = 25h \times 26h \times 5h$, # of cells = **52 million**
- Turbulent boundary conditions at the **inflow** (Klein's method)
- # of CPU hours = **84672** Cray XC30 hours (**1008** cores) for each simulation
- Two test cases. Simulations for $\boldsymbol{Da_{coag} = 1}$ and $\boldsymbol{Da_{coag} = 1/3}$ $\rightarrow Da_{coag} = \frac{\tau_{conv}}{\tau_{coag}}$

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2. Methodology
3. Results
4. Conclusions

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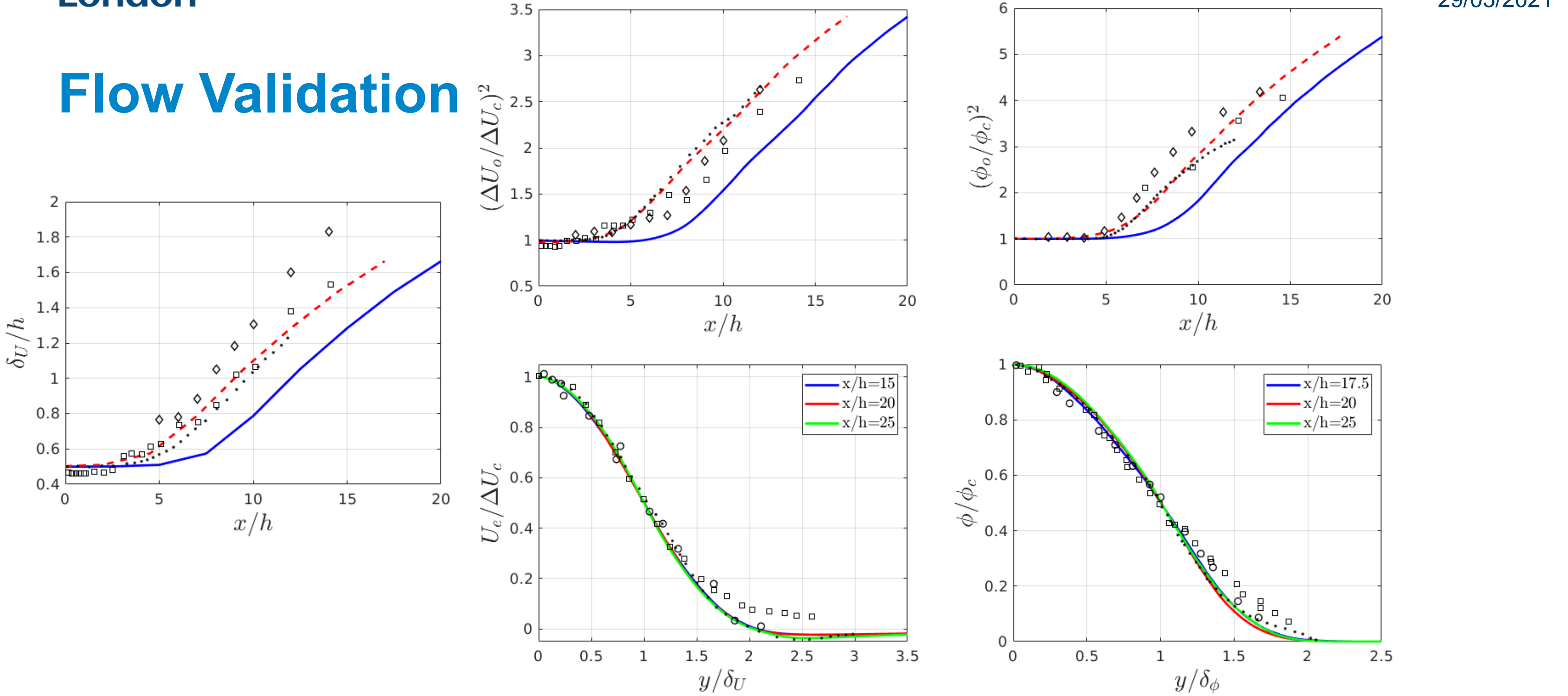
Flow Validation



