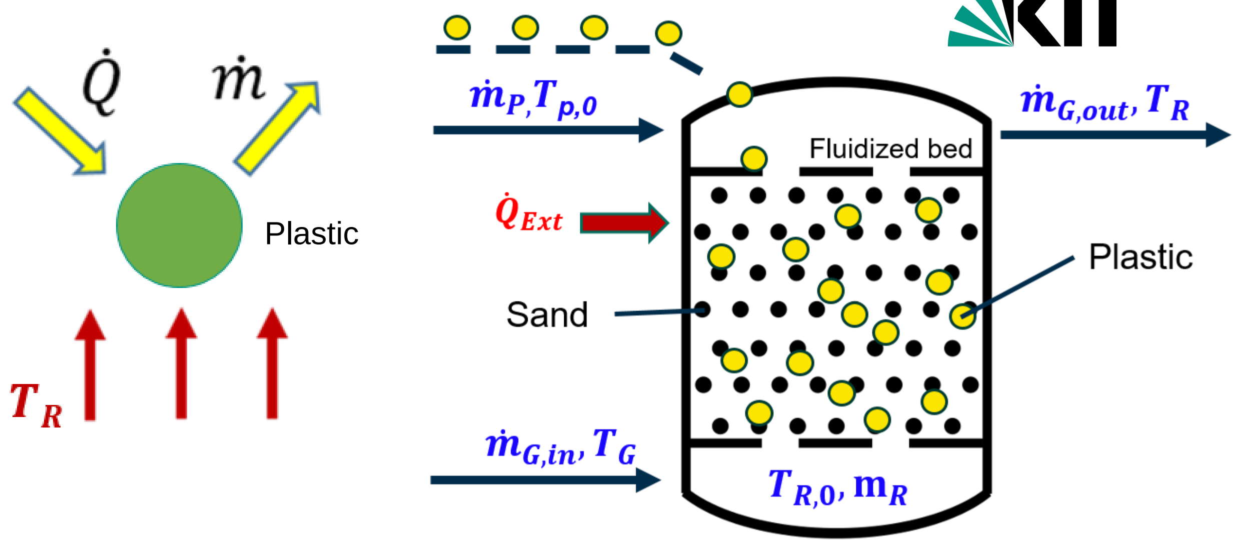
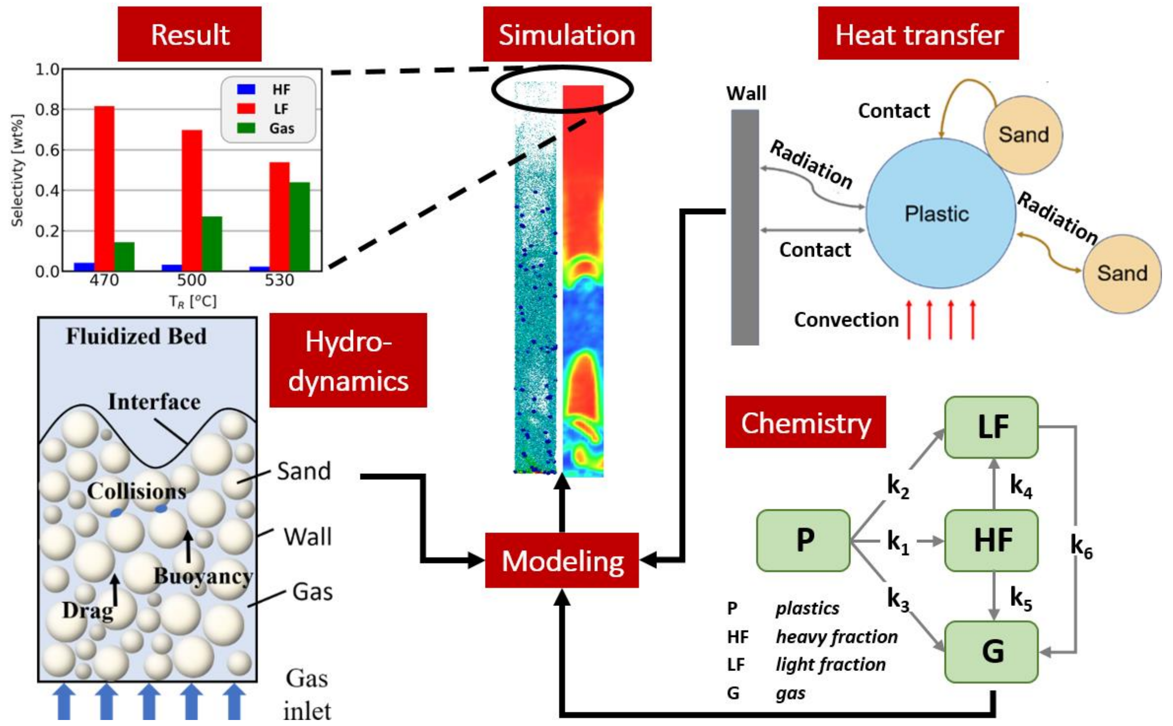
# Numerical Simulation of Plastic Pyrolysis

Reduced-order (0D)




CFD (3D)

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# Outline

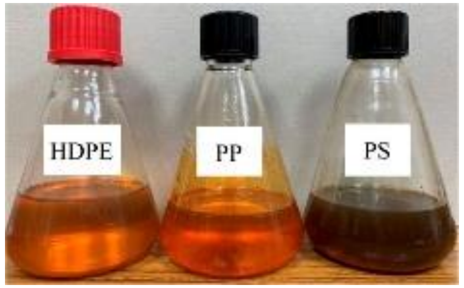
- Motivation
- Modeling of plastic pyrolysis
  - Single-particle model (0D)
  - Particle-resolved simulation (3D)
  - Eulerian-Lagrangian simulation of fluidized bed (3D)
  - Homogeneous reactor model (reduced-order, 0D)
- Summary

