Simulation of Spray Coating in a Spouted Bed using Recurrence CFD

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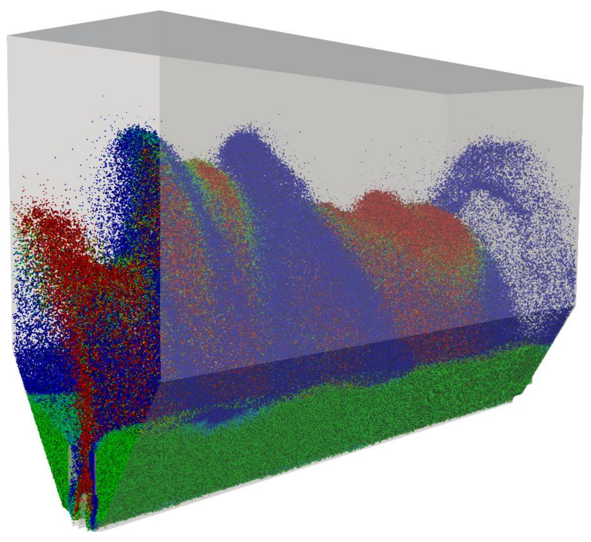
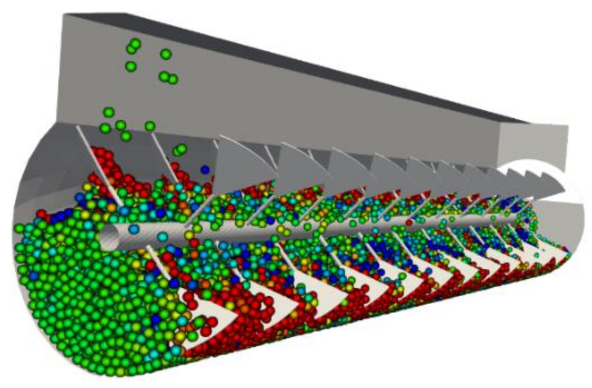
Background

- Many processes in chemical industry show chaotic & **recurrent** behavior
  - Fluidized Beds: Bubbling & Clustering
  - Spouted Beds: Instable Spouting
  - Bubble Columns: Multiphase Turbulence
  - System states deviate from average
- Simulation of these apparatuses is possible, but the resolution of dynamics is numerically expensive
  - Description of transport processes much less computationally expensive
- Main interest lies in chemistry & transport phenomena, not recurrent dynamics

How can the time scales between dynamics and transport phenomena be bridged?



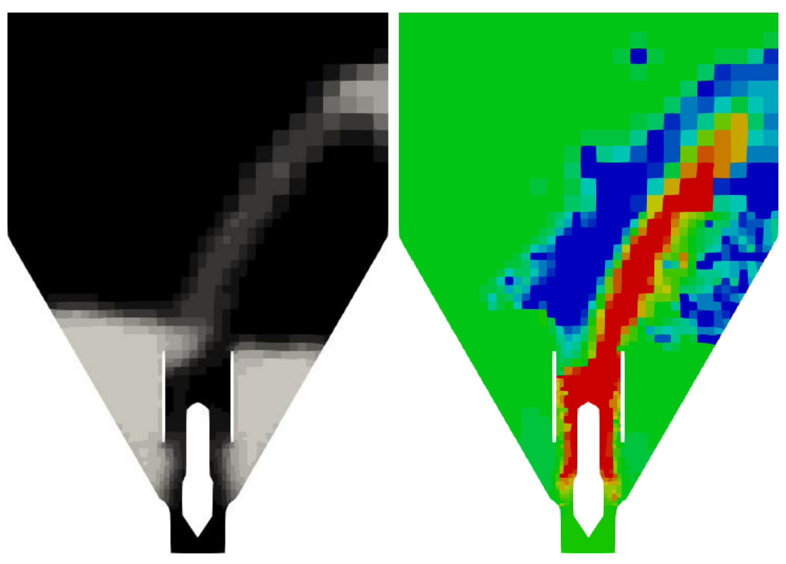
Pilot-scale continuous spouted bed showing recurrent oscillations



Paddle mixer exhibiting recurrent mixing patterns

Method[1]