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PSD Correlations

- Reynolds decomposing the PBE leads to unknown correlations.

$$\frac{\partial n}{\partial t}+u_j\frac{\partial n}{\partial x_j}=\frac{\partial}{\partial x_j}\left(D_p\frac{\partial n}{\partial x_j}\right)+\frac{1}{2}\int_0^v\beta(w,v-w)n(w)n(v-w)dw-\int_0^\infty\beta(v,w)n(v)n(w)dw \quad (3)$$

$$\boldsymbol{n}=\overline{\boldsymbol{n}}+\boldsymbol{n}' \quad (4)$$

$$\frac{\partial\bar{n}}{\partial t}+\bar{u}_j\frac{\partial\bar{n}}{\partial x_j}+\frac{\partial\left(\overline{u'_j n'}\right)}{\partial x_j}-\frac{\partial}{\partial x_j}\left(D_p\frac{\partial\bar{n}}{\partial x_j}\right)$$
$$=\frac{1}{2}\int_0^v\beta(w,v-w)\bar{n}(w)\bar{n}(v-w)dw-\int_0^\infty\beta(v,w)\bar{n}(v)\bar{n}(w)dw \quad (5)$$
$$+\frac{1}{2}\int_0^v\beta(w,v-w)\overline{n'(w)n'(v-w)}dw-\int_0^\infty\beta(v,w)\overline{n'(v)n'(w)}dw$$

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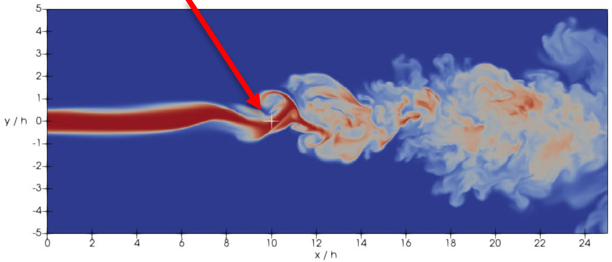
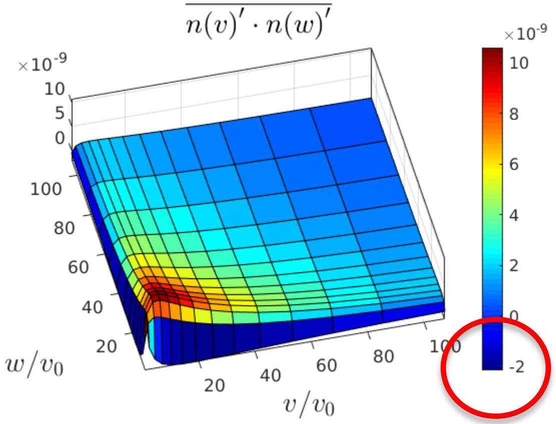
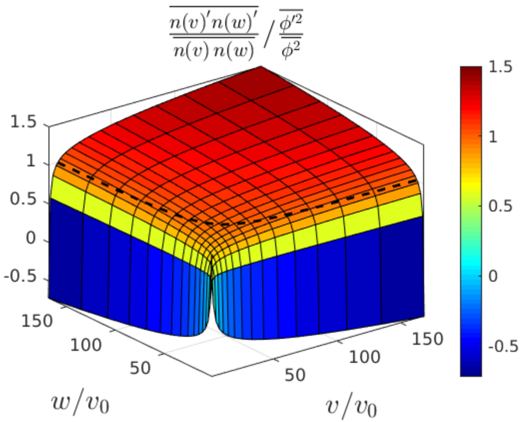
PSD Correlations

