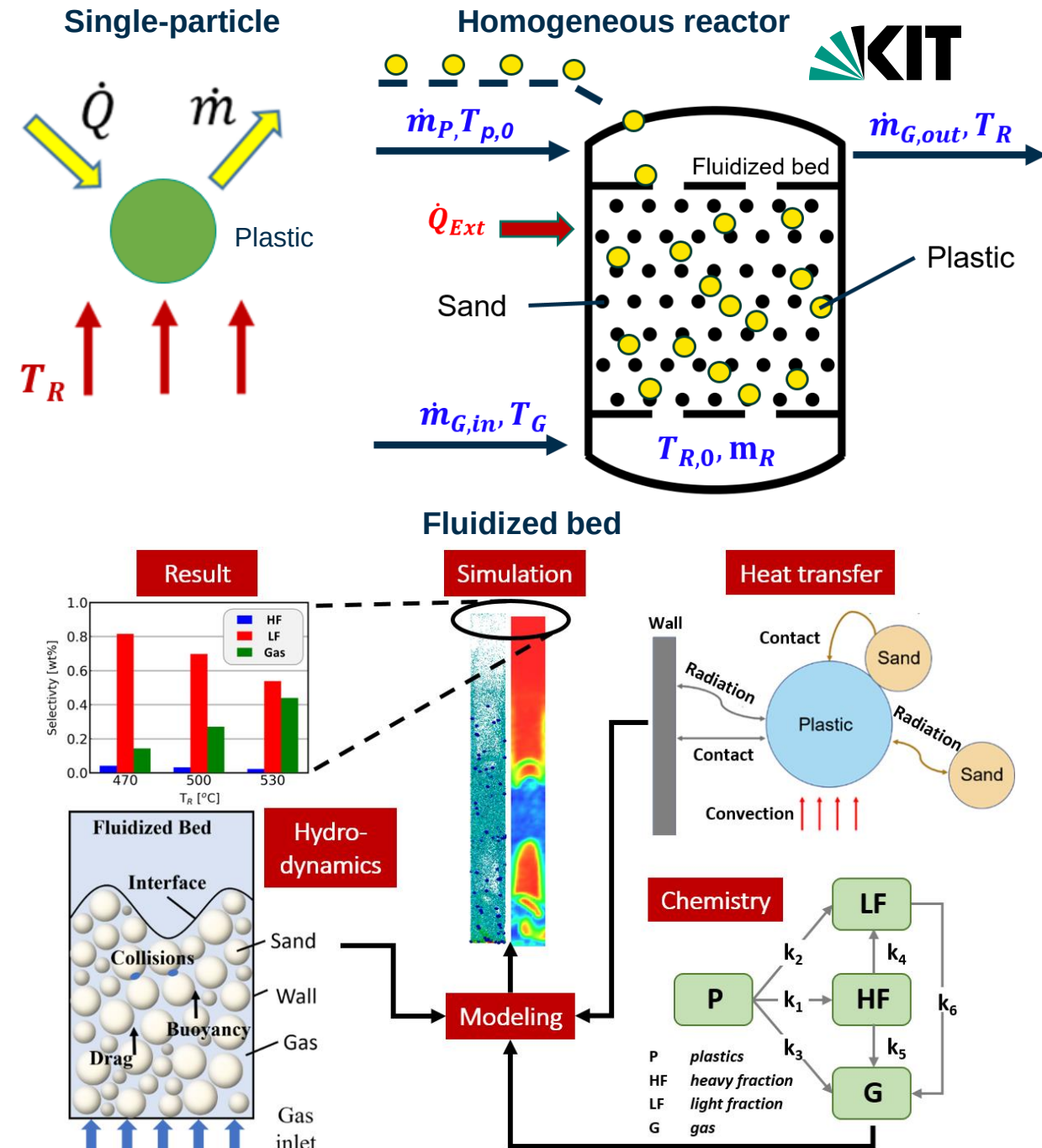


Progress and Challenges in Modeling Plastic Pyrolysis

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Modeling plastic pyrolysis: why?

- ❑ **Plastic wastes:** ~ 400 Mt/year, ~10% recycled [1]
- ❑ Chemical recycling via **pyrolysis**
 - Converting plastic waste into secondary raw materials
 - Capable of mixed/contaminated plastics
- ❑ Challenges: **scale-up**
 - High cost for large-scale experiments
 - Real-flow effects, non-linear

Plastic waste



Pyrolysis



Pyrolysis oil



Ideal

Scale/Dimension/Number/Physics ↑

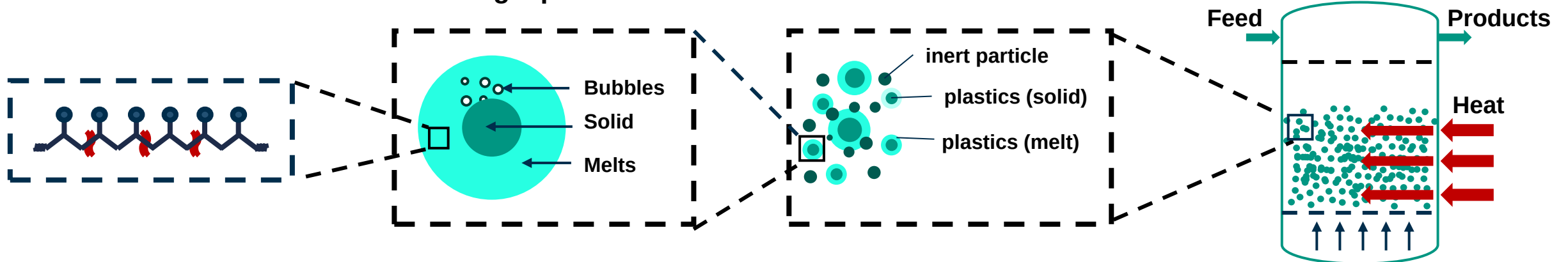
Real-flow

Reaction kinetics

Single particle

Particle interactions

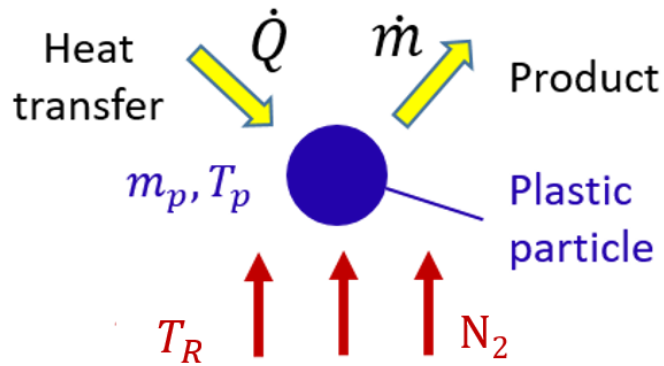
Reactor



[1] PlasticsEurope – Plastics the Facts: <https://plasticseurope.org/knowledge-hub/plastics-the-facts/>

1. Single-Particle Model

- ❑ Ideal/spherical
- ❑ Homogeneous/thermally-thin
- ❑ Convective heating vs. pyrolysis reaction



