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Study of turbulent precipitation in a T-mixer with DNS and DPB

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Code used: Pantarhei

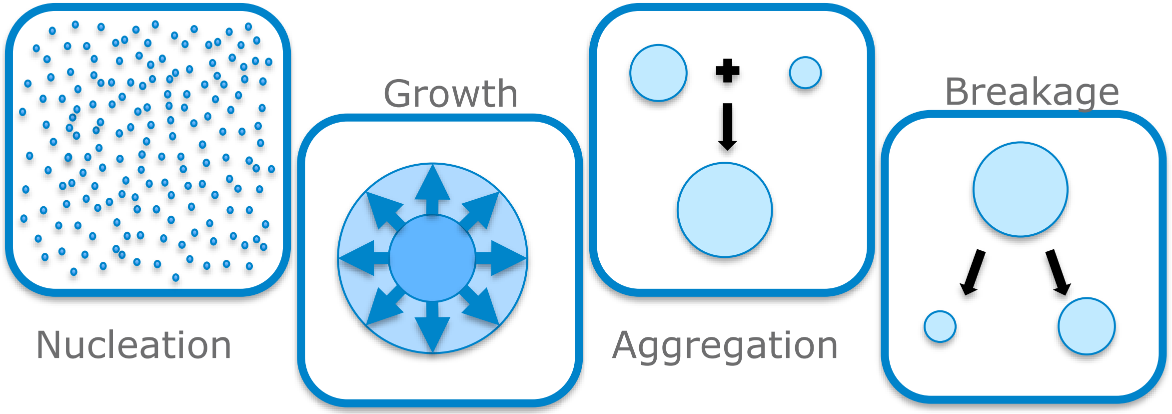
kAU used: 8000 kAUs

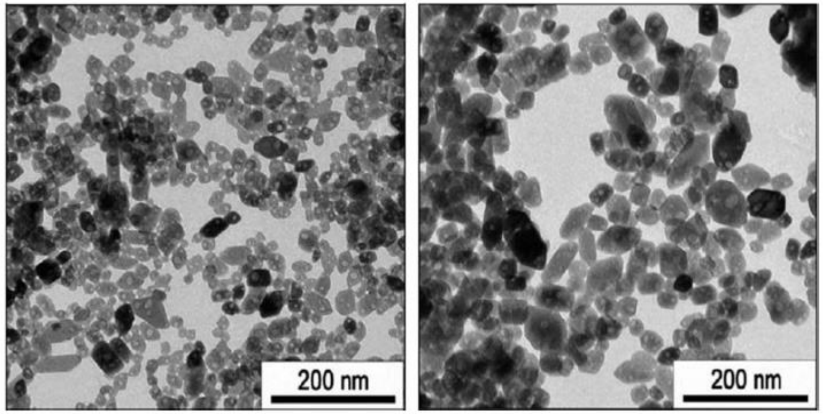
What is particle precipitation?

-A process that forms particulate product

- Mixing reactants
- Supersaturated Solution
- Reaction between chemical species
- Phase change

The product quality usually correlates with the particle size distribution (PSD)





L.Metzger, et.al (2016)

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Challenges

- Precipitation rate is highly sensitive to the local composition
- Fast reaction-precipitation
- Different mechanisms are acting simultaneously
- PSD is changing rapidly in space and in time
- Local information can hardly be captured by experiments

Motivation

- Numerical simulations open a door to understand the physics in turbulent precipitation
- Develop a coupled DNS-DPB approach for simulating particulate process in turbulent flow
- Understand the role of mixing

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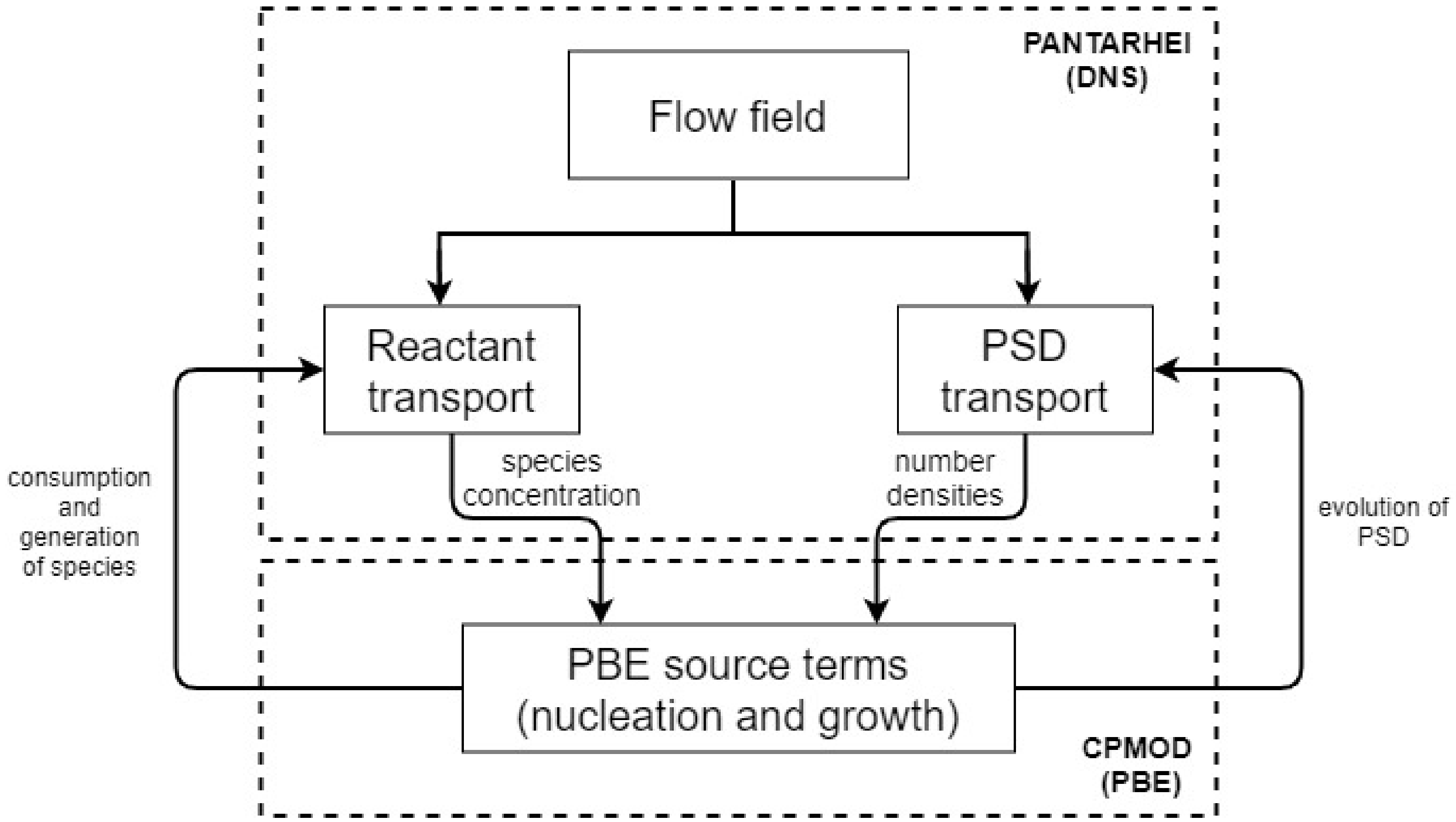
Coupling between DNS and Population balance modelling



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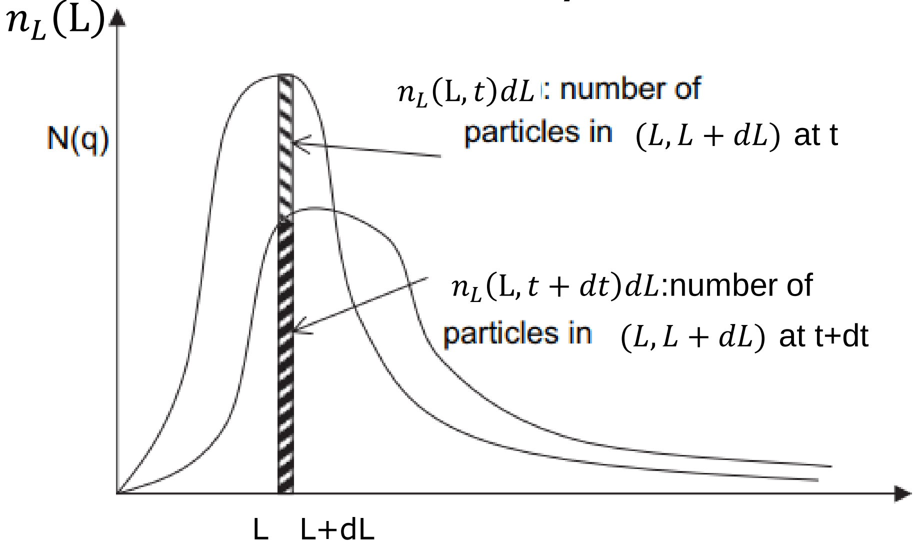
Population balance modelling