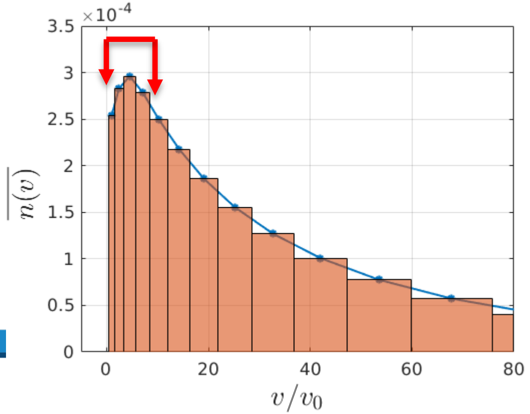
Point (10,0,0) , Da=1





- $\overline{n(v)' \cdot n(w)'}$ were mostly positive
- $\overline{n(v)' \cdot n(w)'} < 0$ close to the jet break-up point
- Were found for distant combinations of particle volumes (e.g., $\overline{n_1{}' \cdot n_4'}$, $\overline{n_1{}' \cdot n_5'}$, …)
- $\dfrac{\overline{n(v)' \cdot n(w)'}}{\overline{n(v)} \cdot \overline{n(w)}}$ receives rather uniform values close to that of the passive scalar.





Source Terms and Turbulent Fluctuations

- The same analysis is done also for the moments of the PSD

$$M_k = \int_0^{\infty} v^k \, n(v) dv \tag{6}$$

- $\boldsymbol{M_0} \equiv N$, $\boldsymbol{M_1} \equiv \Phi$, $\boldsymbol{M_2} \propto$ light scattering

$$\frac{\partial M_k}{\partial t} + u_j \frac{\partial M_k}{\partial x_j} = \frac{\partial}{\partial x_j}\left(D_p \frac{\partial M_k}{\partial x_j}\right)$$
$$+ \frac{1}{2} \iint_0^{\infty} (v+w)^k \, \beta(v,w) n(v) n(w) dv dw - \frac{1}{2} \iint_0^{\infty} \left(v^k + w^k\right) \, \beta(v,w) n(v) n(w) dv dw \tag{7}$$

Source Terms and Turbulent Fluctuations

- Reynolds decompositions of the transport equation of moments

$$\frac{\partial \overline{M_k}}{\partial t} + \bar{u}_j \frac{\partial \overline{M_k}}{\partial x_j} + \frac{\partial \left(\overline{u'_j M'_k}\right)}{\partial x_j} = + \frac{\partial}{\partial x_j}\left(D_p \frac{\partial \overline{M_k}}{\partial x_j}\right)$$
$$+ \frac{1}{2}\iint_0^\infty (v+w)^k \beta(v,w)\bar{n}(v)\bar{n}(w)dvdw - \frac{1}{2}\iint_0^\infty \left(v^k + w^k\right)\beta(v,w)\bar{n}(v)\bar{n}(w)dvdw \quad (8)$$
$$+ \frac{1}{2}\iint_0^\infty (v+w)^k \beta(v,w)\overline{n'(v)n'(w)}dvdw - \frac{1}{2}\iint_0^\infty \left(v^k + w^k\right)\beta(v,w)\overline{n'(v)n'(w)}dvdw$$

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Source Terms and Turbulent Fluctuations

- For $\boldsymbol{k} = \mathbf{0}$ $\rightarrow$

$$\underbrace{-\frac{1}{2}\iint_0^\infty \beta(v,w)\overline{n(v)n(w)}dvdw}_{\boldsymbol{A_0}} = \underbrace{-\frac{1}{2}\iint_0^\infty \beta(v,w)\bar{n}(v)\bar{n}(w)dvdw}_{\boldsymbol{B_0}} \quad \underbrace{-\frac{1}{2}\iint_0^\infty \beta(v,w)\overline{n'(v)n'(w)}dvdw}_{\boldsymbol{C_0}} \tag{9}$$

- Is $\boldsymbol{C_0}$ positive or negative in the domain**?**
- Can we neglect $\boldsymbol{C_0}$ **?** (common practise)