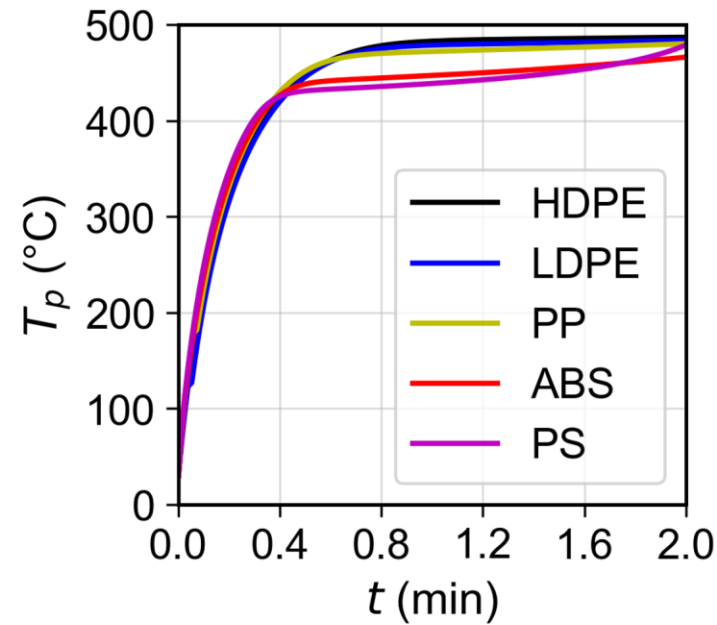
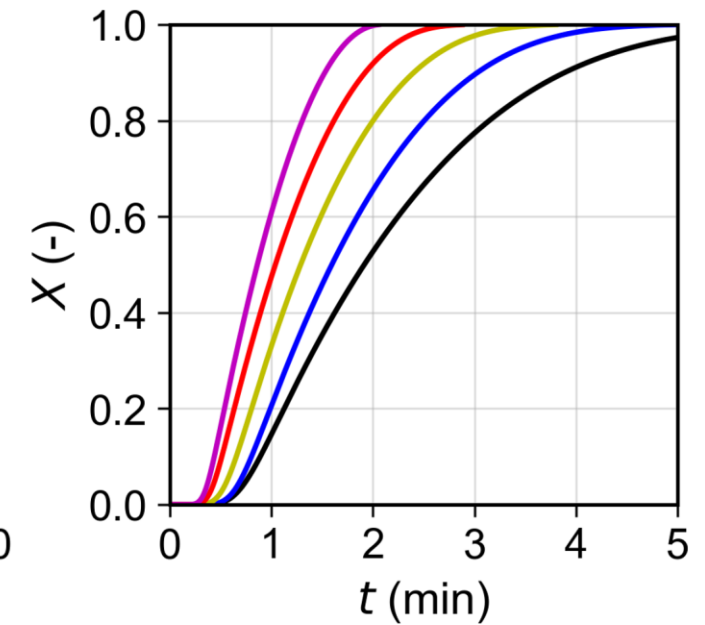
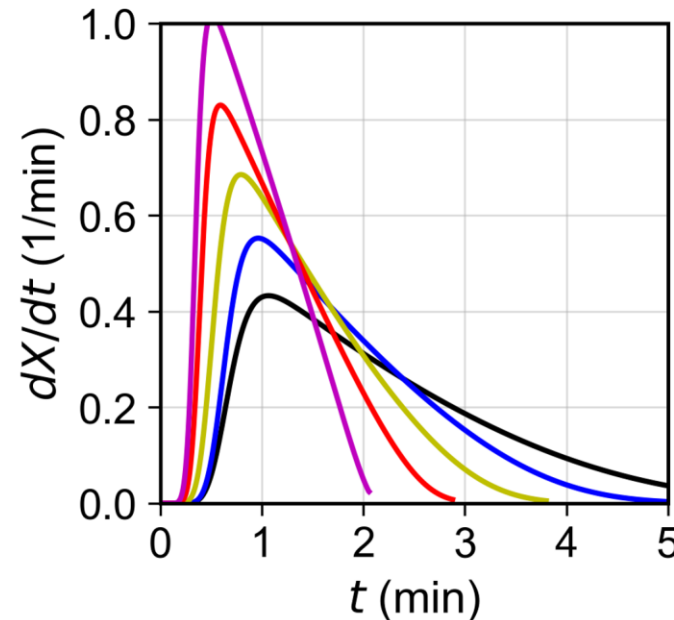
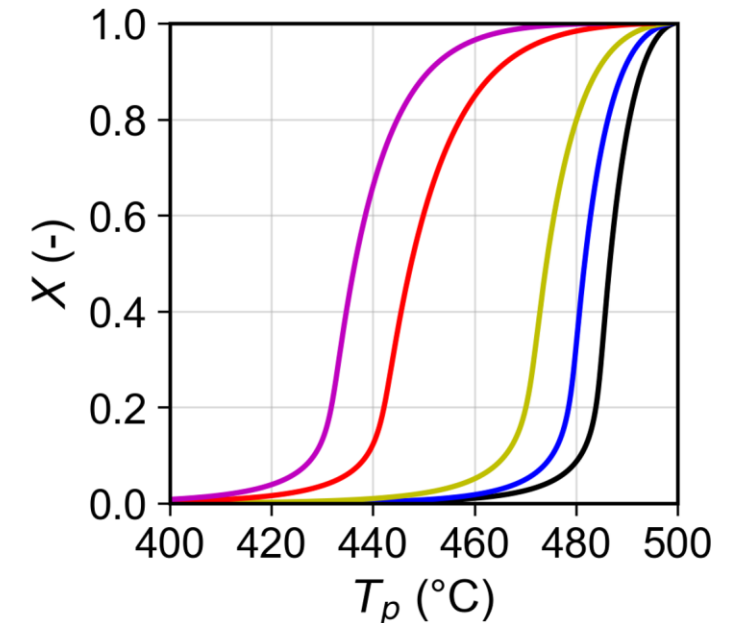
Mass and energy balance

$$-\frac{dm_p}{dt} = \dot{r} \quad \text{Reaction rate}$$

$$m_p c_{p,p} \frac{dT_p}{dt} = \alpha A_p (T_R - T_p) - \Delta h_r \dot{r}$$

Heat transfer coefficient

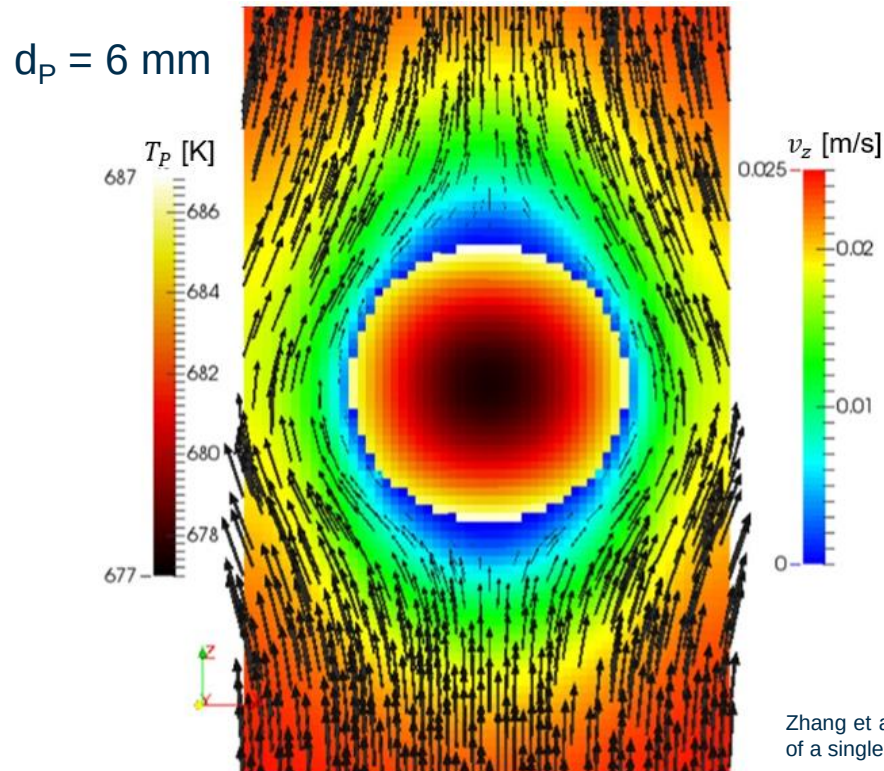
Reaction enthalpy



F. Zhang et al., Numerical simulation of thermal decomposition of polyethylene with a single-particle model. In "Advances in Computational Heat and Mass Transfer", vol. 1, Springer Cham, 2024.
 F. Zhang et al., Assessment of the interplay between convective heat transfer and reaction kinetics during plastic pyrolysis, Particuology, accepted, 2026.

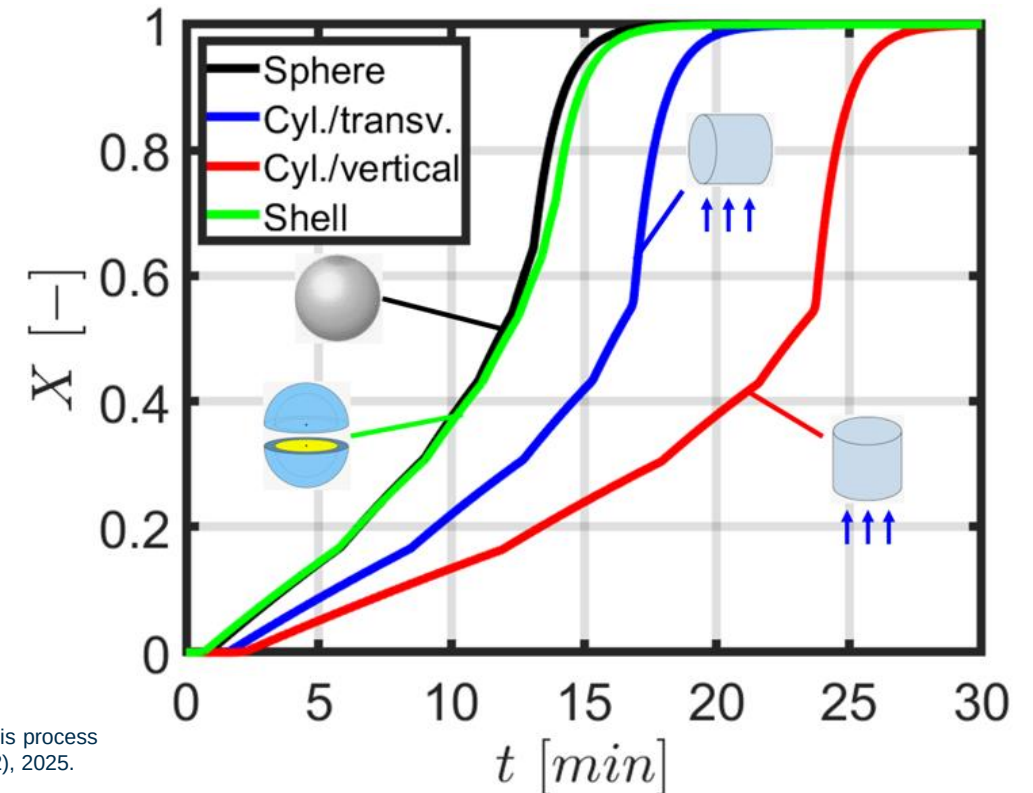
2. Particle-resolved simulation (3D)

- ❑ Non-ideal, thermally-thick
- ❑ Eulerian-Eulerian simulation
- ❑ Resolution of particle-internal gradients and boundary layers



Zhang et al., Particle-resolved simulation of pyrolysis process of a single plastic particle. Heat Mass Transf. 61 (12), 2025.