- Particle number
  - Discretised into intervals
  - Number density

$$n_L(L) = \frac{dN(L)}{V dL}$$

Evolution of Number density distribution in time



S. Rigopoulos (2010)

Population balance equation (PBE)

$$\overbrace{\frac{\partial n_j}{\partial t} + \boldsymbol{u}\cdot\nabla n_j}^{\text{Number transport}} = \frac{\upsilon}{Sc}\nabla^2 n_j \overbrace{+ B_0 - \frac{\partial G\cdot n_j}{\partial L}}^{\text{Source term}}$$

Convection term

Diffusion term

Nucleation

Growth

Semi-empirical relations

- Assume particles as tracer
- PBE is solved locally in each cell together with the DNS
- The PBE source terms are used also in the computation of ion consumption to achieve coupling with ion transport
- The flow field is captured by DNS, which can be considered as fully resolved
- The only modelling terms are the growth and nucleation rates

N	Total number of particles
n_L	Number density
L	Size interval (Class)
B_0	Nucleation term
B	Generation term
D	Destruction term
G	Growth rate

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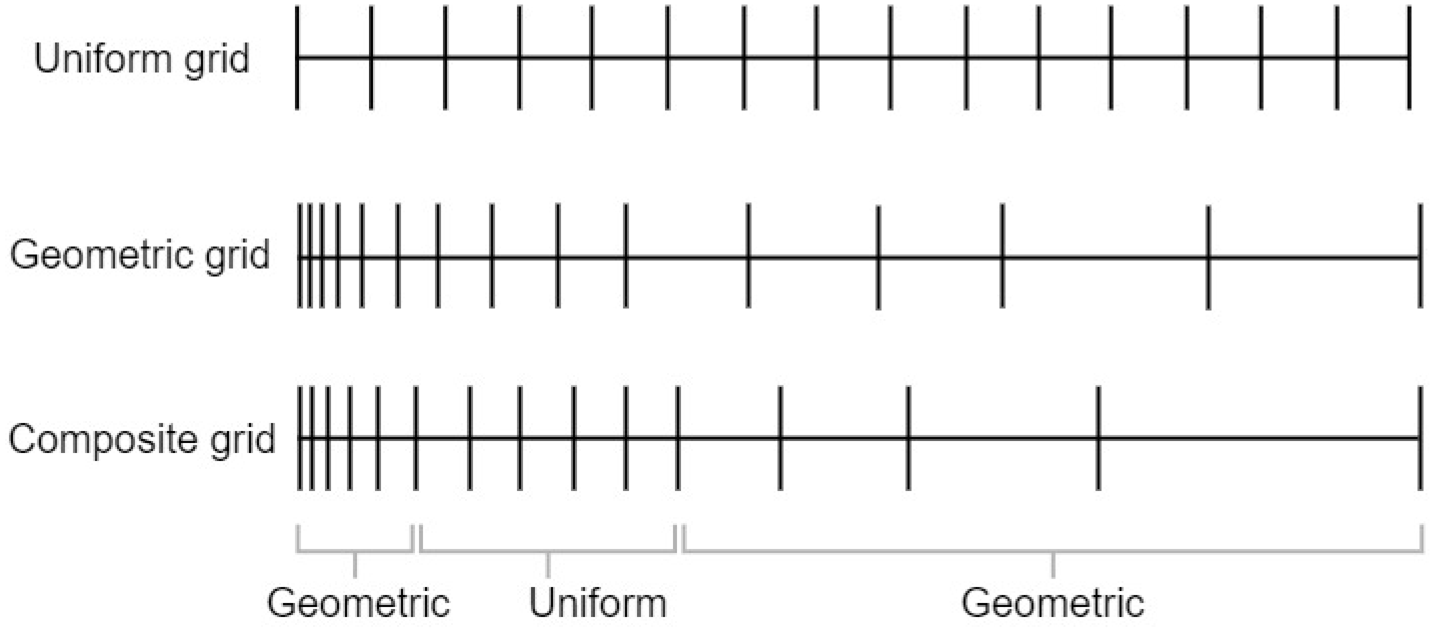
Discretisation on the particle size distribution (PSD)

$$\frac{\partial n(j)}{\partial \mathrm{t}} + \boldsymbol{u} \cdot \nabla n(j) = \frac{\upsilon}{\mathrm{Sc}} \nabla^2 n(j) + B_0 \delta(V_j - V_{nuc}) - \frac{\partial G_j \cdot n(j)}{\partial V}$$

Convective form



- Particle size range is discretised into 45 intervals (j = 1 - 45) with a composite grid
- The composite grid arrangement gives minimal leakage in the interested range compared to the other two arrangements.

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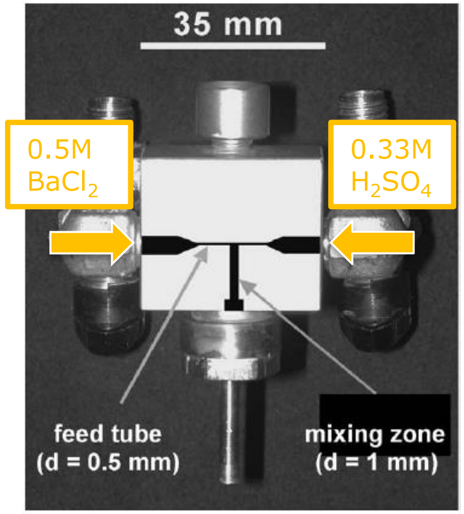
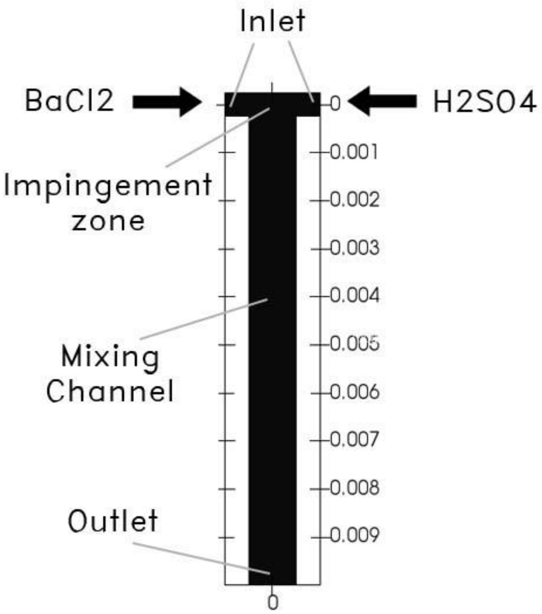
Nanoparticle precipitation in a T-mixer

- Apply the coupled DNS-PBE approach to the nano-particle precipitation of $BaSO_4$ in a T-mixer (H.-C. Schwarzer, 2004)
- What are the effects of mixing on the precipitation process ?
- How the PSD is influenced by local effects ?

$$BaCl_2 + H_2SO_4 \rightarrow BaSO_4 + 2HCl$$



H.-C. Schwarzer, et. Al (2004)



3D Cartesian mesh

21 million cells

Flow field is fully resolved to Kolmogorov scale

6 species:

- Ba^{2+}
- Cl^-
- H^+
- HSO_4^-
- SO_4^{2-}
- $BaSO_4$

45 number densities

→ Total **51** scalars

Flow field & Mixing

- Re = 1135

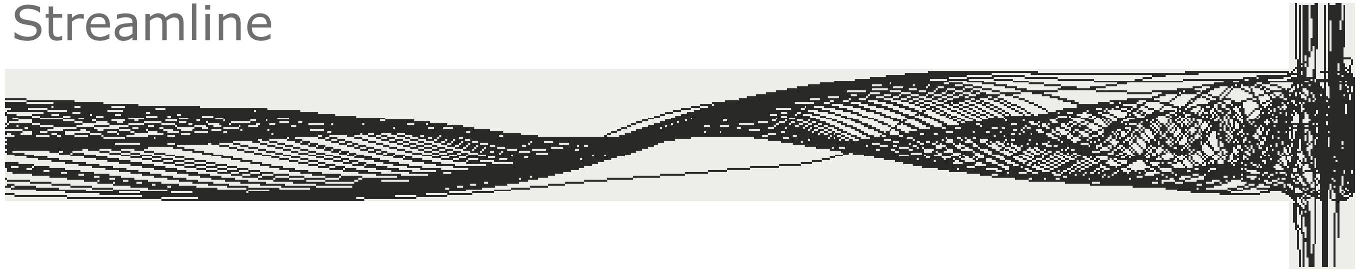
  Turbulent in T-mixers begins at Re>400
  (Telib et al., 2004)

- Helical Pattern

- Intense mixing at impingement zone

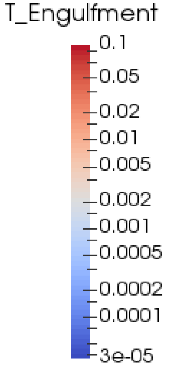
- Fastest mixing time scale in the order of 10^{-5}

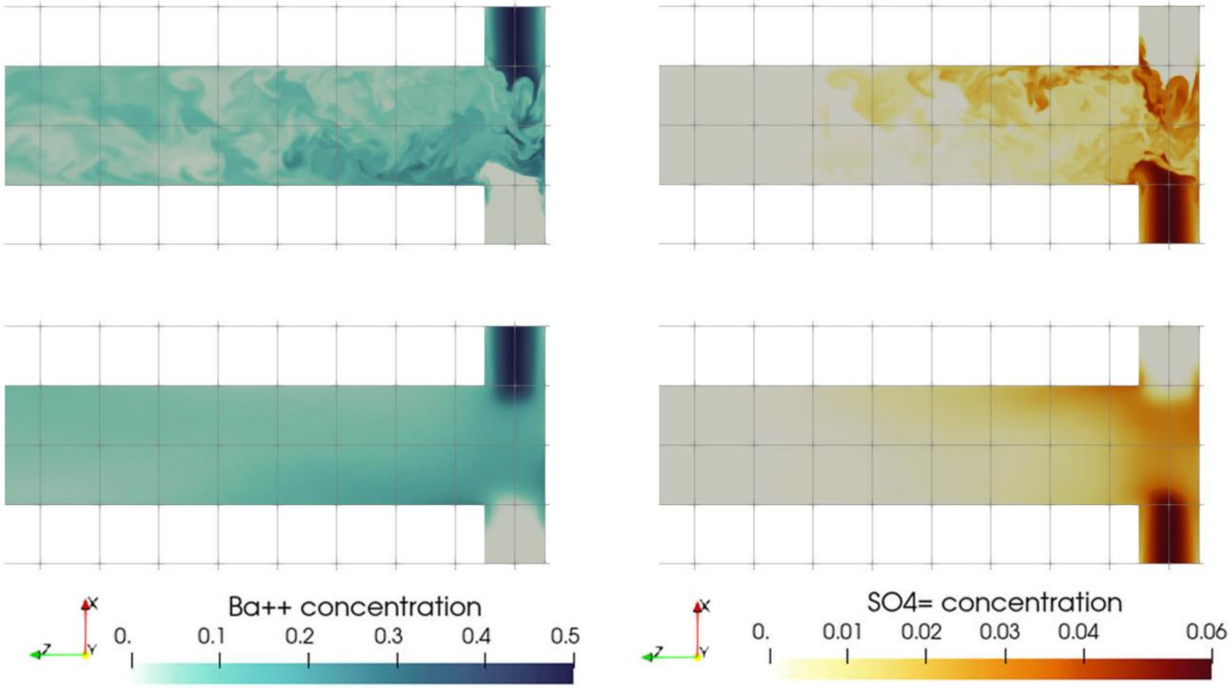
Streamline



Micro-mixing (Engulfment) time scale
(characterizes the timescale of the most energetic vortex)