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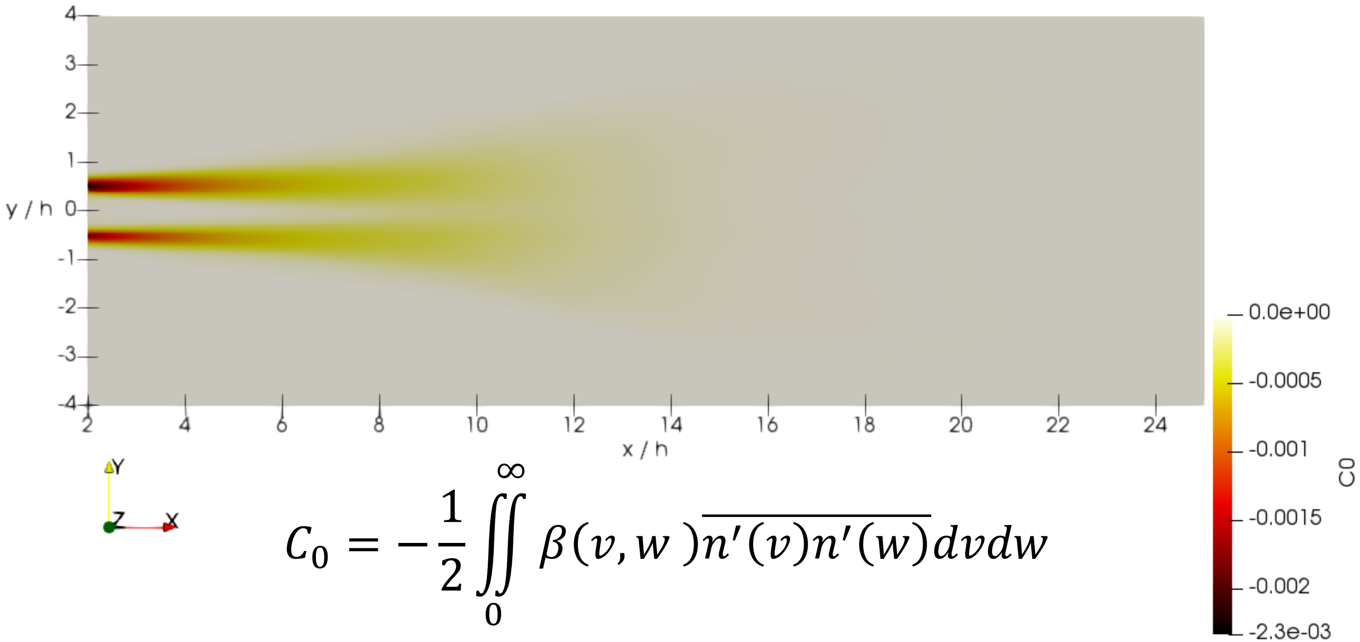
Source Terms and Turbulent Fluctuations

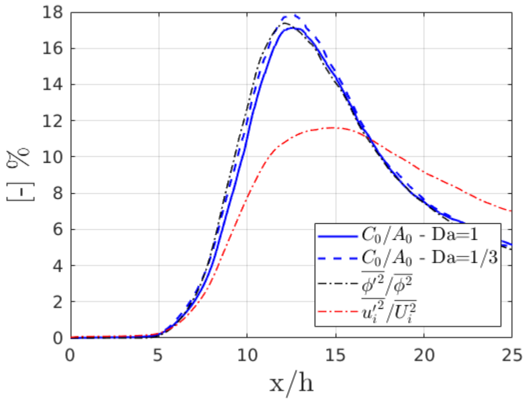
- $C_0 < 0$ found to be negative
- Neglect of this term leads to an overestimation of $\overline{M_0}$

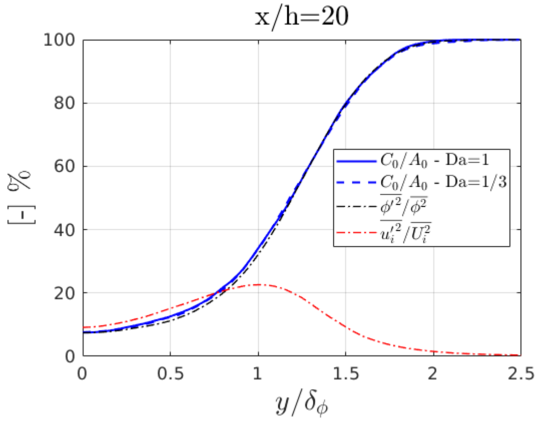


$$C_0 = -\frac{1}{2}\iint_0^\infty \beta(v,w)\overline{n'(v)n'(w)}\,dvdw$$

Source Terms and Turbulent Fluctuations

- How much is the ratio $\frac{C_0}{A_0}$? Can we neglect C_0 ? ➡ up to 40% at jet edges