- ❑ Large deviations between particle-resolved and Lagrangian methods for large particles
- ❑ Significant impact of particle shape



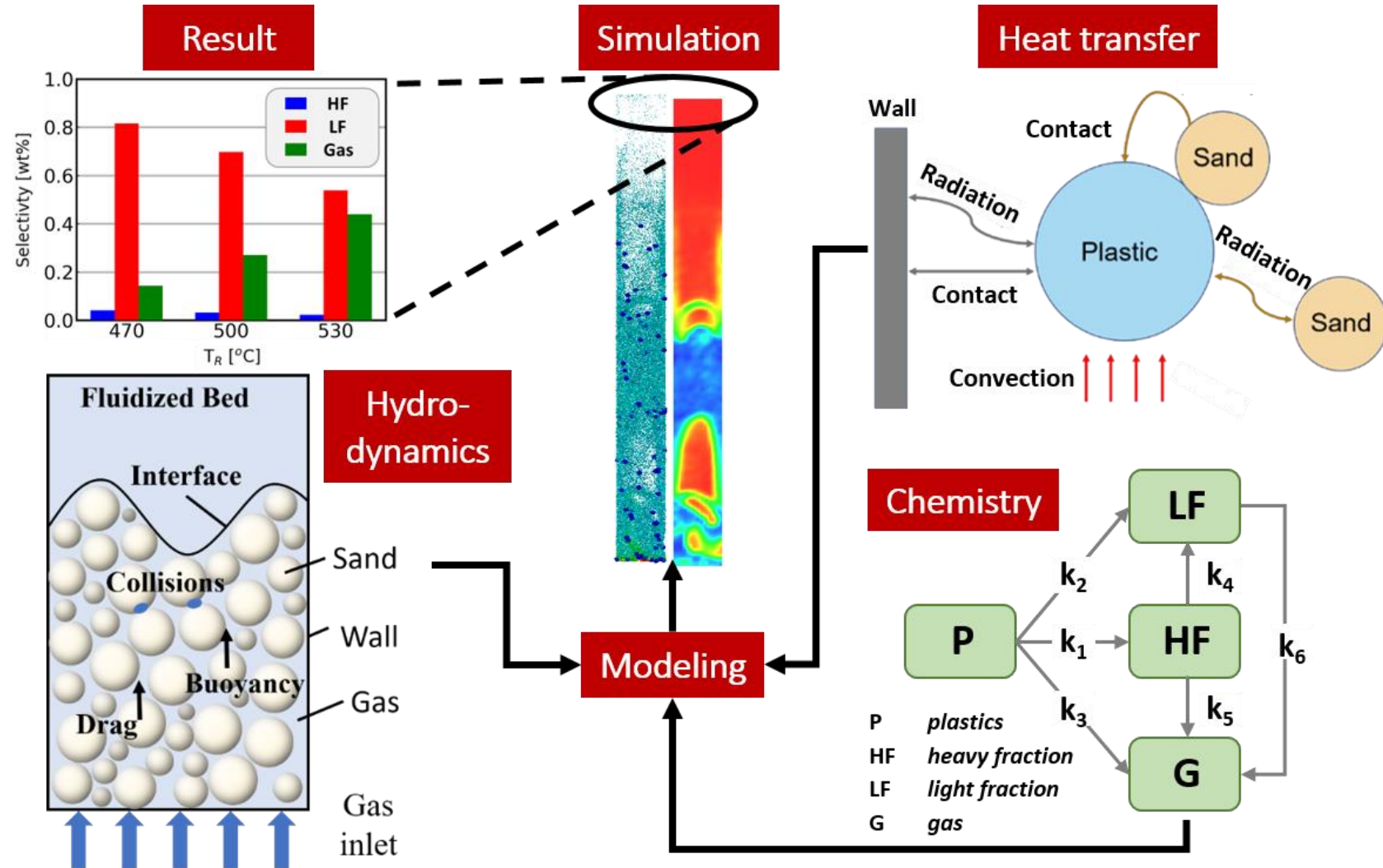
3. Fluidized bed reactor – setups

Fluidized bed reactor (FBR)

- ❑ Bed material: sand, 500 °C
- ❑ PSD: $d_m \sim 0.26$ mm
- ❑ Fluidizing agent: CH_4
- ❑ Polypropylene (PP), 1.5–2.5 mm
- ❑ Continuous vs. batch-wise feeding