$$\tau_E = 17\left(\frac{\upsilon}{\varepsilon}\right)^{\frac{1}{2}}$$





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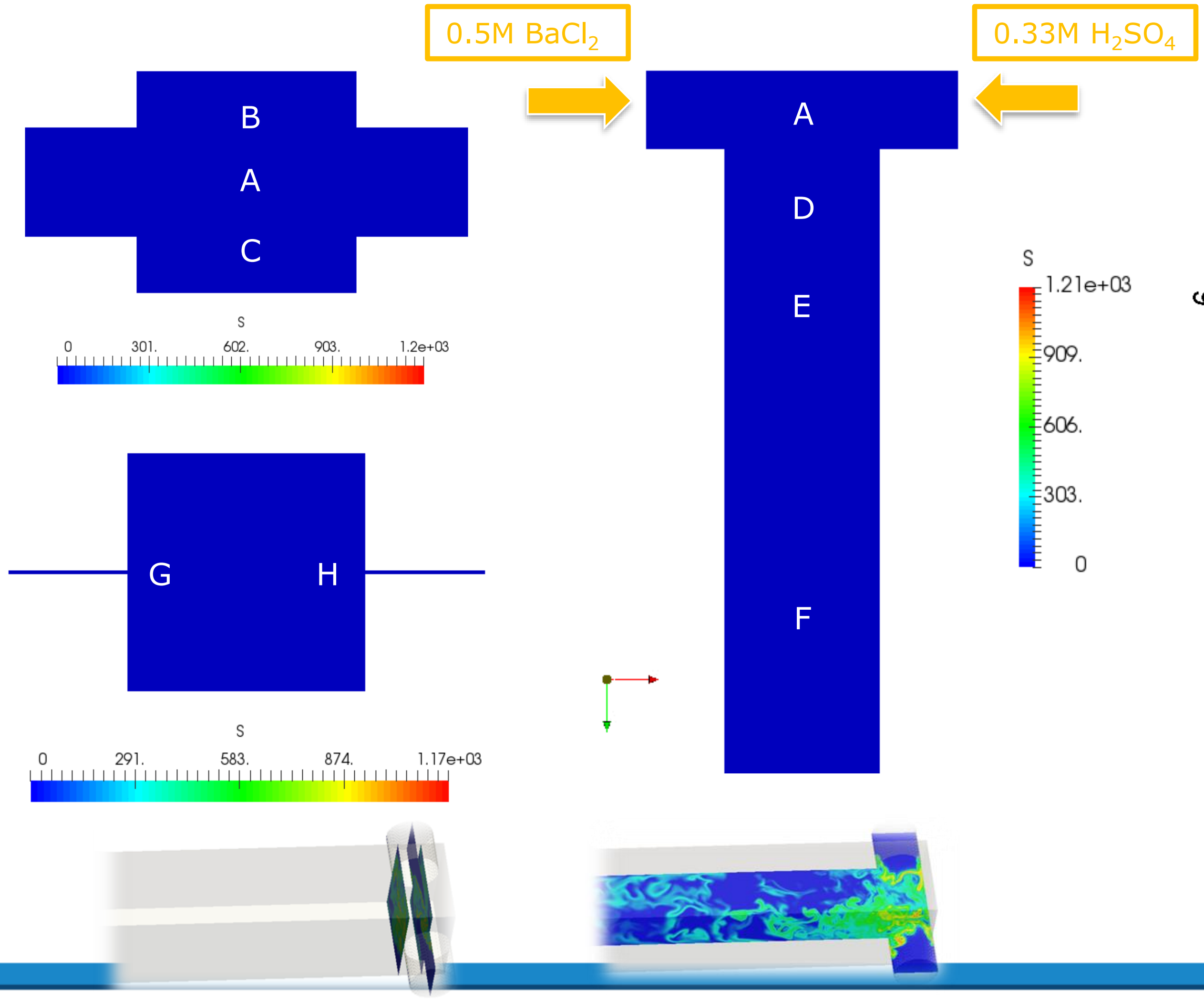
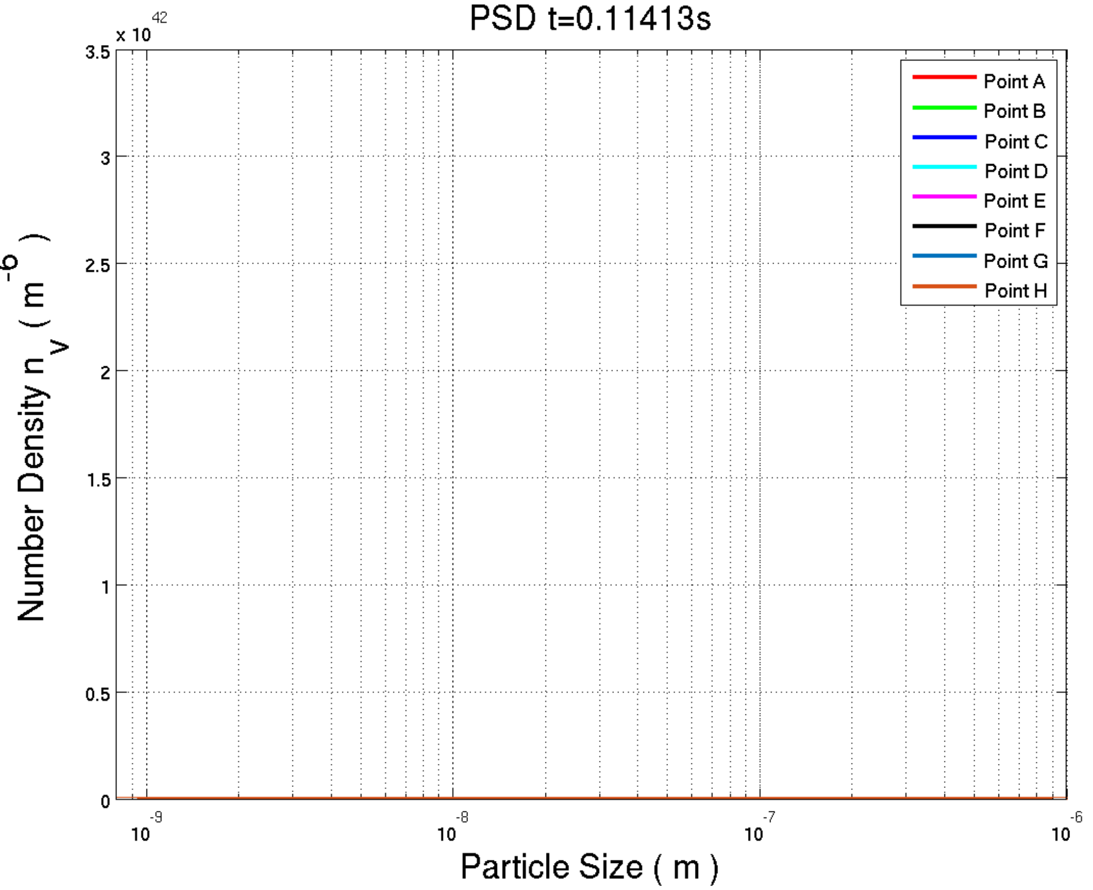
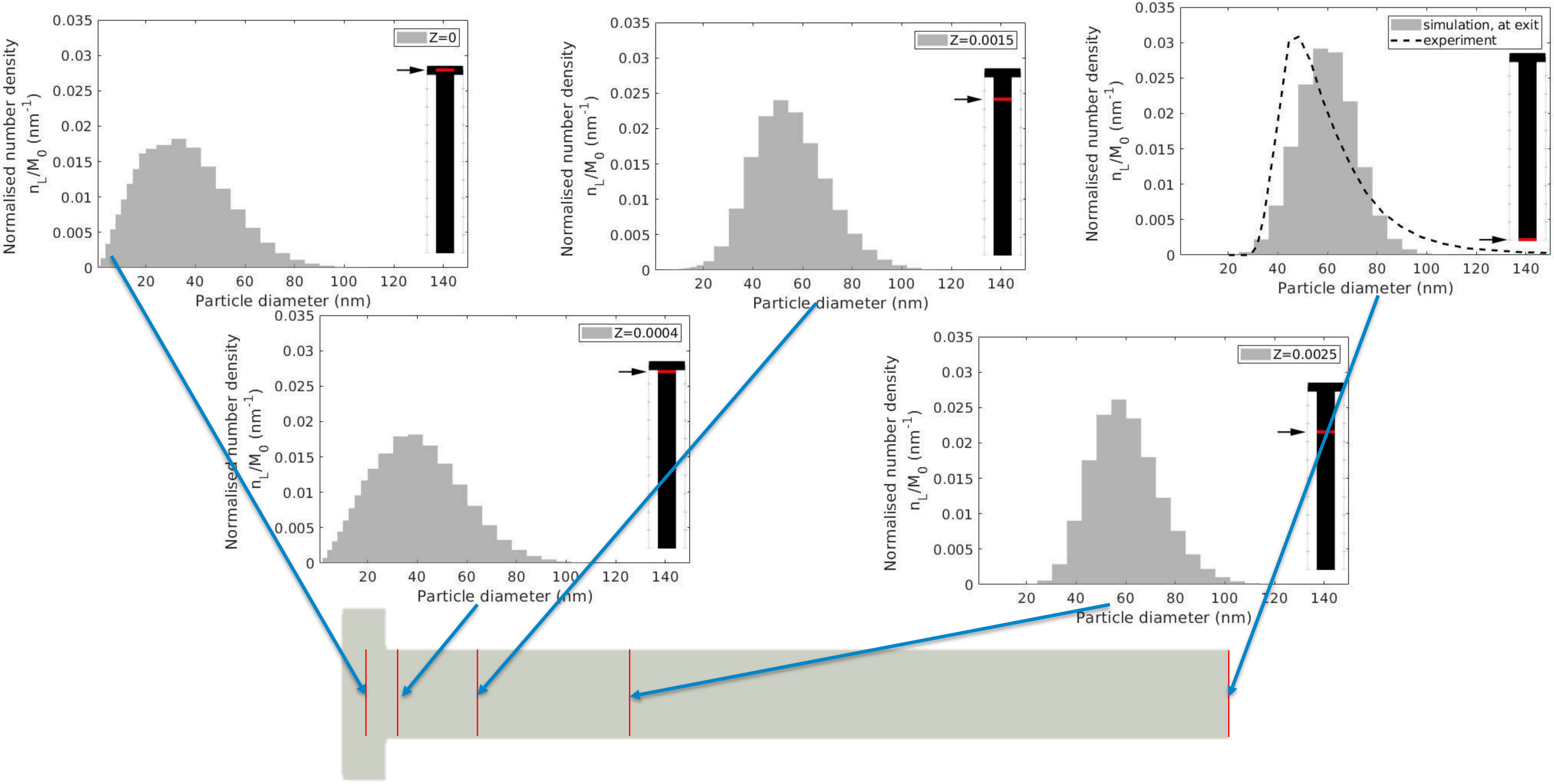
The PSD