1. Step: full CFD simulation



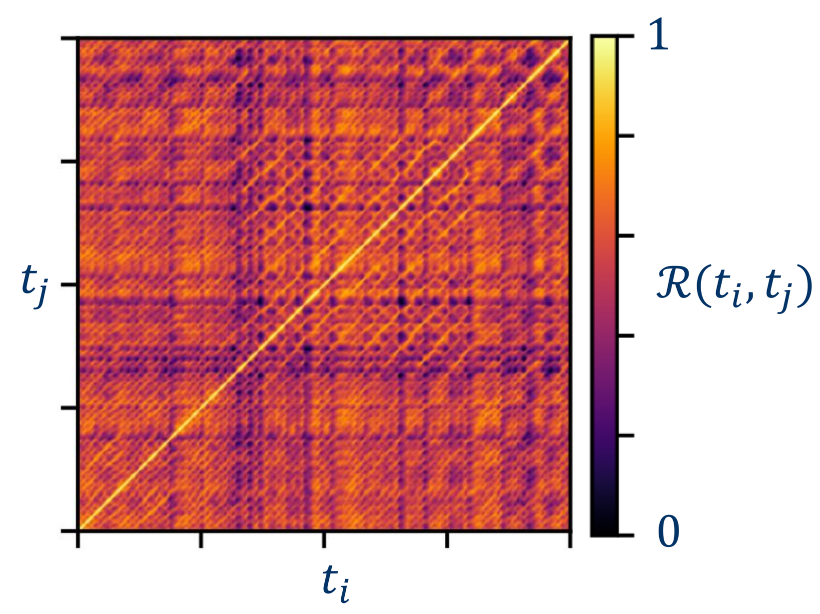
Aim: Capture state spaces of phase dynamics

- For each phase k, sample
  - Volume fraction α_k
  - Velocity $\boldsymbol{U}_k$
  - Any other relevant fields (e.g. pressure, Nusselt number)
- Satisfy temporal resolution crit.

$$\Delta t_{\text{sample}} \ll \frac{<\varphi>}{<\dot{\varphi}>} \quad \text{for fields } \varphi$$

- Cover most of the state space (i.e. bubbling modes)

2. Step: Recurrence Matrix



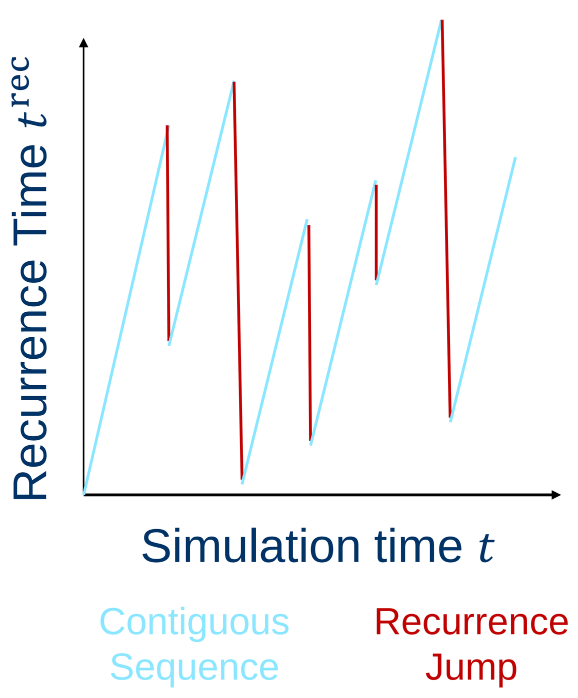
Aim: Quantify pair-wise similarity of states

- Compare states in database based on spatial phase distribution

$$\mathcal{R}(t_i, t_j) = \frac{1}{N} \int_V \alpha(t_i) - \alpha(t_j) dV$$

$$N = \max_{t_i, t_j} \int_V \alpha(t_i) - \alpha(t_j) dV$$

3. Step: Recurrence Path



Aim: Extrapolate a temporal sequence of system states

- Replay *contiguous sequences* of system states from database
- End of sequence: *Recurrence Jump*
  - Use the *Recurrence Matrix* to find state in database most similar to end of sequence
- Minimize discontinuities, ensure physical meaningfulness