# Why modeling plastic pyrolysis

- ❑ **460 Mt** plastic waste per year, **9%** recycled
- ❑ **Chemical recycling**: converting plastic waste into secondary raw materials
  - Capable of **mixed/contaminated** plastics
- ❑ **Challenges**
  - **High cost** for large-scale experiments
  - **Real-flow** effects

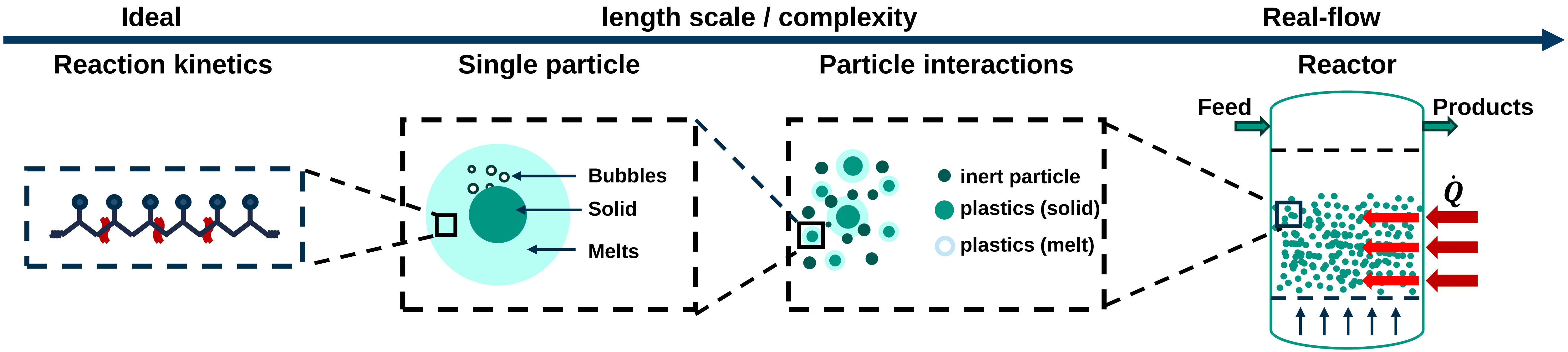
Plastic waste

Pyrolysis




Pyrolysis oil

http://dx.doi.org/10.1039/d3ra08150h



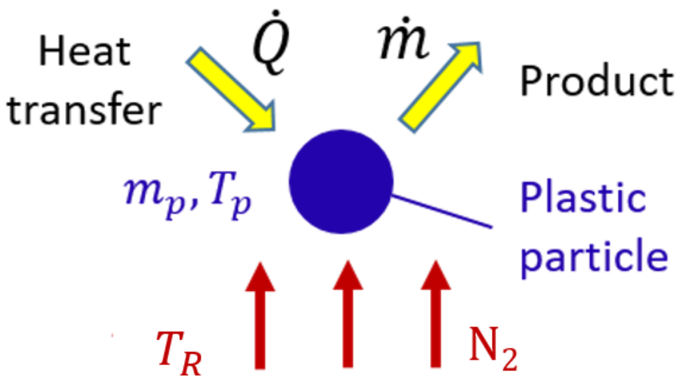
# 1. Single-particle model (0D)

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

Heat transfer coeff. ($\alpha$)

Reaction rate coeff. ($k_r$)

- ❑ **Ideal, thermally-thin/homogeneous**
- ❑ **Heat transfer vs. pyrolysis reaction**



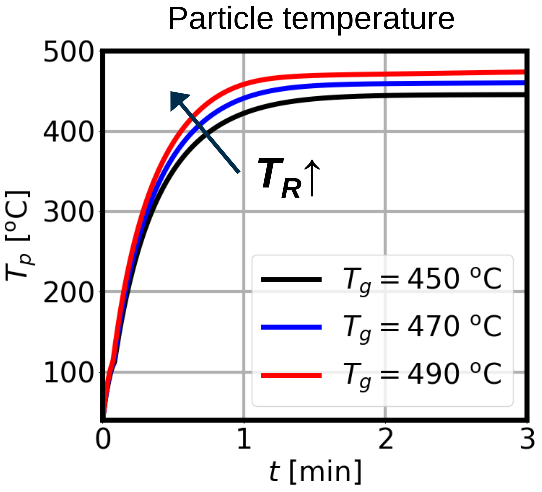

**Mass and energy balance**

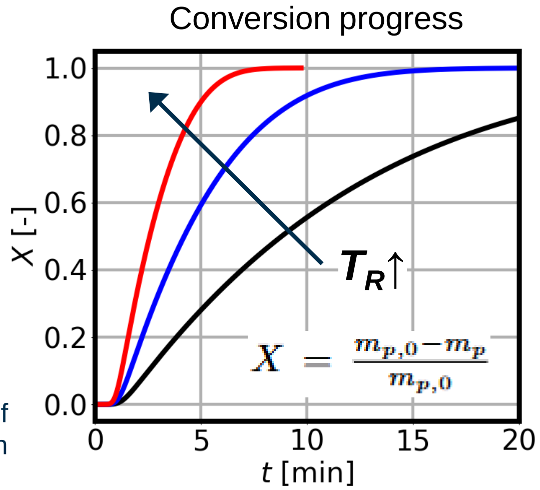
$$-\frac{dm_P}{dt} = \dot{r}$$ — Reaction rate