Mean plane averaged PSD



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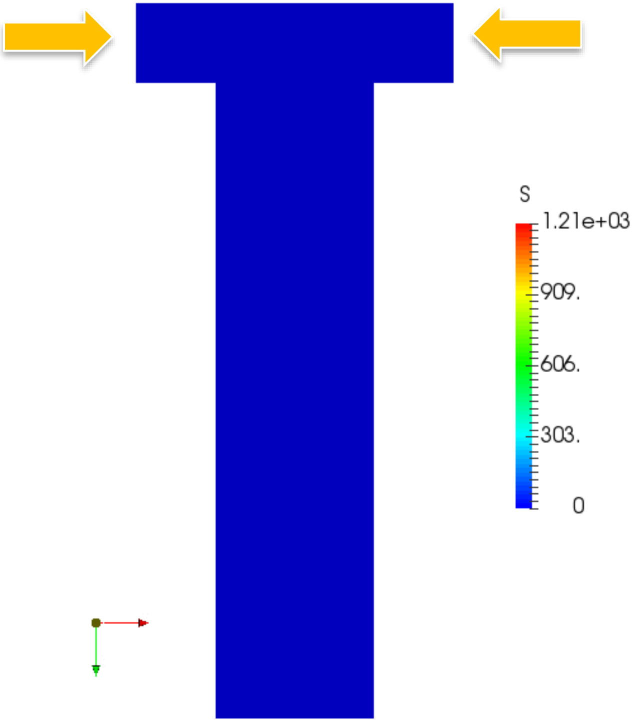
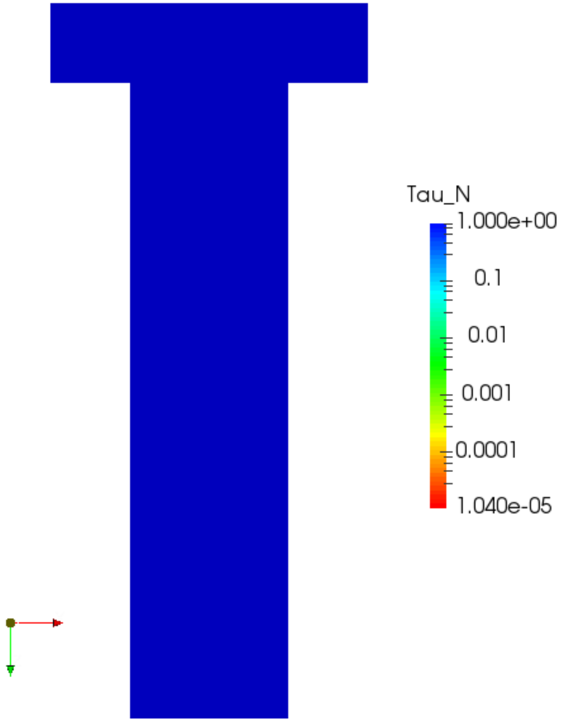
Local kinetics and timescales

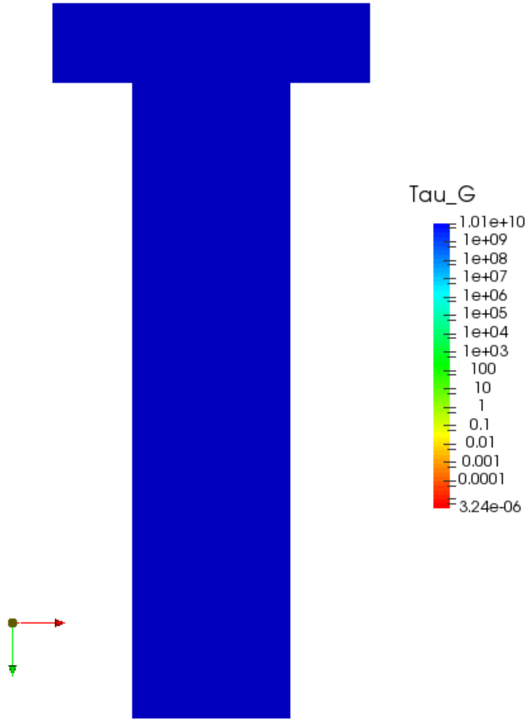
Supersaturation



Nucleation timescale



Growth timescale



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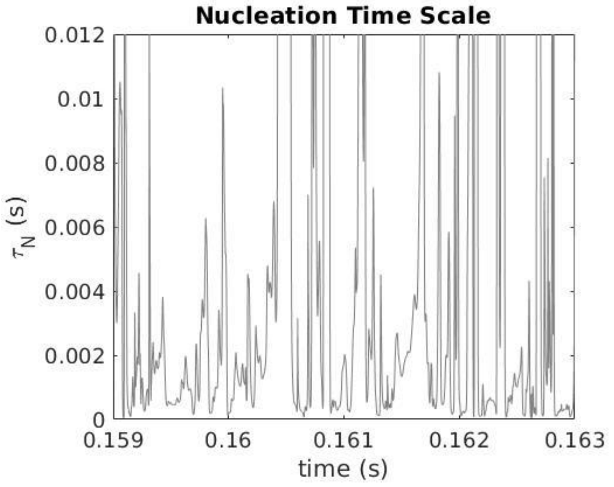
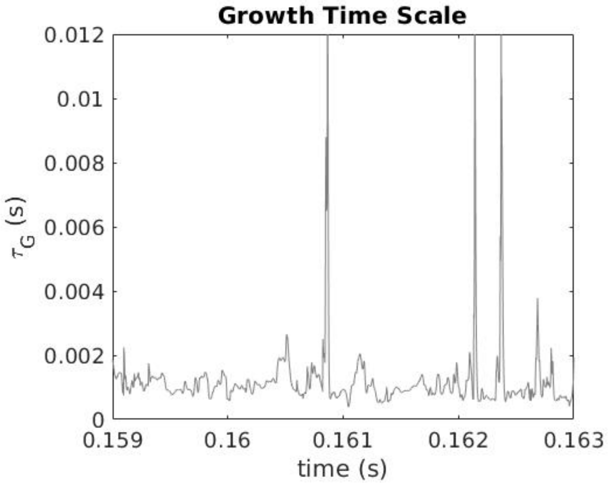
Intermittency

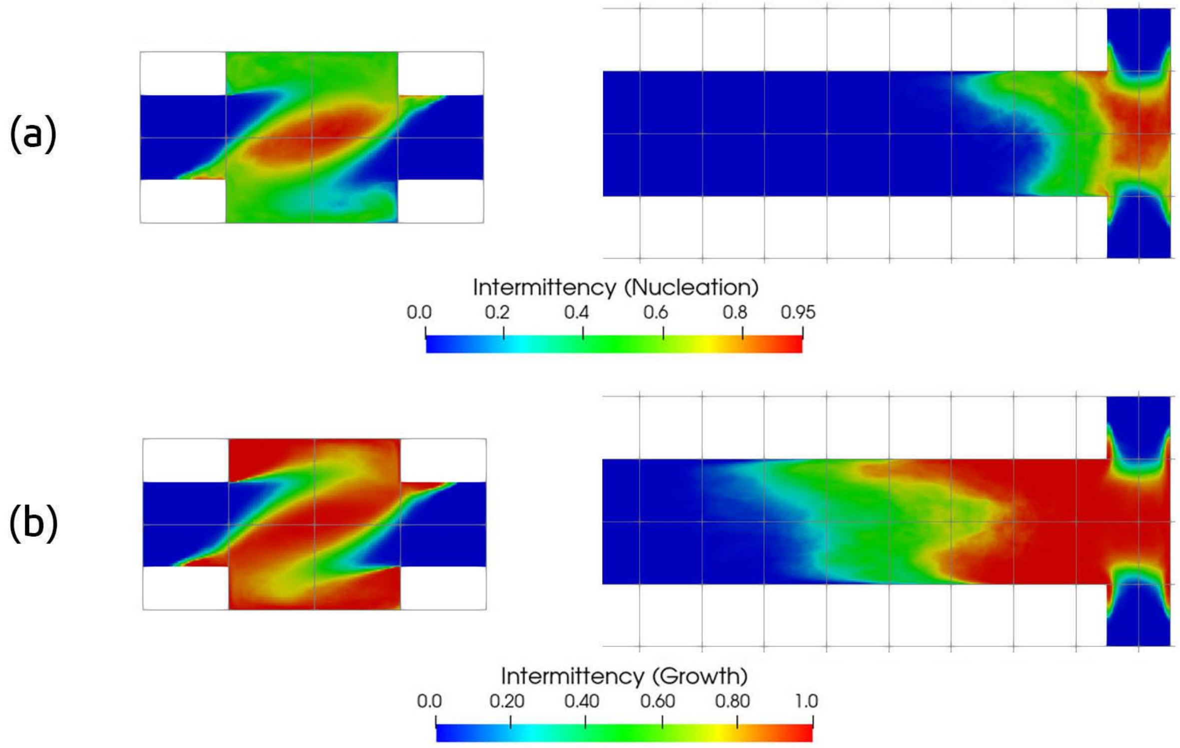
$$\gamma(\mathbf{x}) = \langle I(\mathbf{x}, t)\rangle$$

$$I(x,t) = \begin{cases} 1, & S(\mathbf{x},t) > S_{threshold} \text{ and } \tau(\mathbf{x},t) < \tau_{threshold} \\ 0, & \text{otherwise} \end{cases}$$

Non-linear kinetics and turbulent mixing leads to highly intermittent precipitation rates.