Treatment of Transport Processes

- Evolve transport processes on loaded recurrence fields $\boldsymbol{\phi}^{\text{rec}}/\ \boldsymbol{U}^{\text{rec}},\ \alpha^{\text{rec}}$
- Eulerian Frame of Reference

$$\frac{\partial}{\partial t}(\alpha^{\text{rec}} c_i) + \nabla \cdot (\boldsymbol{\phi}^{\text{rec}} c_i) = \nabla \cdot (\alpha^{\text{rec}} D \nabla c_i) + \dot{S}_{c_i}$$

  - Local mass conservation at recurrence jumps not given
  - Small time steps required
- **Lagrangian Frame of Reference**

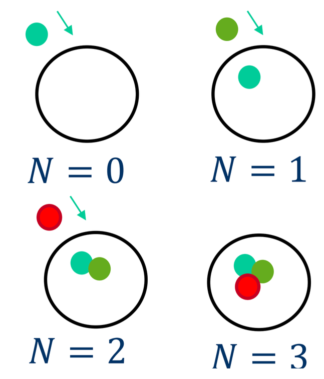
$$\dot{\boldsymbol{x}}_i = \underbrace{\boldsymbol{U}_i^{\text{rec}}}_{\text{ensures velocity}} + \underbrace{\boldsymbol{n}_{\text{rand}} \sqrt{\frac{D_0}{6\pi\Delta t} \max\left(0, \frac{\alpha_i - \alpha_i^{\text{rec}}}{\alpha_i^{\text{rec}}}\right)}}_{\text{ensures phase distribution}}$$

  - Mass conservation guaranteed
  - Large time steps possible

Modelling of Spray Coating

- Inject droplet parcels, strip droplets using a filter correlation [2] and deposit on particle surfaces

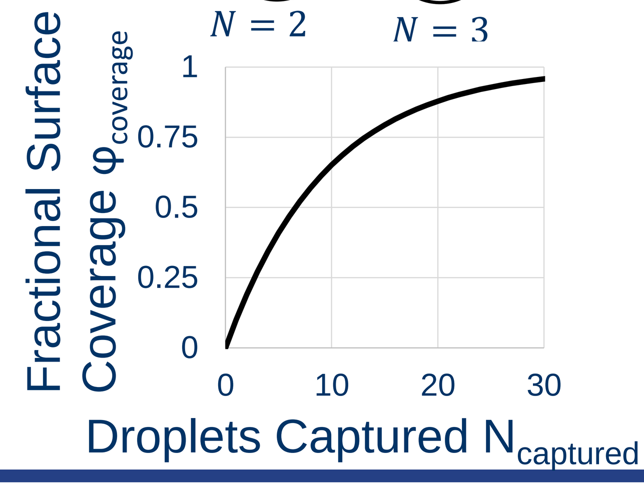
$$\eta_{\text{dep}} = 1.5\ \alpha_{\text{P}} U_{\text{r}}\ \lambda\ d_{\text{P}},$$
$$\lambda = (St^*_{\text{eff}})^{3.2} / \left((St^*_{\text{eff}})^{3.2} + 4.3\right)$$



- Calculate **fractional surface coverage** $\varphi_{\text{coverage}}$

$$\varphi_{\text{coverage}} = \frac{S_{\text{covered}}}{S_{\text{P}}} = 1 - (1 - f)^{N_{\text{captured}}}$$

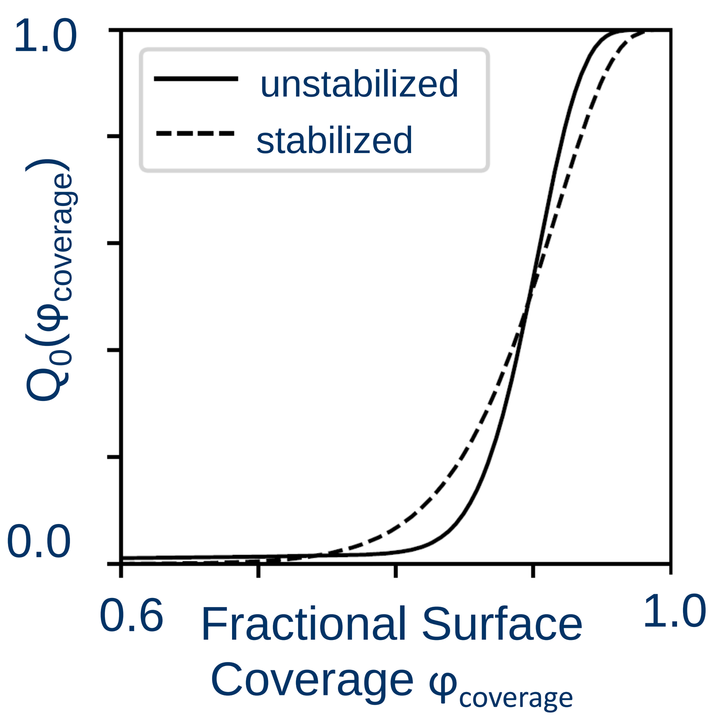
$$f = A_{\text{q,droplet}} / S_{\text{P}}$$