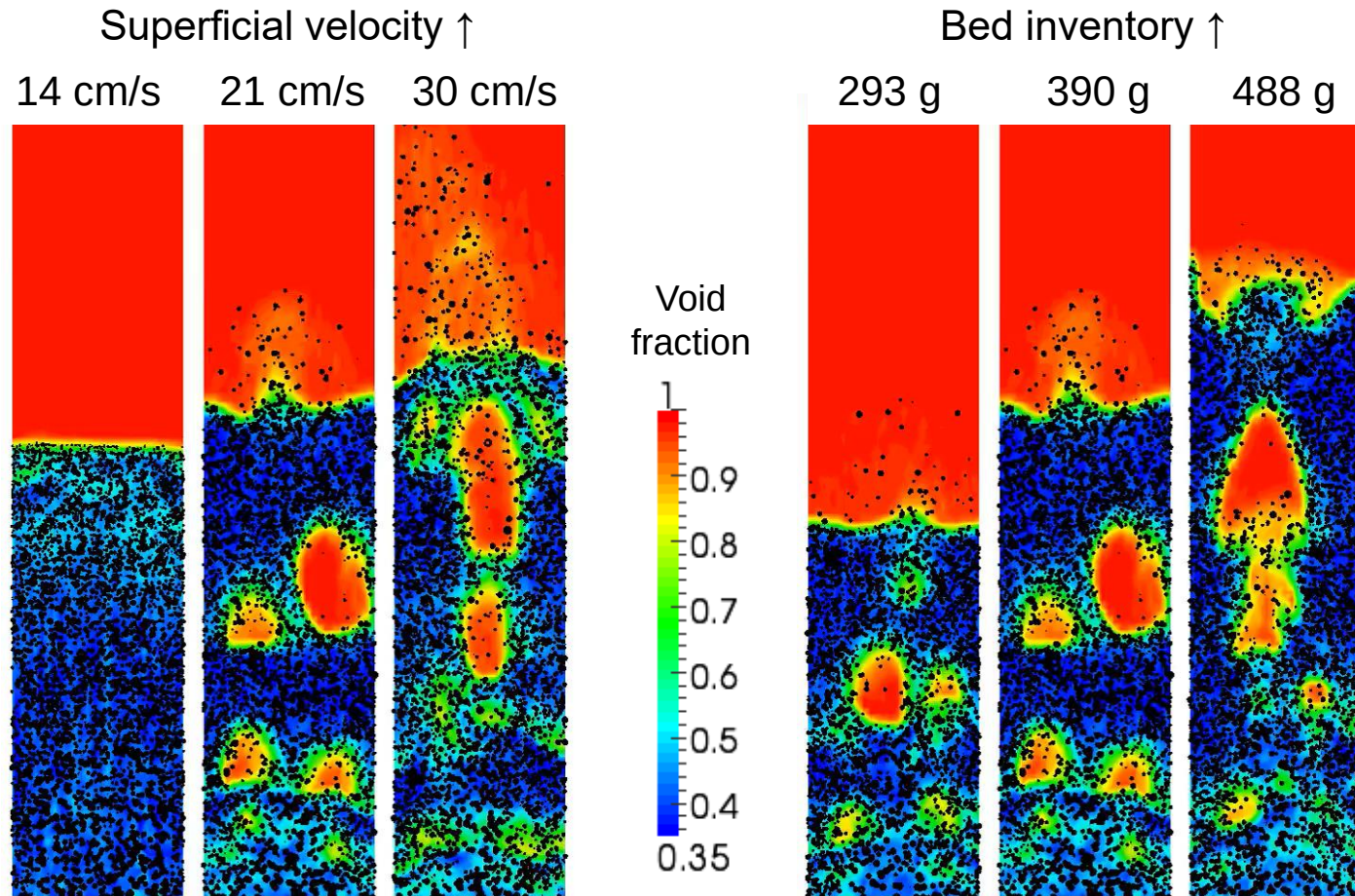
Eulerian–Lagrangian simulation

- ❑ 4-way coupling
- ❑ **Hydrodynamics**
- ❑ Heat transfer
- ❑ Thermo-chemistry



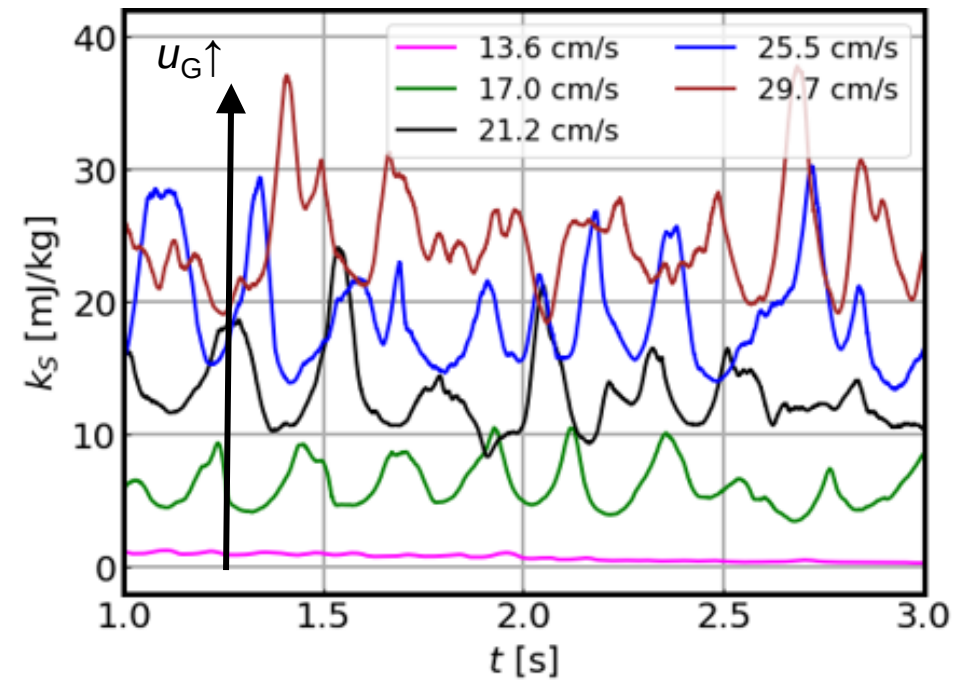
3. Fluidized bed reactor – hydrodynamics

- ❑ Good agreement with measured pressure drop and bubble size
- ❑ Strong increase of FBR's kinetic energy with superficial velocity and bed inventory



Specific kinetic energy

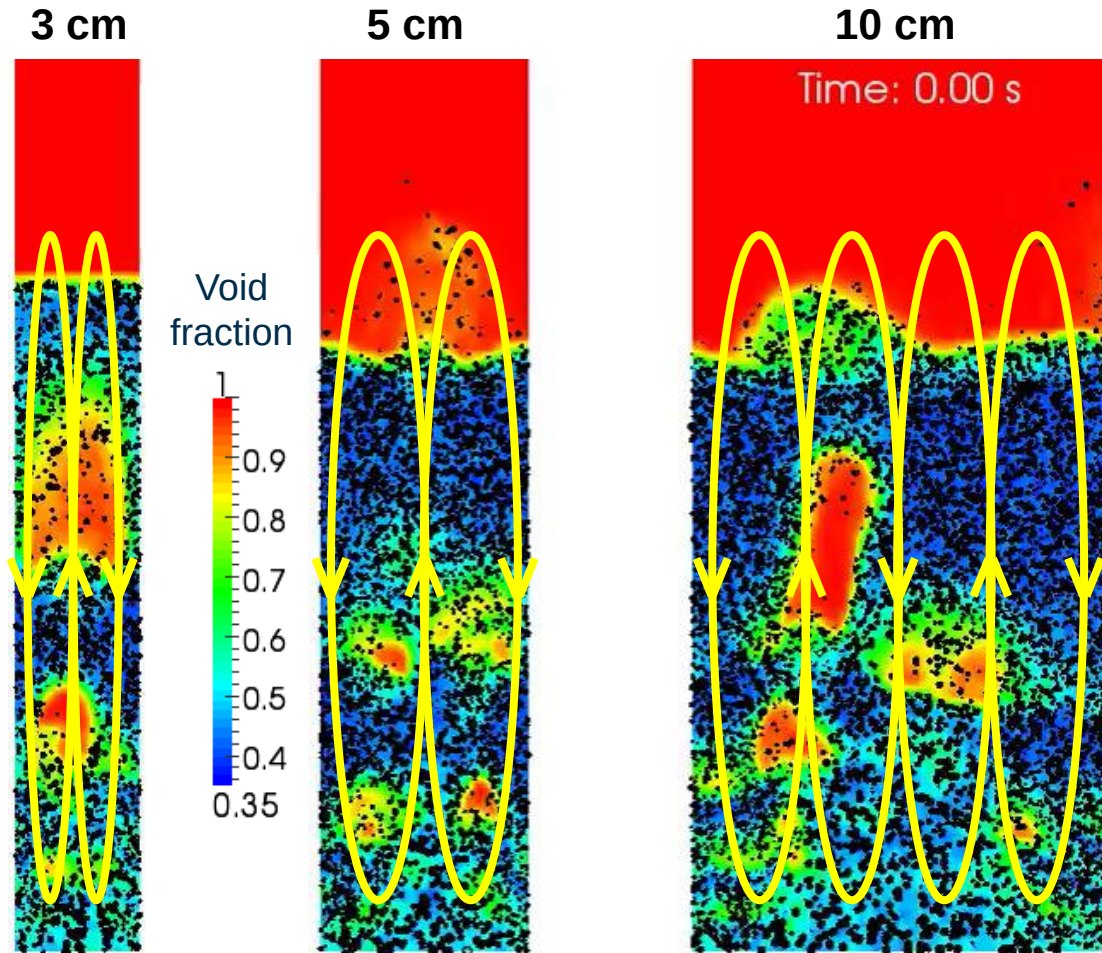
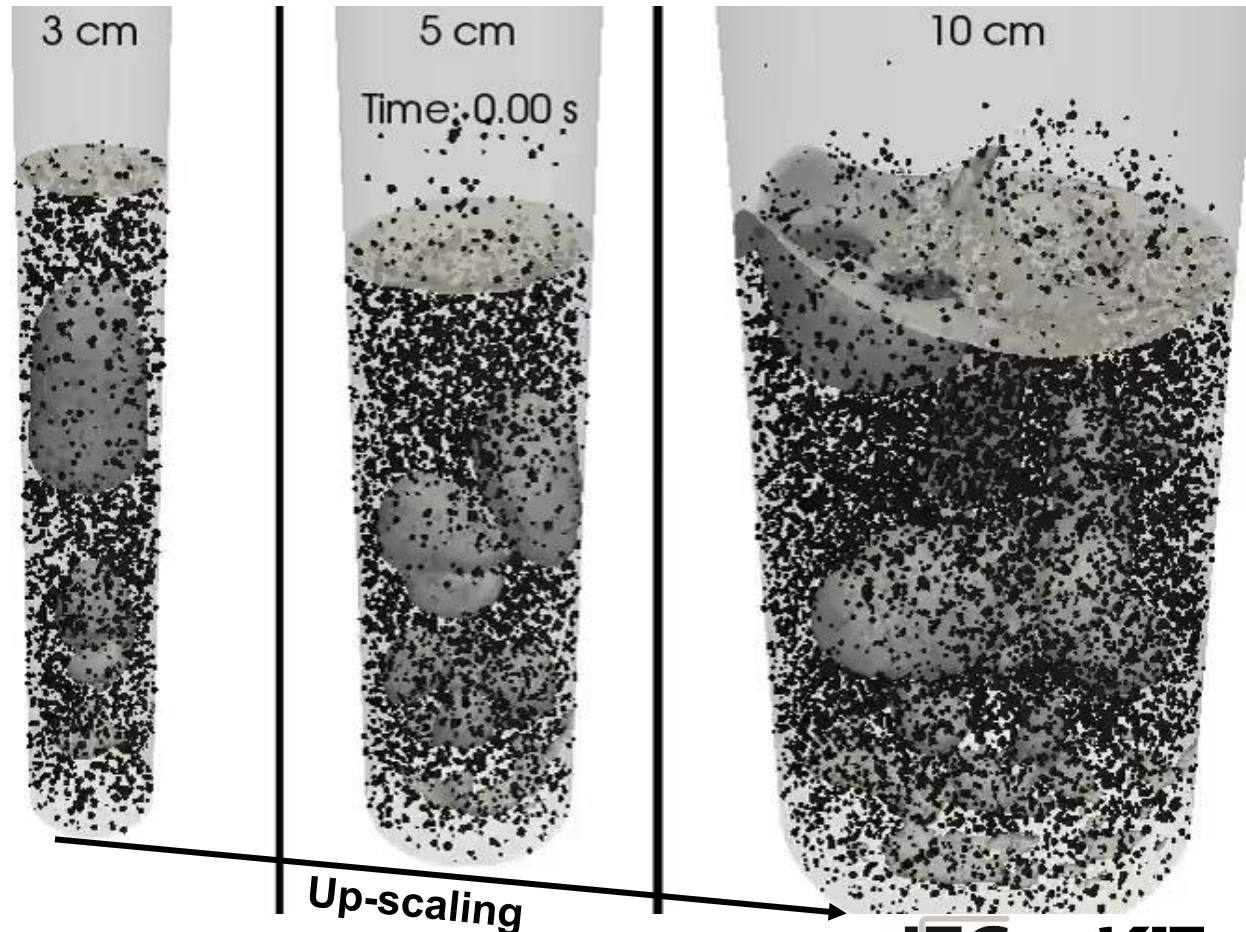
$$k_S = \frac{1}{m_S} \sum_{i=1}^{N_p} \frac{1}{2} m_{p,i} v_{p,i}^2$$