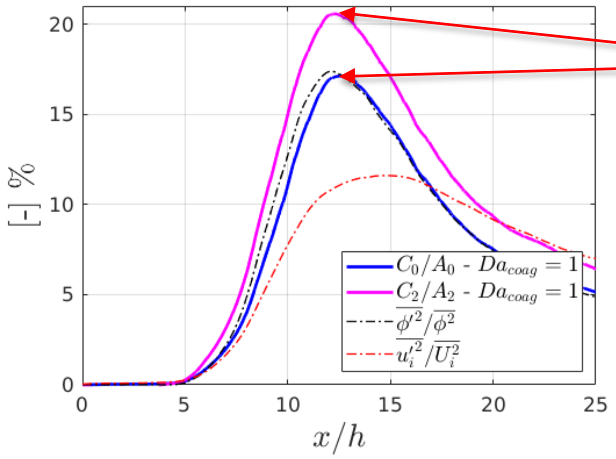




$$\underbrace{-\frac{1}{2}\iint_0^\infty \beta(v,w)\overline{n(v)n(w)}dvdw}_{A_0} = \underbrace{-\frac{1}{2}\iint_0^\infty \beta(v,w)\bar{n}(v)\bar{n}(w)dvdw}_{B_0} \underbrace{-\frac{1}{2}\iint_0^\infty \beta(v,w)\overline{n'(v)n'(w)}dvdw}_{C_0} \quad (9)$$

Source Terms and Turbulent Fluctuations

- For $\boldsymbol{k} = \mathbf{2}$ $\rightarrow$ $$\underbrace{\iint_0^\infty v\, w\beta(v,w)\overline{n(v)n(w)}dvdw}_{\boldsymbol{A_2}} = \underbrace{\iint_0^\infty v\, w\beta(v,w)\bar{n}(v)\bar{n}(w)dvdw}_{\boldsymbol{B_2}} \underbrace{+ \iint_0^\infty vw\beta(v,w)\overline{n'(v)n'(w)}dvdw}_{\boldsymbol{C_2}} \quad (10)$$
- $\boldsymbol{C_2} > 0$ found to be positive
- $\dfrac{\boldsymbol{C_2}}{\boldsymbol{A_2}} > \dfrac{\boldsymbol{C_0}}{\boldsymbol{A_0}}$
- It is attributed to the larger effect of coagulation on M_2 due to the heavier weighting of large particles on the PSD



18% difference

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Conclusions

- The effect of turbulent fluctuations on the coagulation process was studied by performing **DNS** of turbulent coagulation in a planar jet.
- The behaviour of the PSD correlations $\overline{\boldsymbol{n}'(\boldsymbol{v})\,\boldsymbol{n}'(\boldsymbol{w})}$ was studied. The correlations were mostly positive, but it was found that they can also take **negative values**.
- Turbulence-coagulation interaction leads to some unclosed terms in the transport equation of the 0^{th} and 2^{nd} moments. The behaviour of these terms was studied.
- The unclosed terms make a large contribution to the time-averaged coagulation source term and therefore **they cannot be neglected**.

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Thank You!

Contributors:

Dr Stelios Rigopoulos

Dr George Papadakis

Appendix

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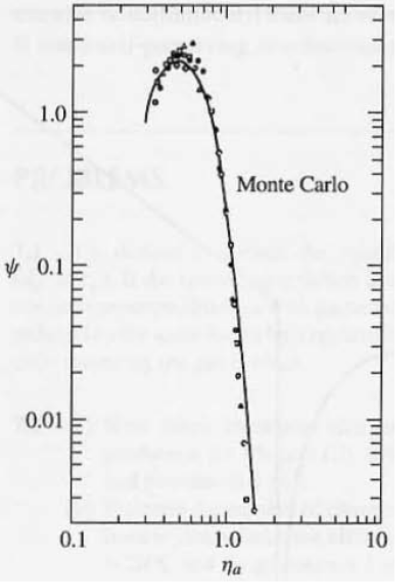
Governing equations