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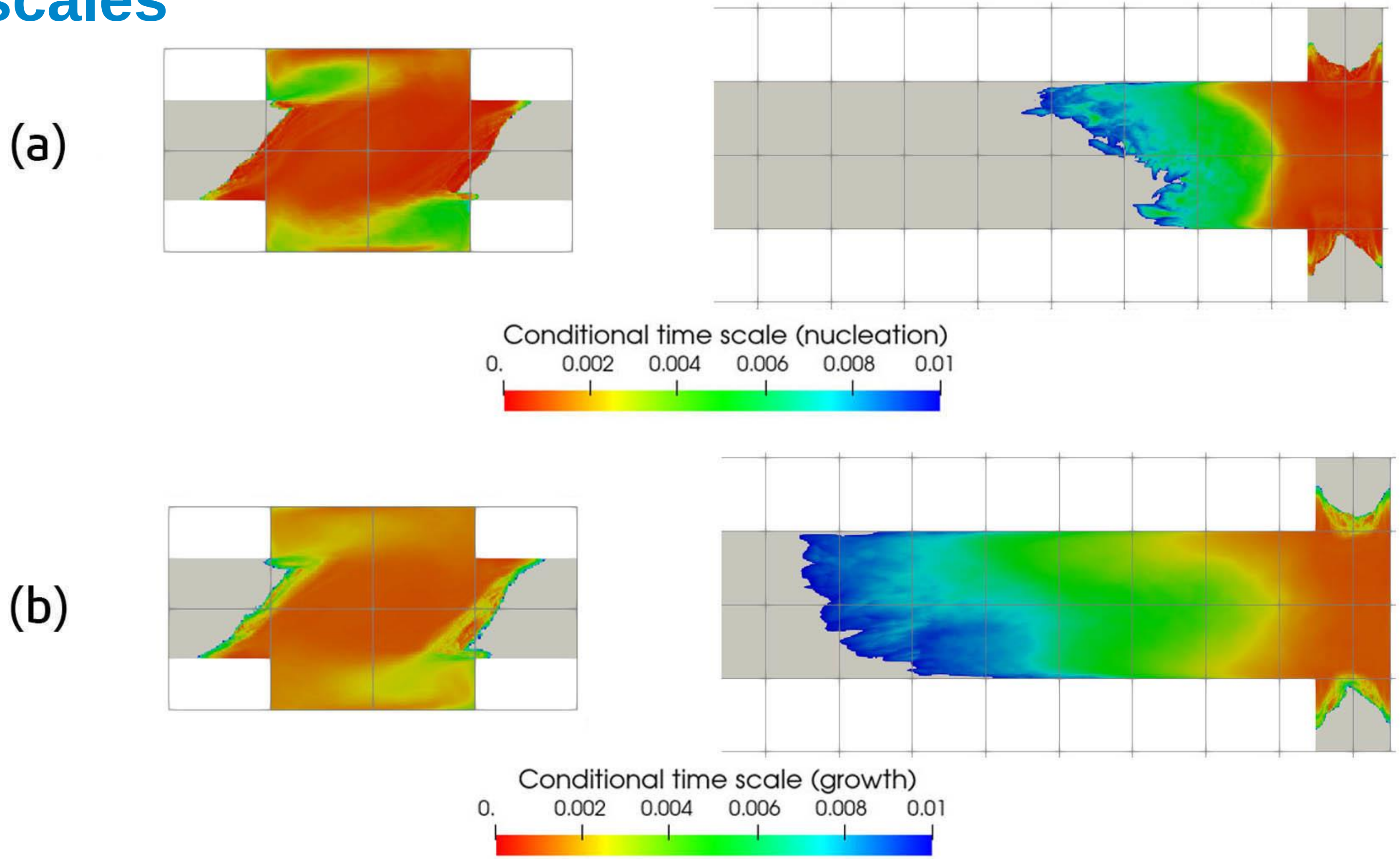
Conditional timescales

$$\tau_{\mathrm{cond}} = \frac{\int_0^T I(\mathbf{x},t)\tau(\mathbf{x},t)dt}{\int_0^T I(\mathbf{x},t)t\,dt}$$



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Damköhler numbers

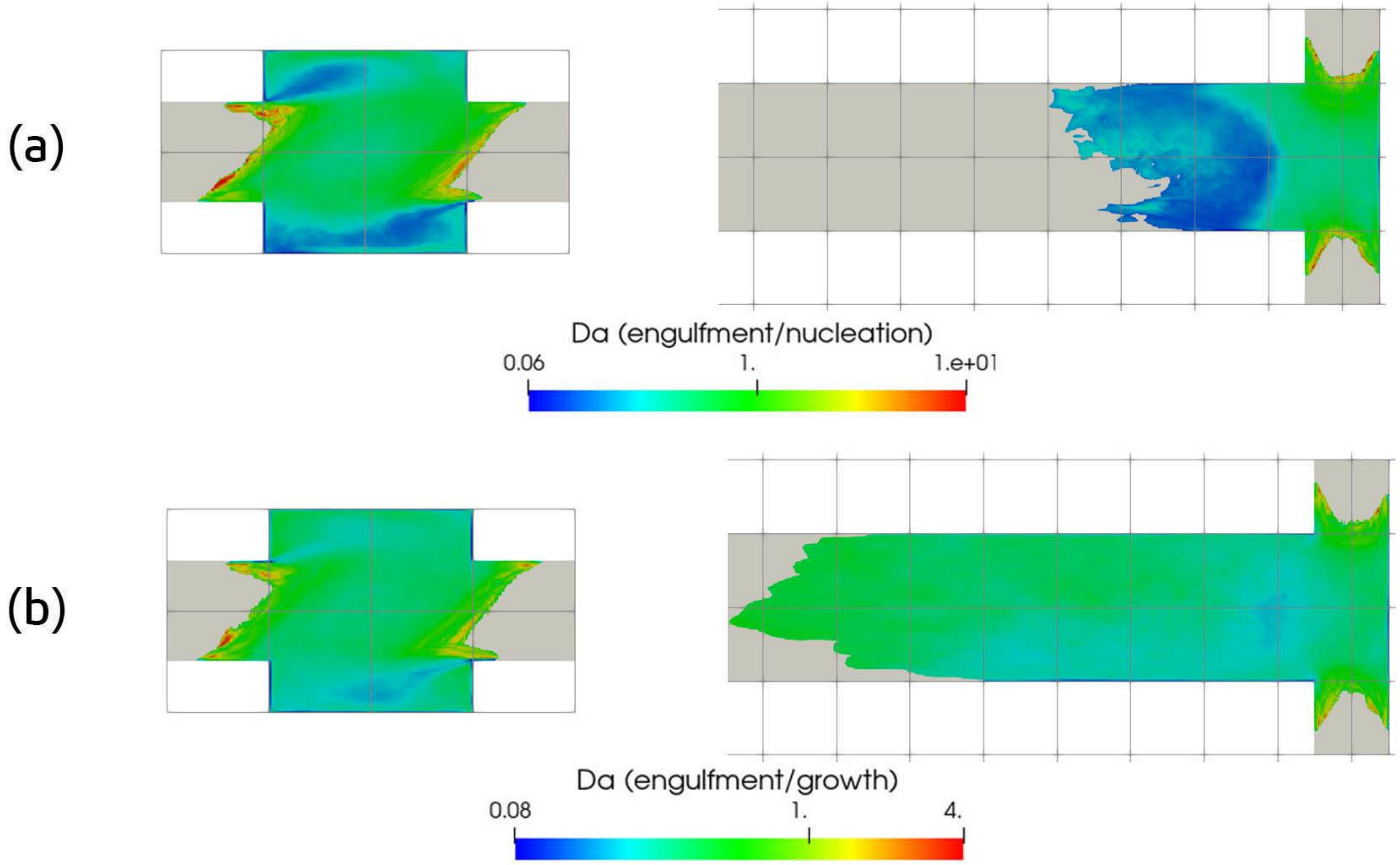
Nucleation and growth have their own timescales.