$$m_P c_{p,P} \frac{dT_P}{dt} = \alpha A_P (T_R - T_P) - \Delta h_r \dot{r}$$

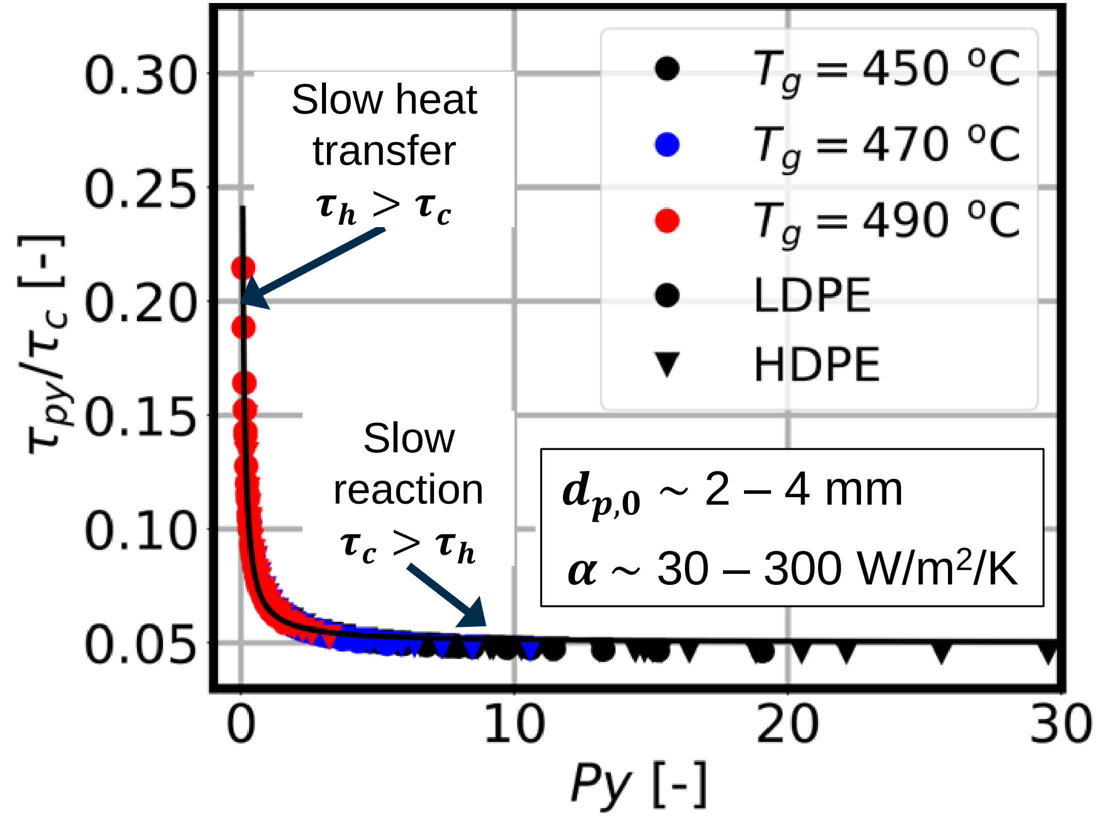
Reaction enthalpy ($\Delta h_r$)

Heat transfer coefficient ($\alpha$)




$\tau_{py}$: pyrolysis duration ~ 1% < $X$ < 99%



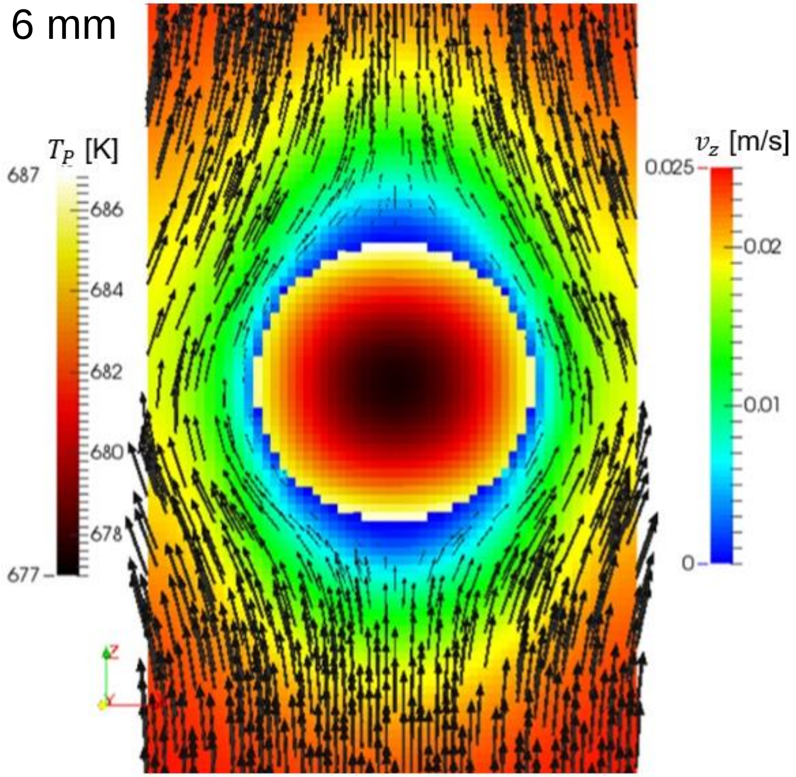

F. Zhang et al. Numerical simulation of thermal decomposition of polyethylene with a single-particle model. In "Advances in Computational Heat and Mass Transfer", vol. 1, Springer Cham, 2024.