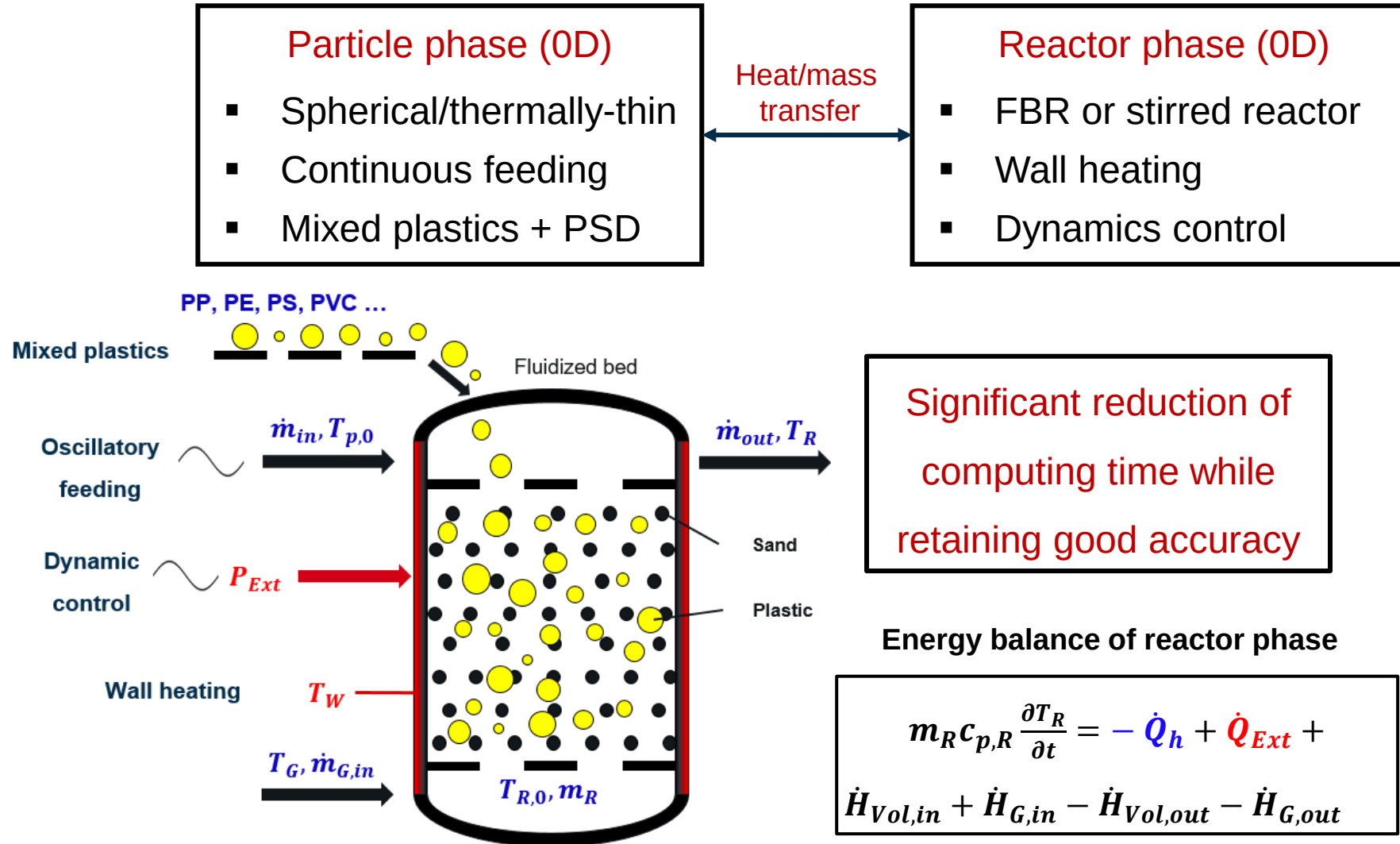
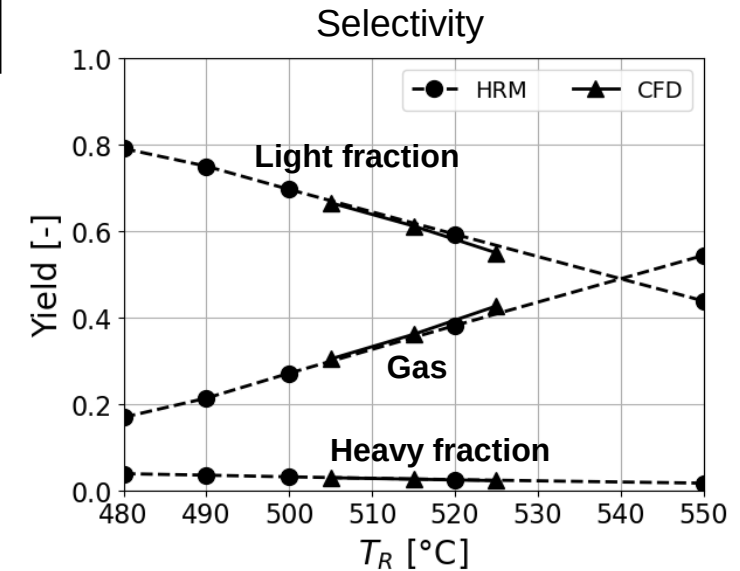
Zhang et al., Assessment of Dynamic Characteristics of Fluidized Beds via Numerical Simulations. Phys. Fluids 36 (2), 023348, 2024.

3. Fluidized bed reactor – hydrodynamics

- ❑ Transition to multiple-column bubbling while **up-scaling**
- ❑ Increase of FBR's kinetic energy with reactor size