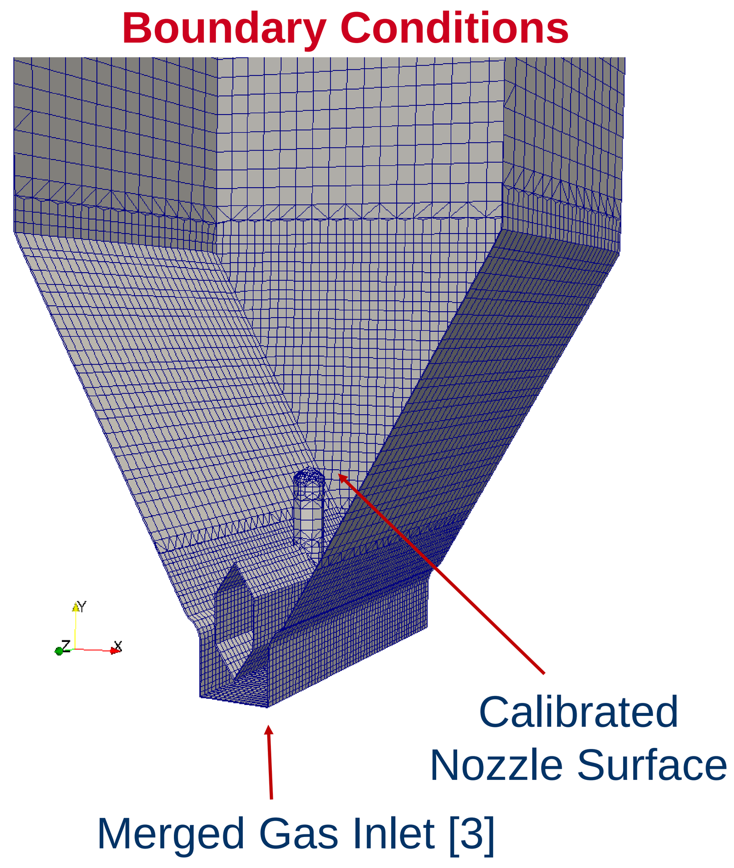
Case Setup and Results

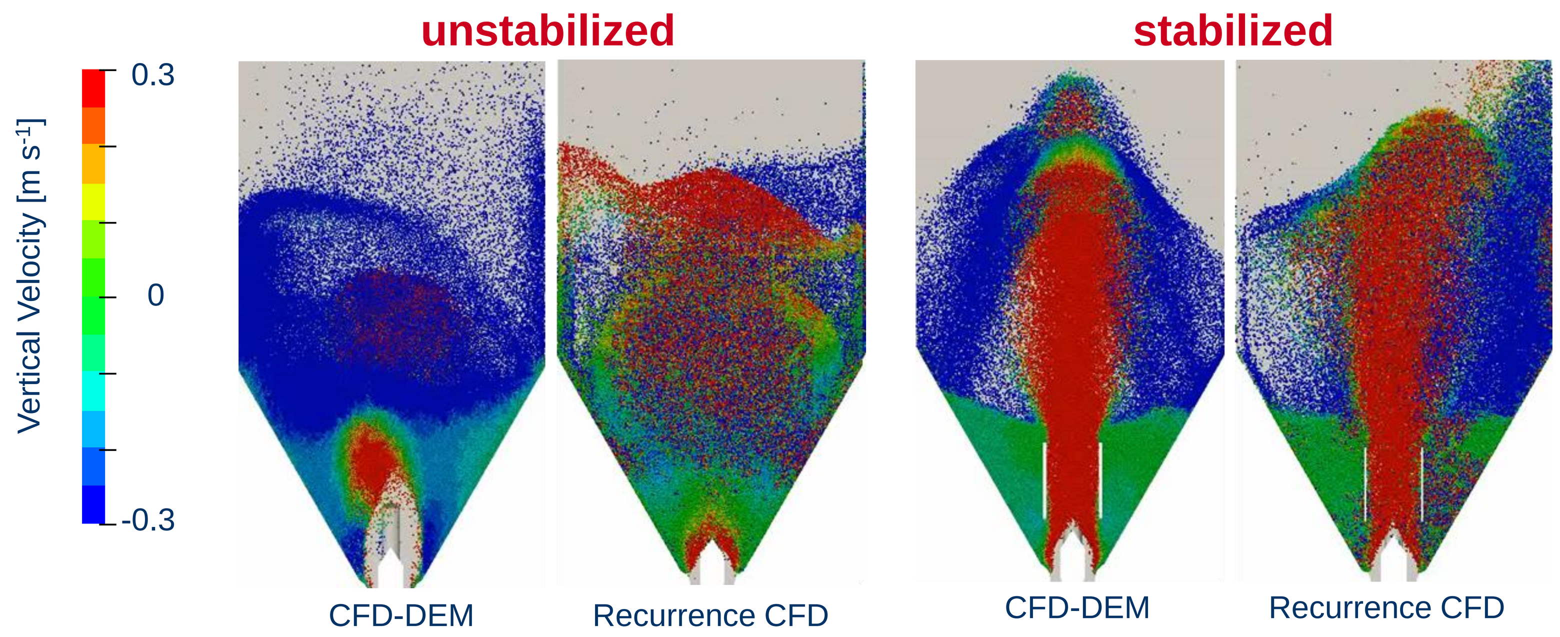
- **Objectives**
  - Demonstrate **validity** of Recurrence CFD for spouted beds [3]
  - Perform **long-term simulations** of spray coating (**1 h**)
  - Evaluate **influence of stabilization** by draft plates on **coating quality**
- **Validation**[4]
  - Against full CFD-DEM simulations
  - Accurate reproduction of both time-averaged and instant void fractions
  - Residence time distributions within a fictitious spray zone agree well
- **Coating Quality**
  - Stabilization by draft plates decreases mixing
  - Less homogeneous surface coverage results from inhibited mixing

Quantity	Value
Particle Diameter d_{P}	1.8 mm
Particle Density ρ_{P}	1040 kg m^{-3}
Bed Mass M_{P}	1.5 kg
Fluidization Air $\dot{V}_{\text{G}}$	230 m^3 h^{-1}
Atomization Air $\dot{V}_{\text{G,noz}}$	5 m^3 h^{-1}
Spray Rate $\dot{M}_{\text{noz}}$	5 g min^{-1}
Apparatus Depth	200 mm
Apparatus Width	250 mm