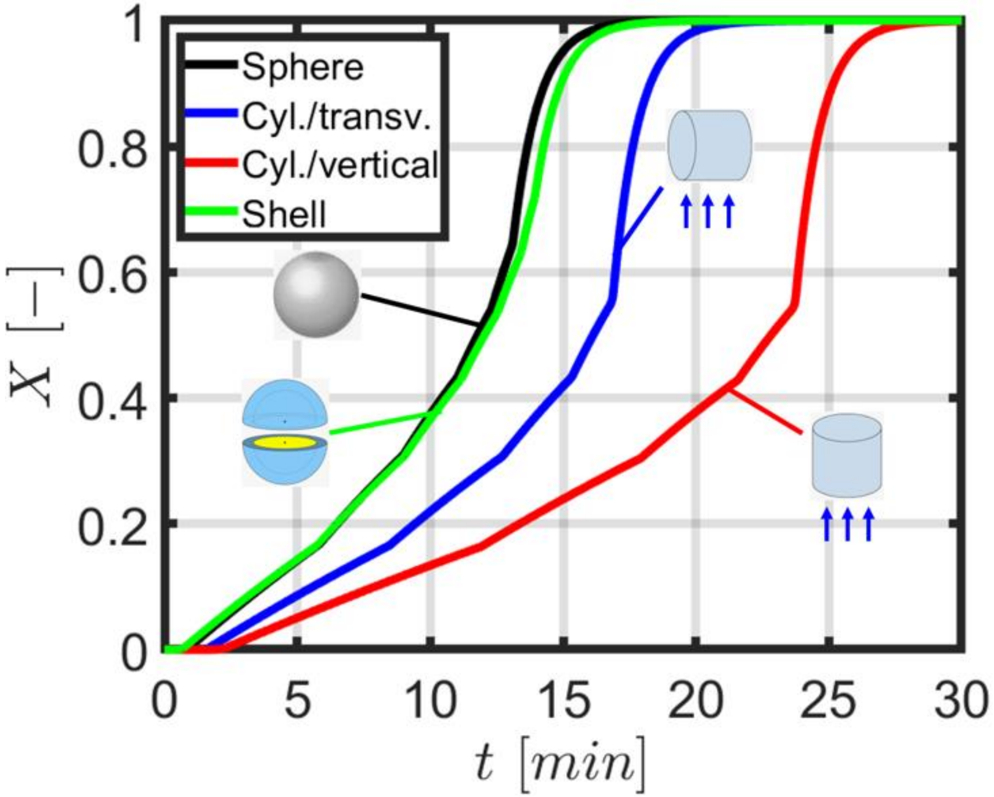
# 2. Particle-resolved simulation (3D)

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

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

$d_P$ = 6 mm




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

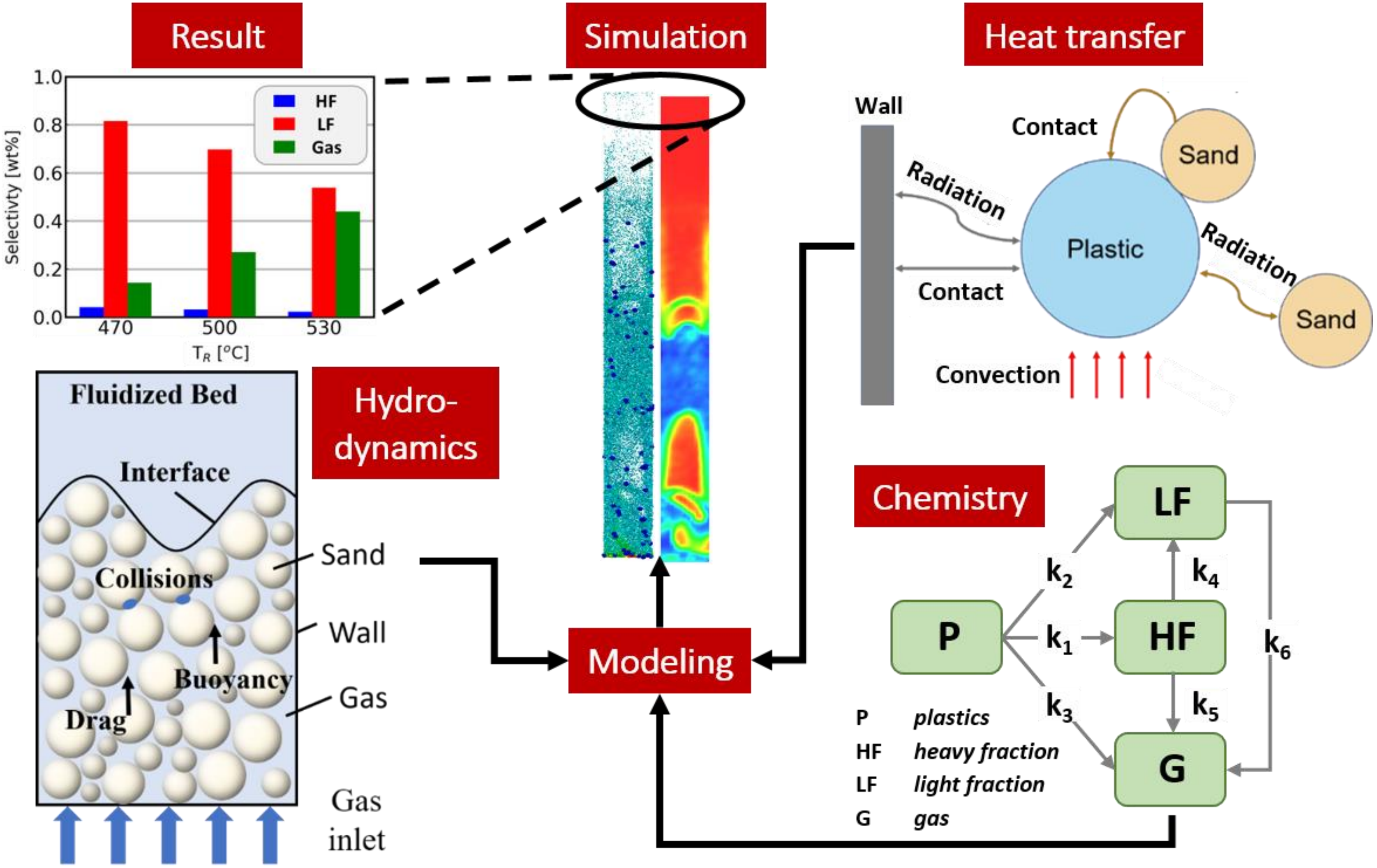
# 3. Eulerian-Lagrangian simulation of fluidized bed – setups

**Fluidized bed**

- Bed material: sand, 500 °C
- PSD: $d_m$ ~ 0.23 mm
- Fluidizing agent: $CH_4$
- Plastic: polypropylene (PP), 1.5 – 2.5 mm, 25 °C
- Continuous/batch-wise feeding