Two Damköhler numbers can be defined:

$$Da_{nuc} = \frac{\tau_{flow}}{\tau_{cond,n}}$$

$$Da_G = \frac{\tau_{flow}}{\tau_{cond,G}}$$

Neither mixing- nor kinetic-controlled



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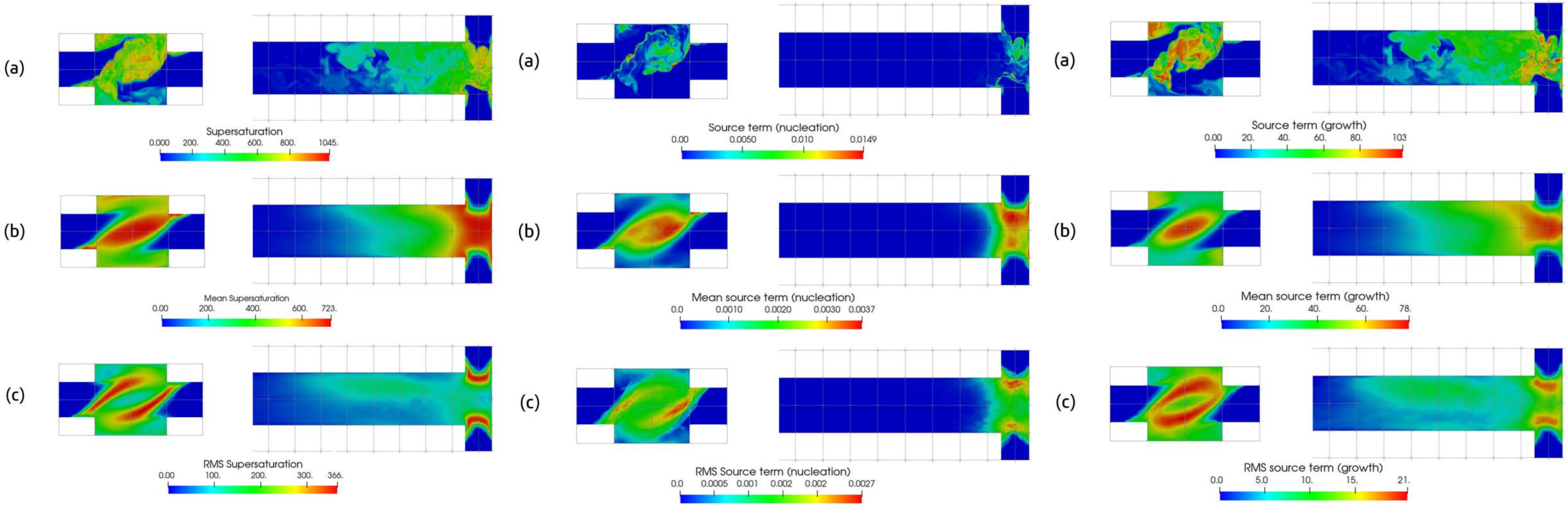
Consumption rates

Instantaneous | Mean | RMS

Supersaturation | Source due to nucleation | Source due to growth



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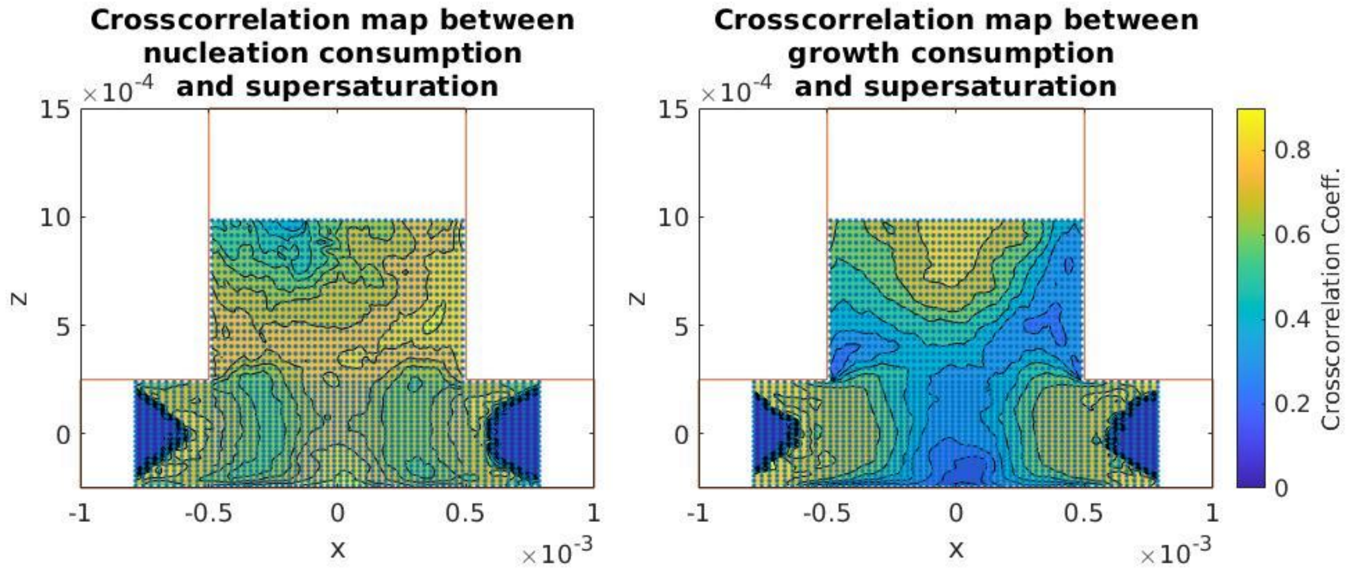
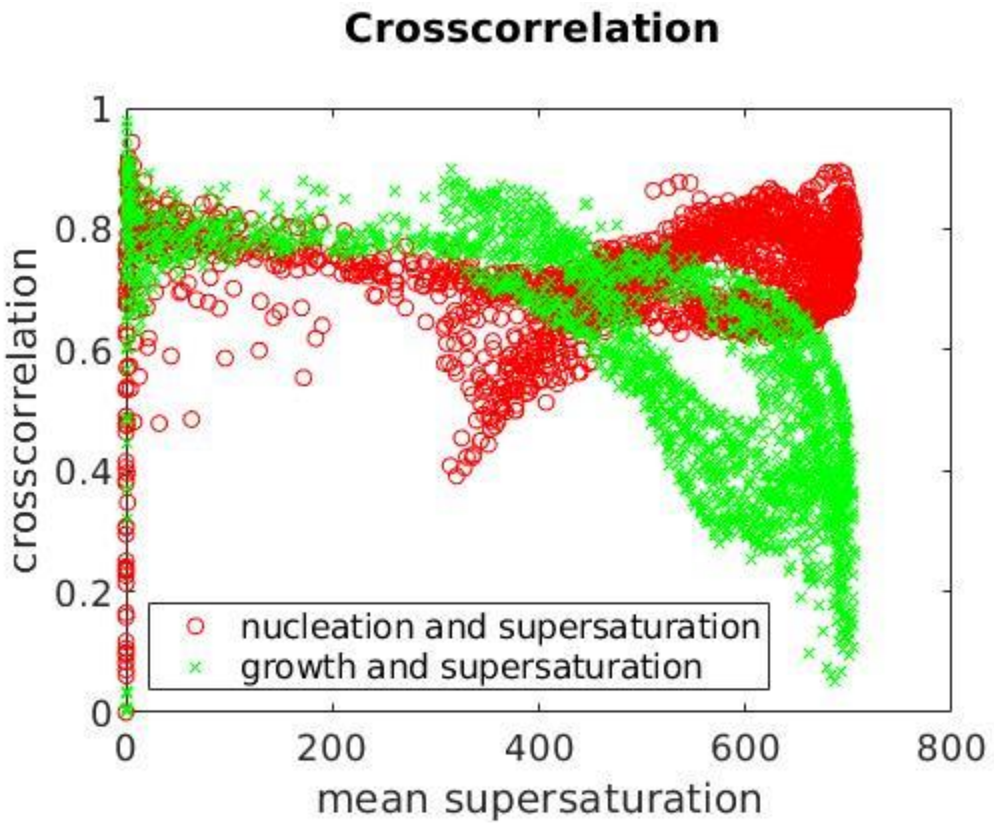
Correlations

Cross-correlation coefficients at 3000 points in the impingement zone and its immediate downstream