CFD Time Step Δt_{CFD}	2.5·10^{-5} s
DEM Time Step Δt_{DEM}	1·10^{-6} s
Performance CFD-DEM	~1 s / day
Performance rCFD	**2100 s / day**
Field Sampling Rate	200 Hz
Simulation Time	13 s
Drag Law	Beetstra
Contact Law	Hertzian
rCFD Time Step Δt_{rCFD}	5·10^{-3} s
Size of Database	10 s / 16 GB



Mesh and Boundary Conditions





References

[1] Lichtenegger T., Pirker S.: *Recurrence CFD - A novel approach to simulate multiphase flows with strongly separated time scales*, CES (2019).

[2] Kolakaluri, R.: *Direct Numerical Simulations and Analytical Modeling of Granular Filtration*, PhD thesis, Iowa State University (2013).

[3] Kieckhefen, P., Pietsch, S., Höfert, M., Schönherr, M., Heinrich, S., Kleine Jäger, F.: *Influence of gas inflow modelling on CFD-DEM simulations of three-dimensional prismatic spouted beds*, Powder Technology (2018).

[4] Kieckhefen, P., Lichtenegger, T., Pietsch, S., Pirker, S., Heinrich, S.: *Simulation of Spray Coating in a Spouted Bed using Recurrence CFD*, Particuology (2018).