**Challenges**

- Hydrodynamics
- Heat transfer
- Reaction kinetics

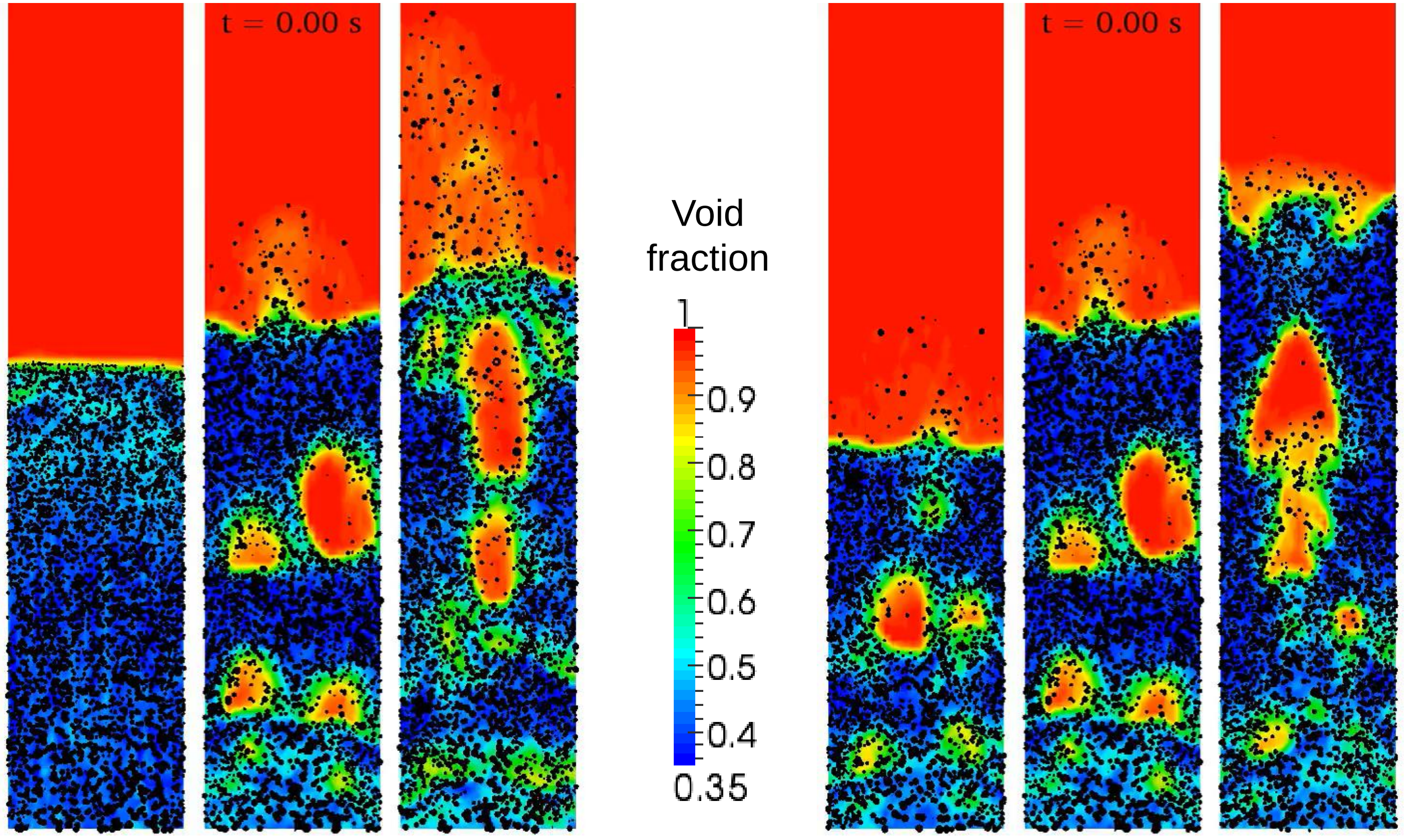


# 3. Eulerian-Lagrangian simulation of fluidized bed – hydrodynamics

- Good agreement with experiments for pressure drop & bed height

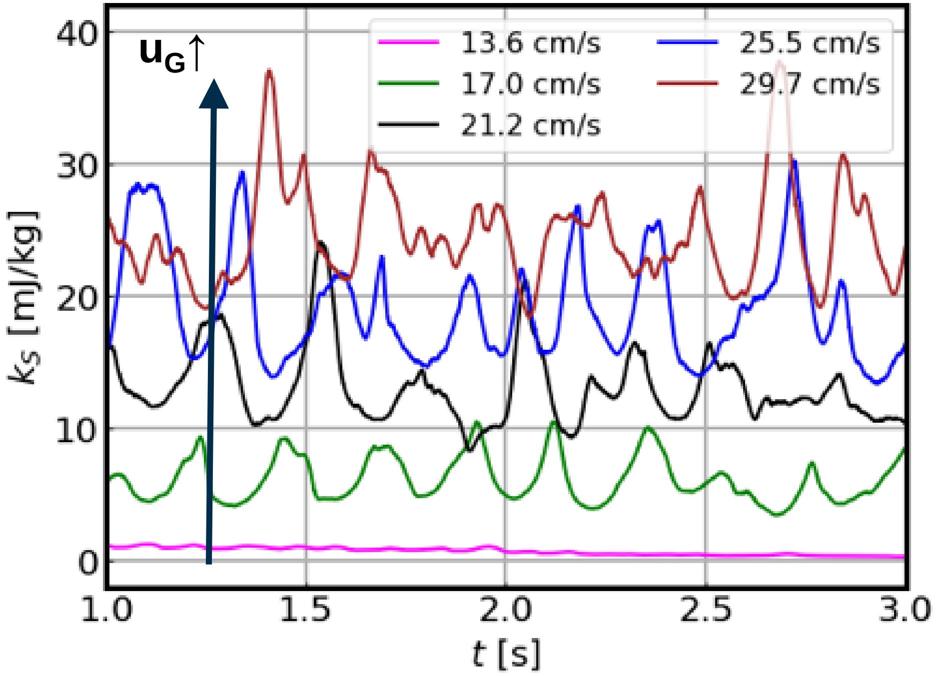
**Superficial velocity ↑** **Bed inventory ↑**