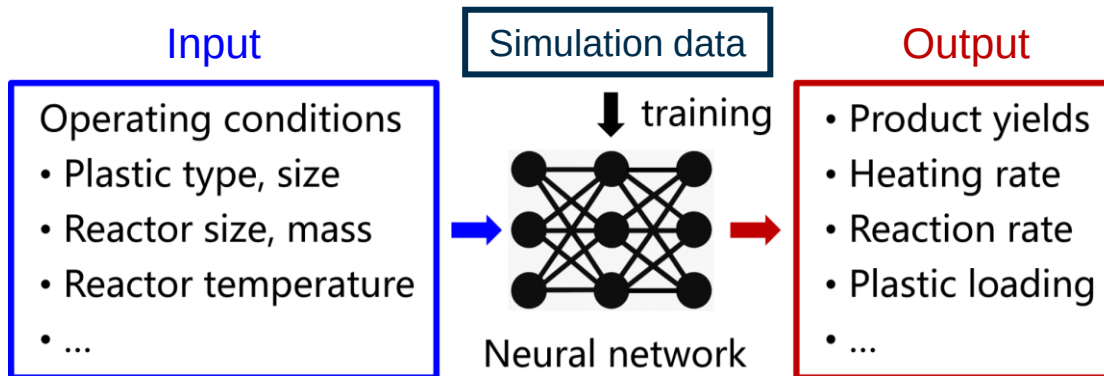
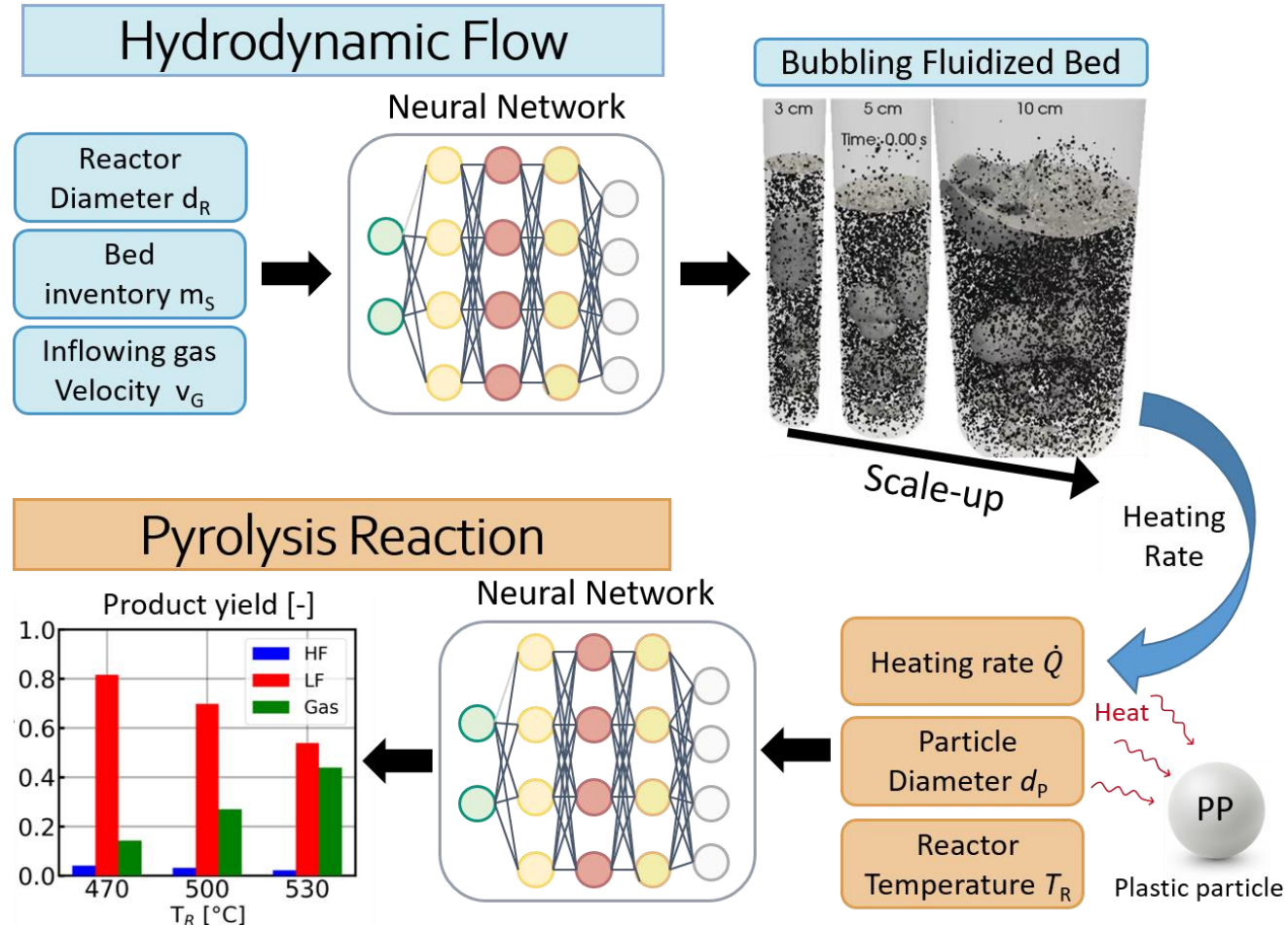


4. Homogeneous reactor (reduced order model - ROM)



5. Neural network model

- Direct prediction from operating conditions with machine learning
- Training on simulation data
- Speed-up factor ~ 20,000
- Surrogate model for rapid screening
- Data-driven scale-up model



Conclusion

■ Multi-scale modeling

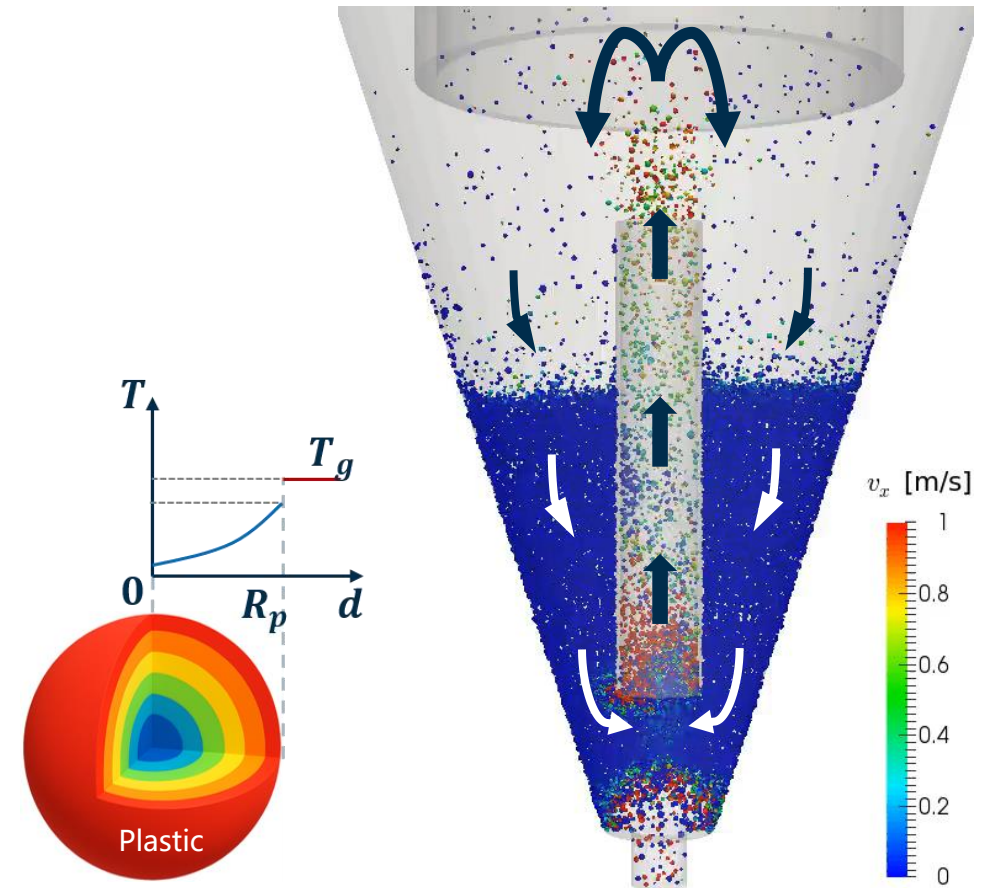
- Homogeneous particle (0D)
- Resolved particle (1D, 3D)
- Fluidized bed (3D)
- Homogeneous reactor (ROM)
- Neural network (data-driven)

■ Challenges

- Plastic melting/morphology
- Gas-solid flow/heat transfer
- Thermo-chemistry/mixed plastics
- Scale-up/computational effort
- Digital reactor scale-up
 - Multi-scale thermo-physical closures
 - Detailed/simplified chemistry
 - ROM, ML surrogate models

■ Future trends

Thank you for listening!



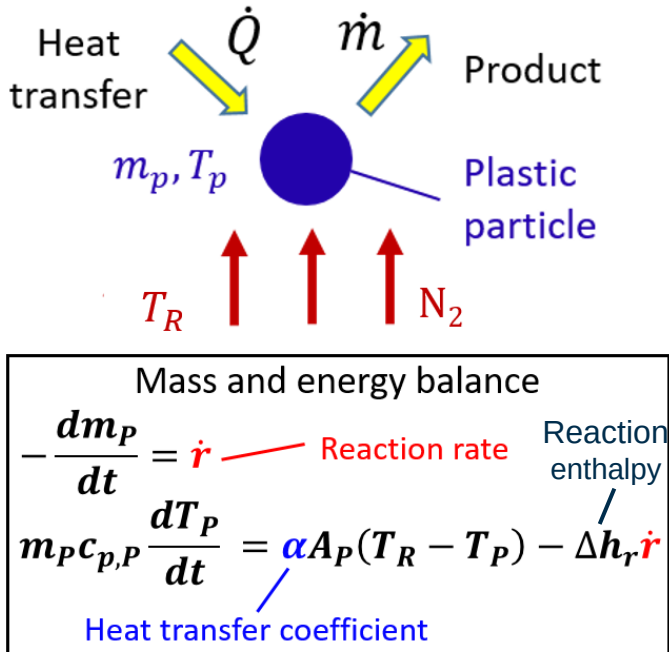
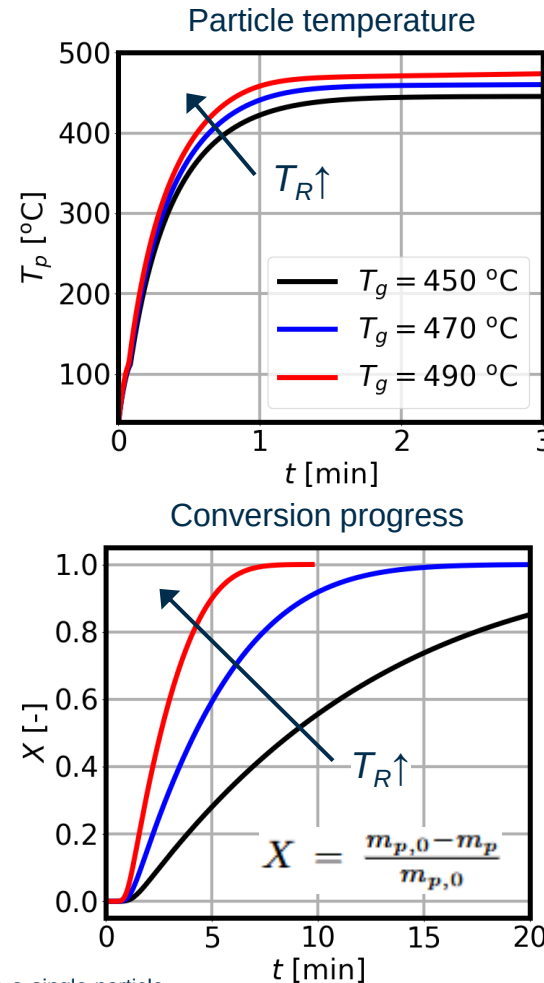
Appendix