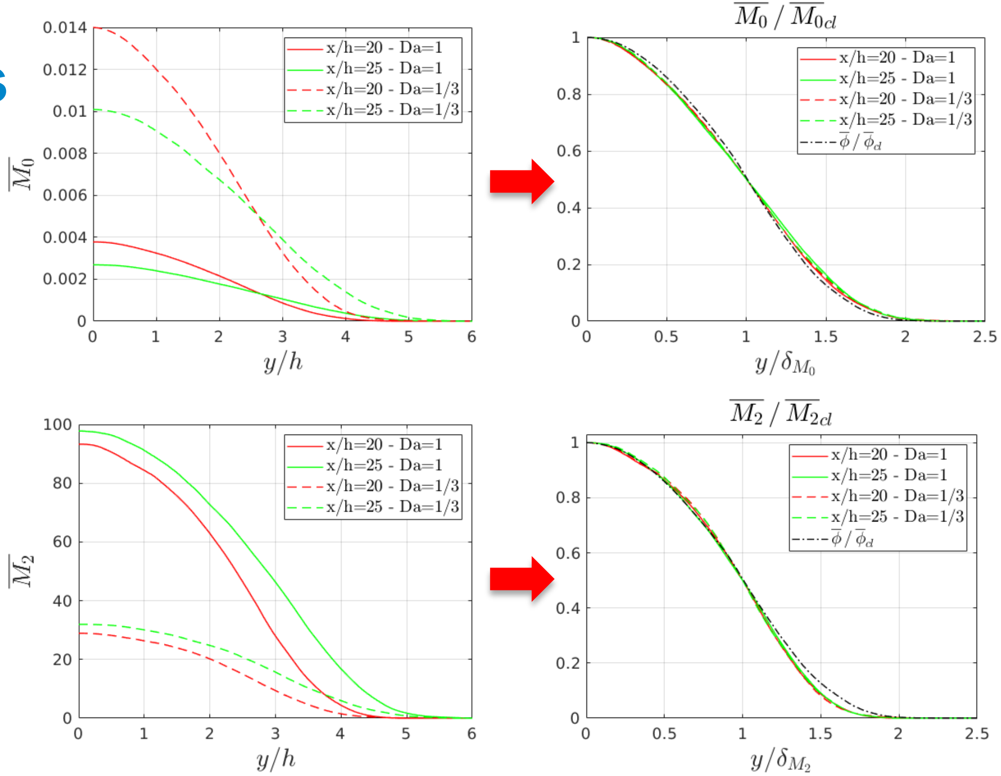
- PBE admits self-similar solutions when the variables are properly normalised for the case of pure coagulation.
- $$\tau_{SP} = \frac{5}{\left(\frac{3}{4\pi}\right)^{\frac{1}{6}}\left(\frac{6k_bT}{\rho_p}\right)^{\frac{1}{2}} v_o^{\frac{1}{6}}\ N_0}$$ Time to reach the self-preserving PSD
- $$\tau_{conv} = \frac{h}{U_o}$$ Convection time scale for planar jet
- $$\boxed{\boldsymbol{Da_{coag}} = \frac{\boldsymbol{\tau_{conv}}}{\boldsymbol{\tau_{SP}/5}}}$$ Coagulation Damköhler Number



(Friedlander, 2000)

Self-similarity of moments

- The cross-stream profiles collapse to a single curve under self-similarity scaling
- **Independent of the Da_{coag}**



Conclusions

- **DNS** of turbulent coagulation in a planar jet where performed.
- The behaviour of the PSD correlations $\overline{\boldsymbol{n}'(\boldsymbol{v})\,\boldsymbol{n}'(\boldsymbol{w})}$ was studied and it was found that they can also take negative values.
- Reynolds Decomposition of the transport equations of moments leads to some unclosed terms. These terms were found to make a large contribution to the mean source term and since **they cannot be neglected**.
- The cross-stream profiles of the **moments** for the case of coagulation become **self-similar** when they are properly normalised.