14 cm/s 21 cm/s 30 cm/s 293 g 390 g 488 g




Specific kinetic energy

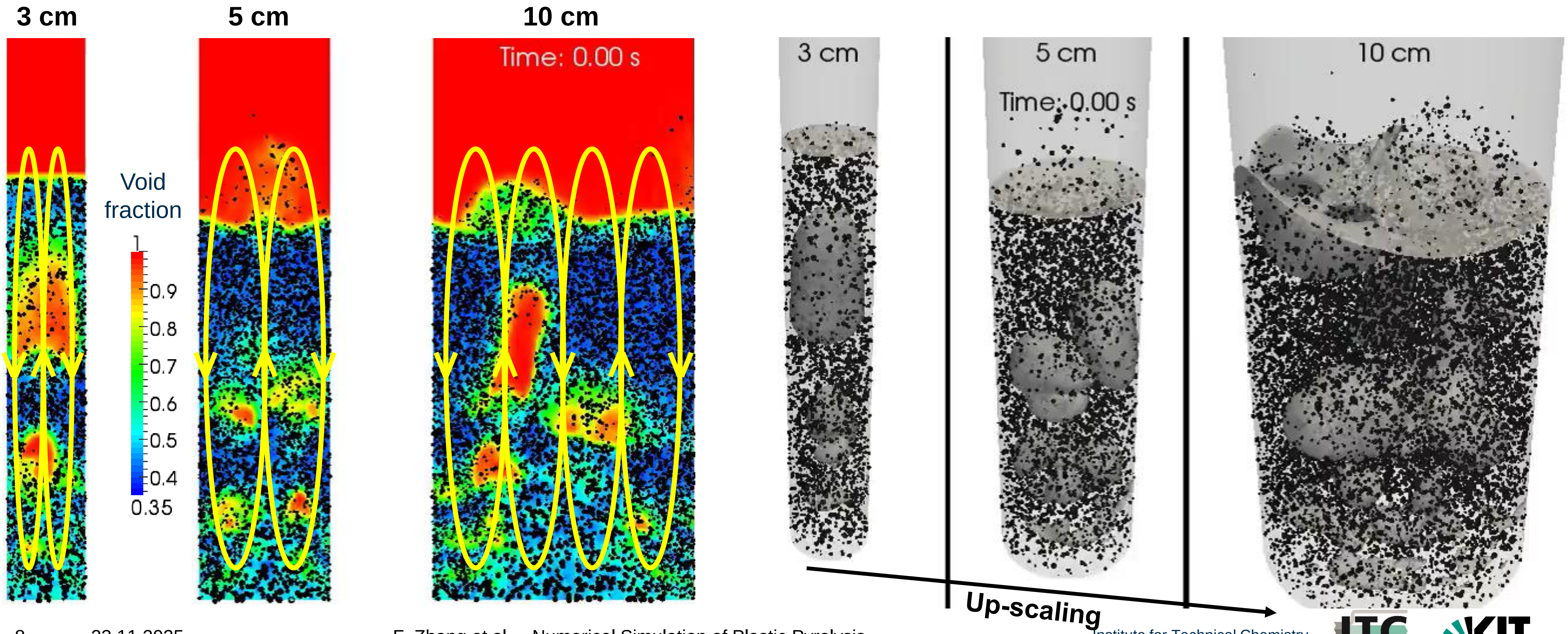
$$k_S = \frac{1}{m_S} \sum_{i=1}^{N_p} \frac{1}{2} m_{p,i} v_{p,i}^2$$




Zhang et al. Assessment of dynamic characteristics of fluidized beds via numerical simulations. Phys. Fluids 2024.

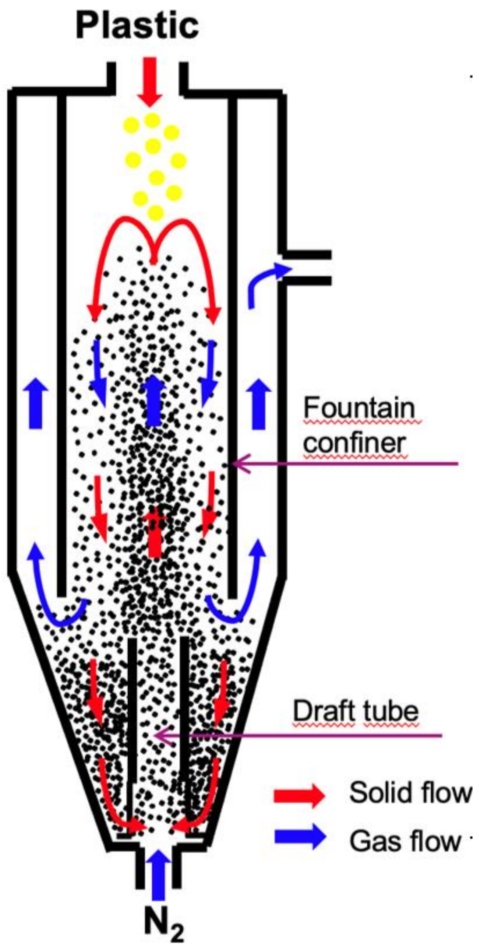
# 3. Eulerian-Lagrangian simulation of fluidized bed – up-scaling