Outline

- Motivation
- Modeling of plastic pyrolysis
 - Homogeneous particle
 - Particle-resolved modeling
 - Fluidized bed reactor
 - Reduced order model (ROM)
 - Data-driven prediction
- Summary

1. Single-Particle Model

- Ideal/spherical
- Homogeneous/thermally-thin

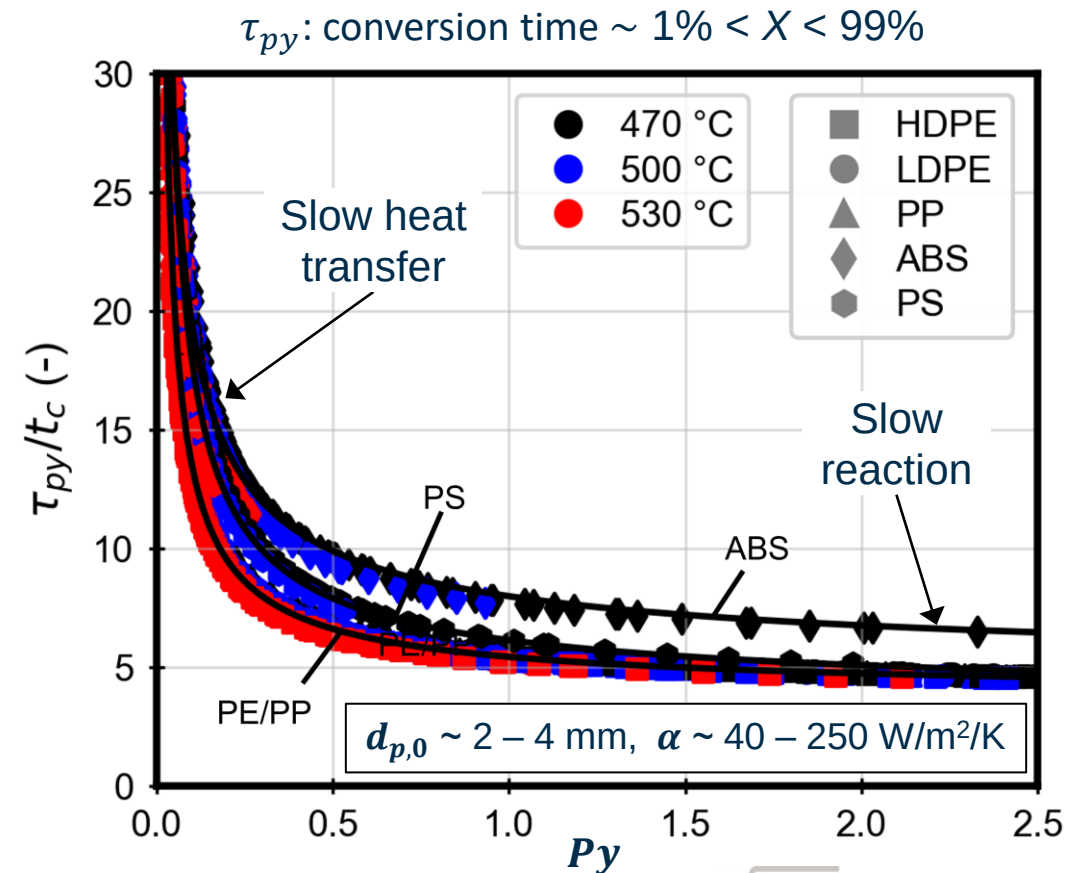


- Heat transfer vs. pyrolysis reaction

$$Py = \frac{\text{Time scale of chem. react.}}{\text{Time scale of heat transfer}} = \frac{t_c}{t_h} = \frac{\alpha}{k_r \rho_P c_{p,P} d_{p,0}}$$

Heat transfer coefficient α

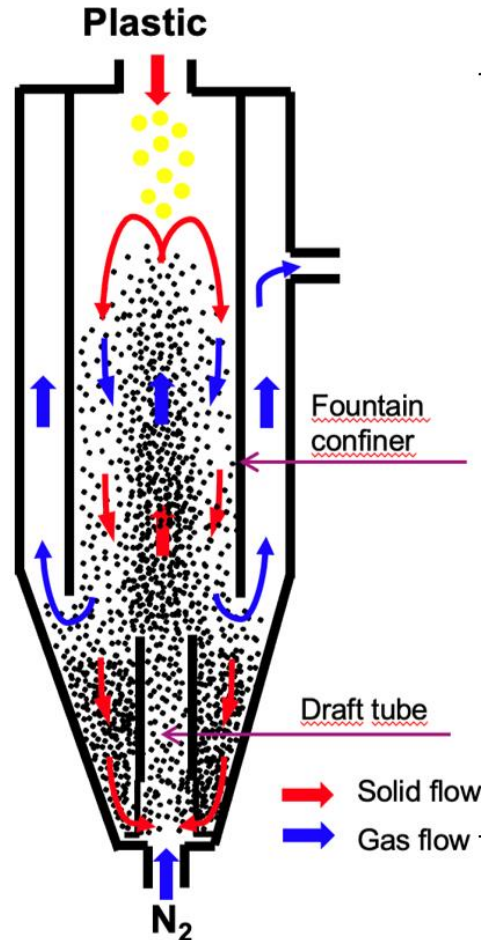
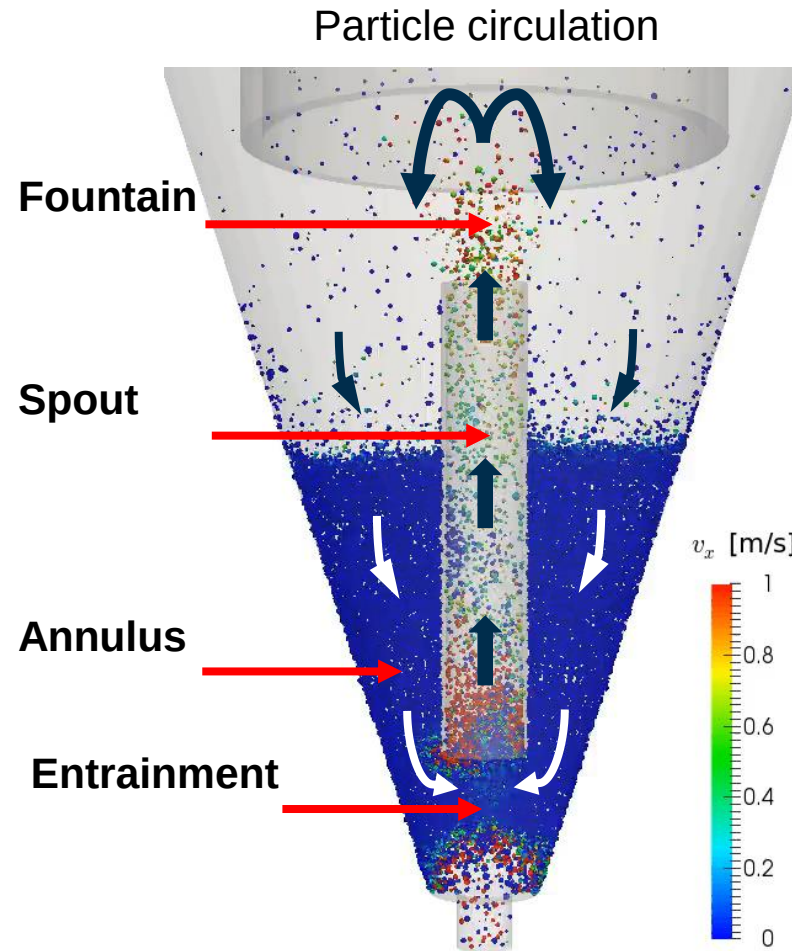
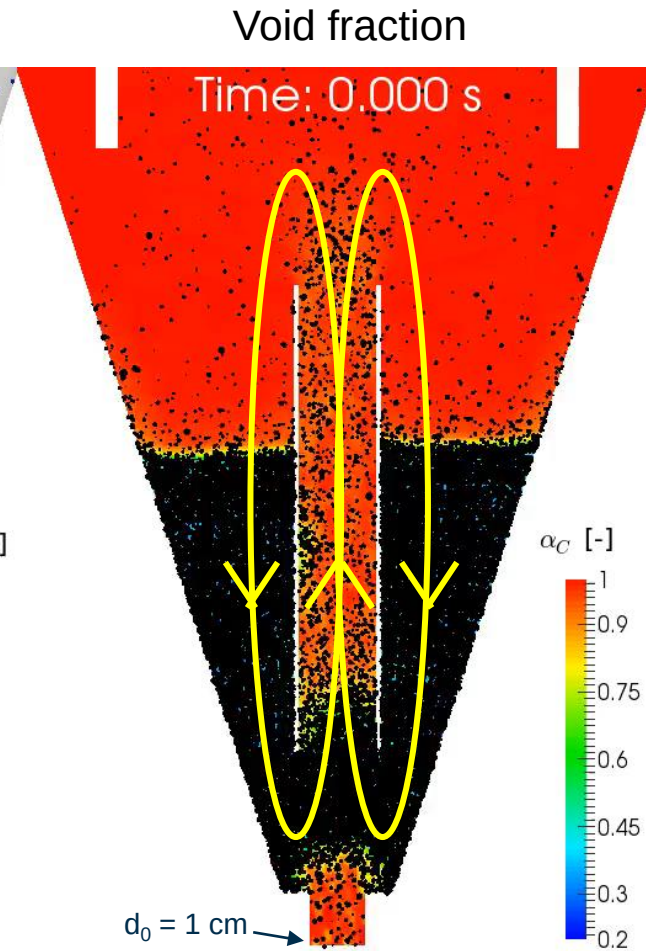
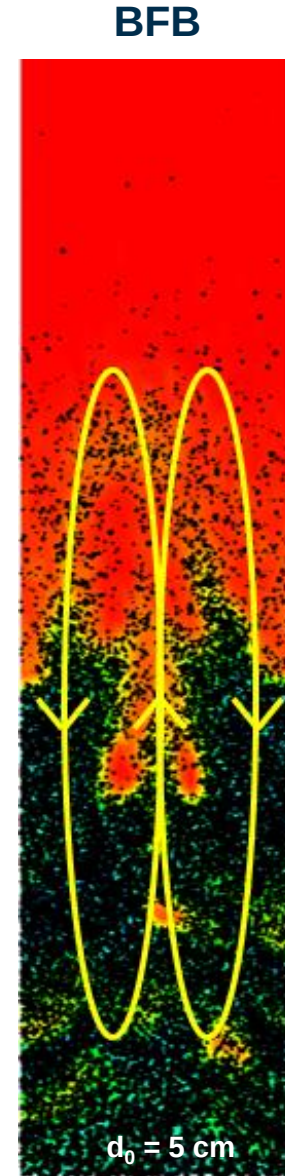
Reaction rate coefficient k_r