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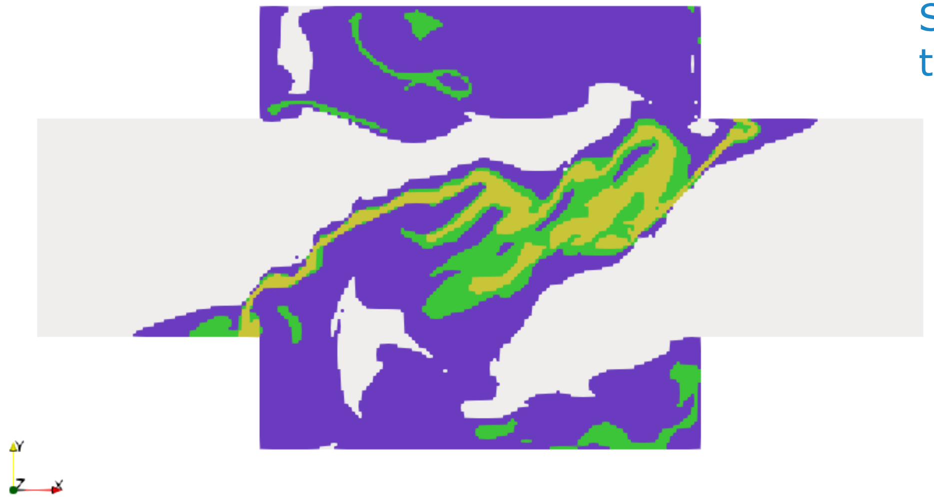
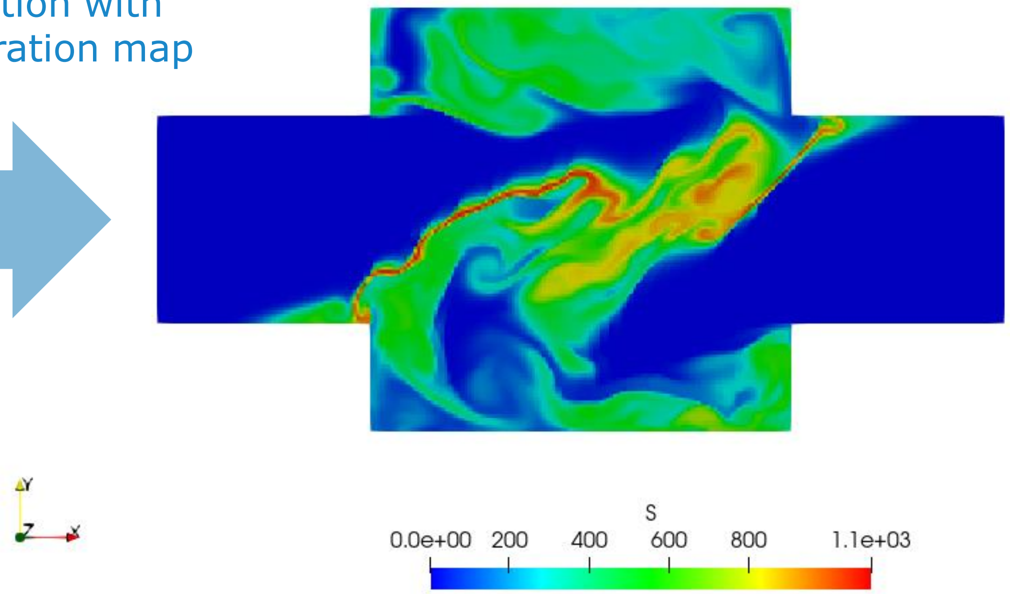
Locally dominant zone and its relation with supersaturation



Strong correlation with the supersaturation map



Growth dominant zone

Competing zone

Nucleation dominant zone

Nucleation dominance: $S > 700$

Competing: $400 < S < 800$

Growth dominance: $S < 550$

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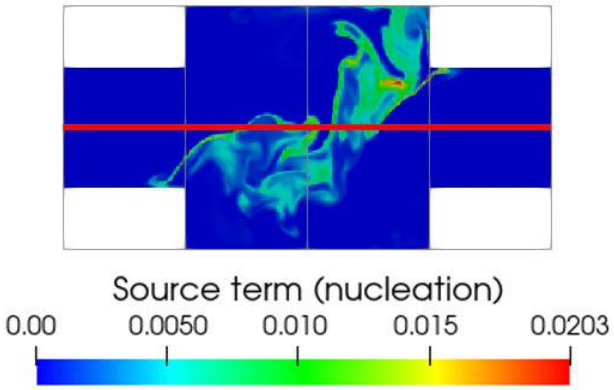
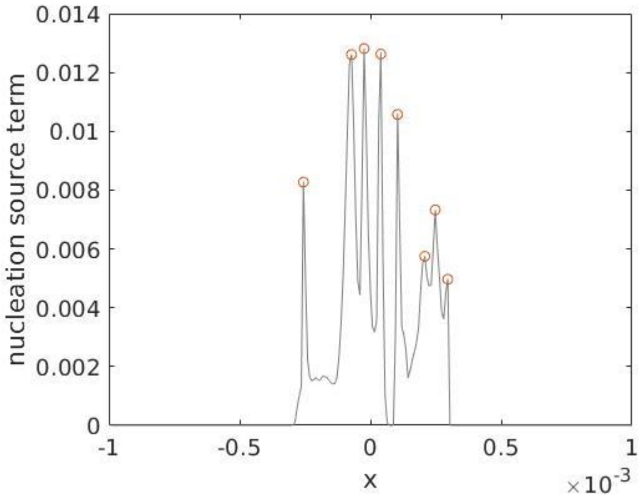
Nucleation burst

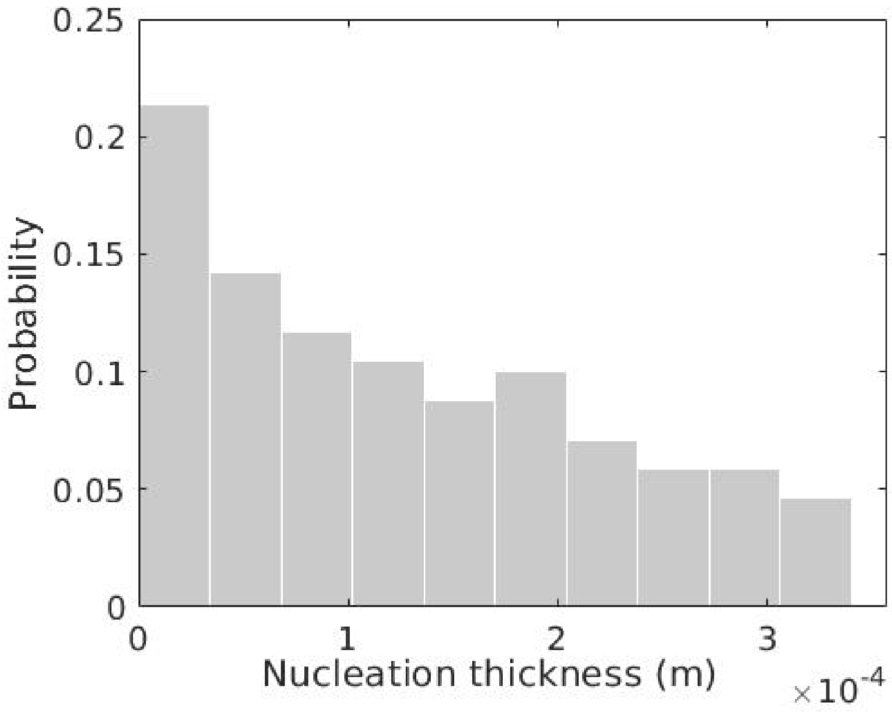
The non-linearity in the nucleation kinetics leads to thin and intense nucleation sites.

These nucleation bursts contribute to seed formation

All thickness measured are above Kolmogorov scale (on average 20 times larger)







Conclusions

- A coupled DNS-DPE approach employed in simulating turbulent precipitation of BaSO4 nanoparticles in a T-mixer
- The comparison of the nucleation, growth and mixing timescales shows inseparable scale between mixing and precipitation
- Although most reactants are consumed in the form of growth, nucleation controls the number of seed particles that plays a determinant role on the PSD
- Different local dominant mechanism that corresponds to the supersaturation build up can be found in the process, of which the distribution is controlled by mixing
- The current works try to include aggregation that alters the growth environment

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Thank you