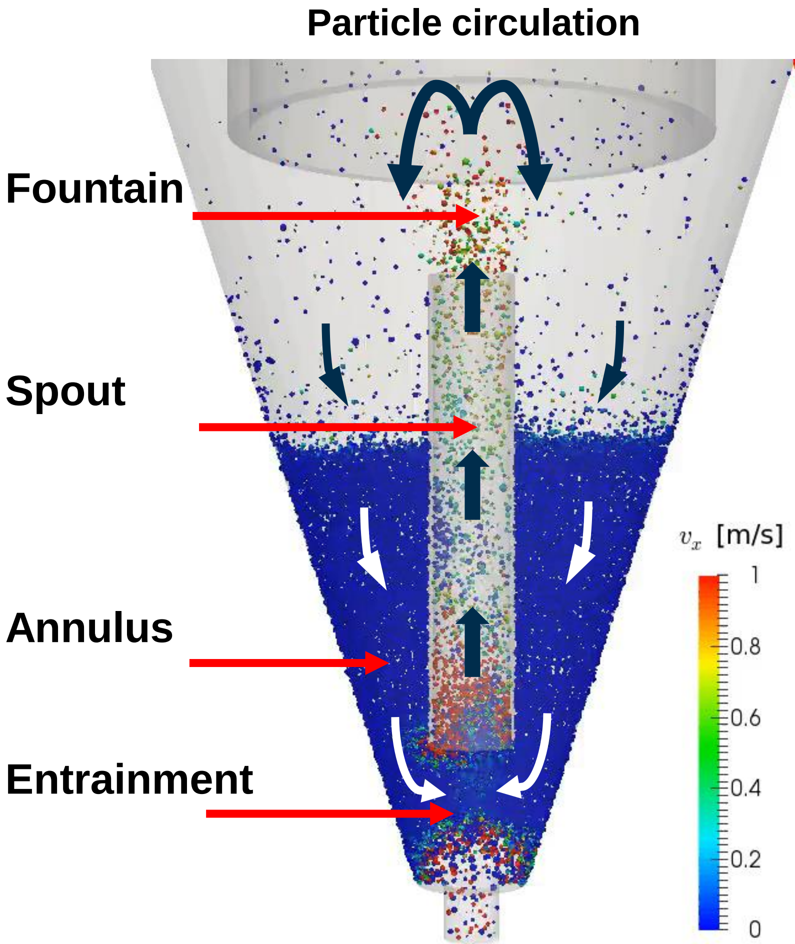
- Transition from **single- to multiple-column** bubbling while up-scaling

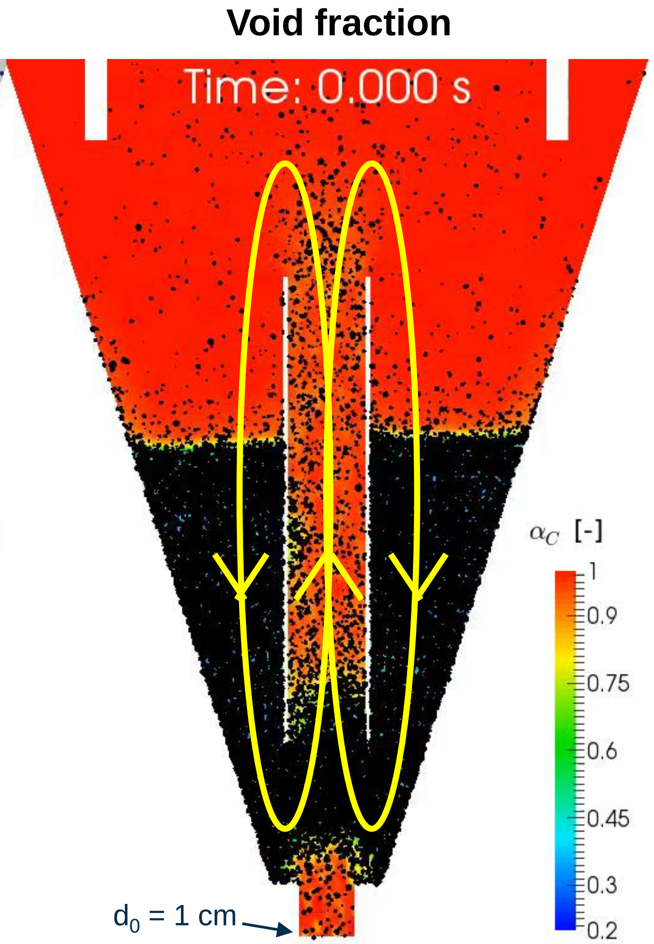


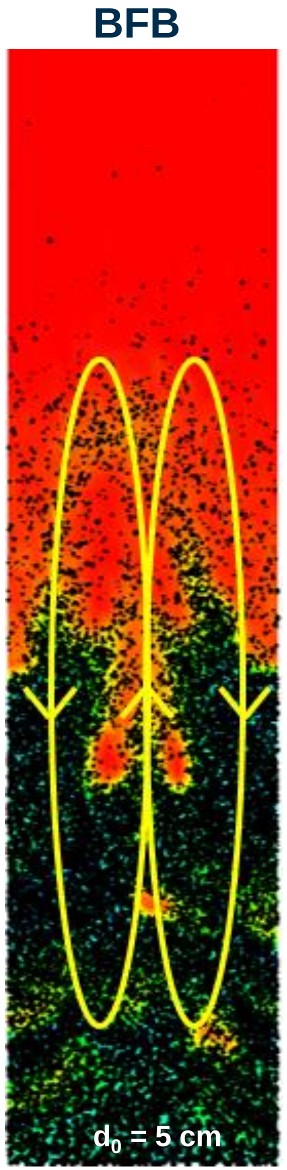
# 3. Eulerian-Lagrangian simulation of conical spouted fluidized bed

- **Conical** reactor wall
- High gas velocity $u_{G,CSFB} >> u_{G,BFB}$
- Higher kinetic energy than BFB
  → Avoid defluidization and clogging