3. Simulation of conical spouted fluidized bed

- **Conical** reactor wall
- High gas velocity $u_{G,CSFB} \gg u_{G,BFB}$

- Higher kinetic energy than BFB
→ Avoid defluidization and clogging

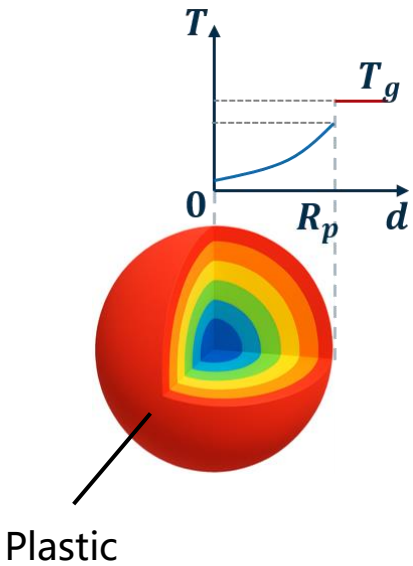




Modeling of Plastic Pyrolysis

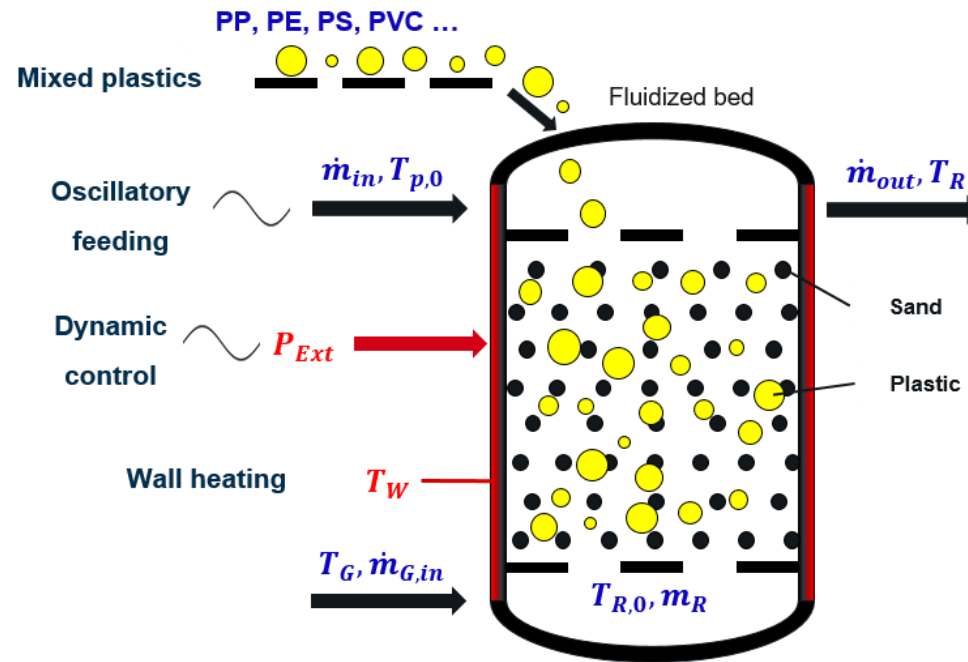
Single plastic particle

- Heat transfer vs. reaction
- Homogeneous (0D)
- Particle-resolved (1D)



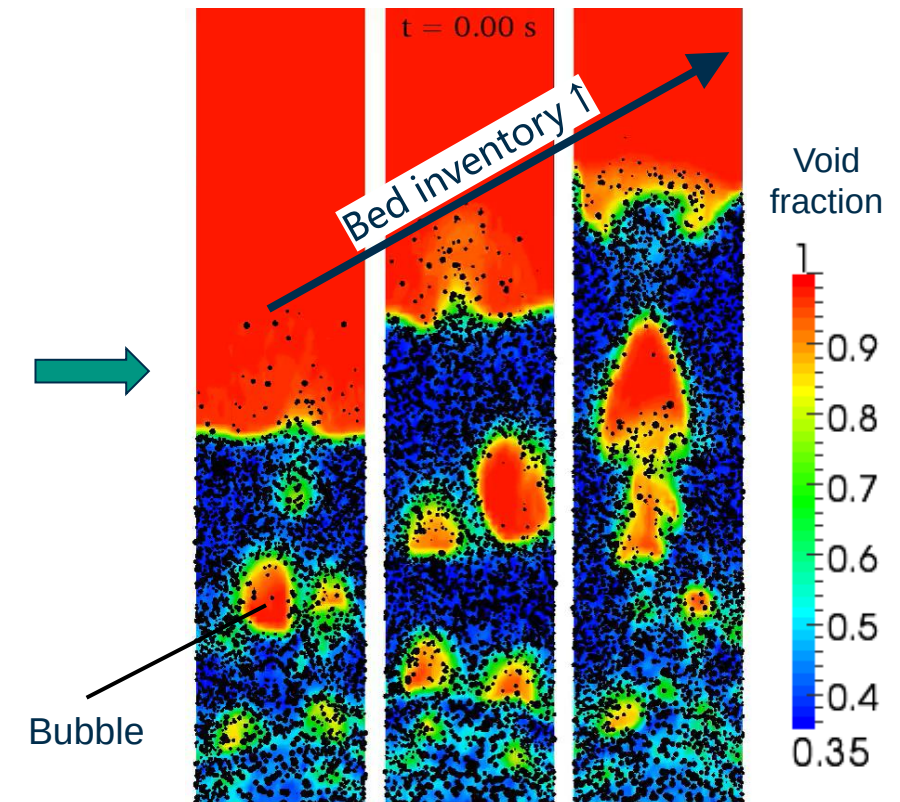
Stirred tank (reduced-order, 0D)

- Continuous feeding of mixed plastics
- Dynamic control of reactor temperature



Bubbling fluidized bed

- Spatially-resolved (CFD, 3D)
- Effect of hydrodynamics



F. Zhang et al. Particle-resolved simulation of pyrolysis process of a single plastic particle. *Heat Mass Transf.* 61 (12), 2025.

F. Zhang et al. Assessment of Dynamic Characteristics of Fluidized Beds via Numerical Simulations. *Phys. Fluids* 36 (2), 023348, 2024.