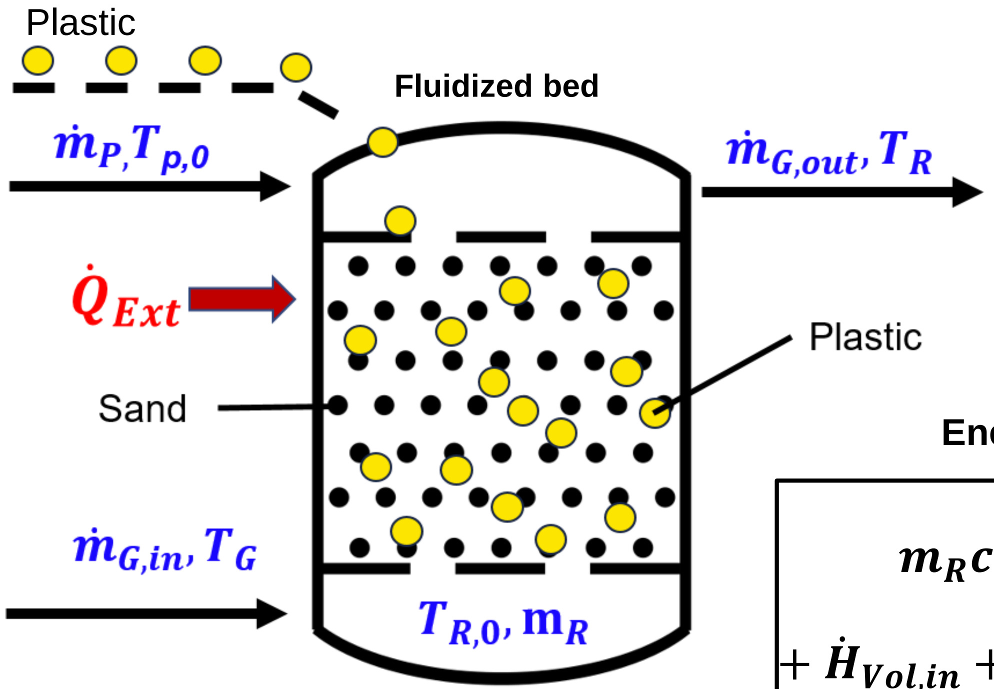



# 4. Homogeneous reactor model (reduced-order, 0D)

**Particle phase**
- Spherical/thermally-thin
- Continuous feeding
- Mass & energy balance for each individual particle

Heat transfer

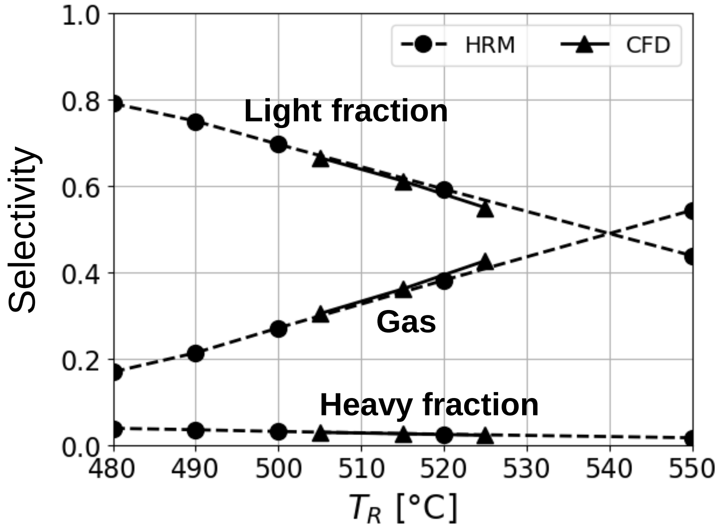
**Reactor phase**
- Fluidized bed or stirred reactor
- External heating
- Energy balance

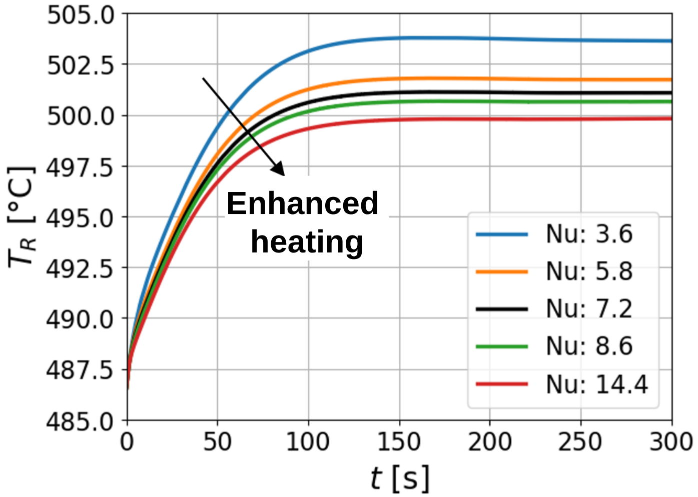



**Significantly reduced computing time while retaining overall accuracy**

**Energy balance of reactor**

$$m_R c_{p,R} \frac{\partial T_R}{\partial t} = -\dot{Q}_h + \dot{Q}_{Ext} + \dot{H}_{Vol,in} + \dot{H}_{G,in} - \dot{H}_{Vol,out} - \dot{H}_{G,out}$$



# Conclusion

- **Progresses**
  - **Homogeneous particle** heat transfer vs. chemical reaction
  - **Resolved particle** particle morphology
  - **Fluidized bed** hydrodynamics, scale-up, conical spouted bed
  - **Homogeneous reactor** improved computing efficiency
- **Challenges**
  - **Particle morphology** shape, agglomeration, attrition, breakage …
  - **Thermo-physics** melting, heat transfer, thermo-physical data …
  - **Reaction kinetics** random chain break, heterogeneous reaction …
  - **Multi-scale** disparity between length and time scales
- **Future trends**
  - **Reduced-order model** mixed plastics, size distribution, oscillatory feeding …
  - **Data-driven/ML model** hydrodynamics/heat transfer/pyrolysis, scale-up …

# Thank you for listening!