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Particle-resolved numerical simulation of pyrolysis process of a non-ideal plastic particle

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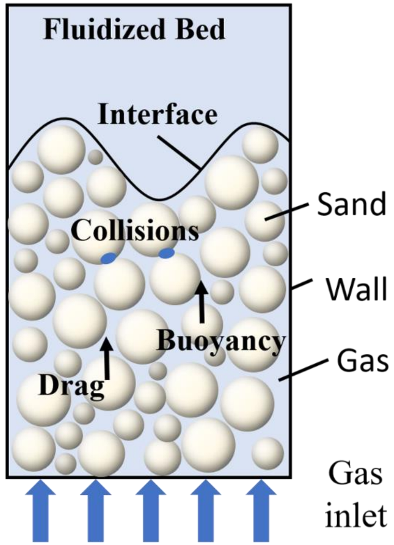
Institute for Technical Chemistry (ITC)



Multiphysics

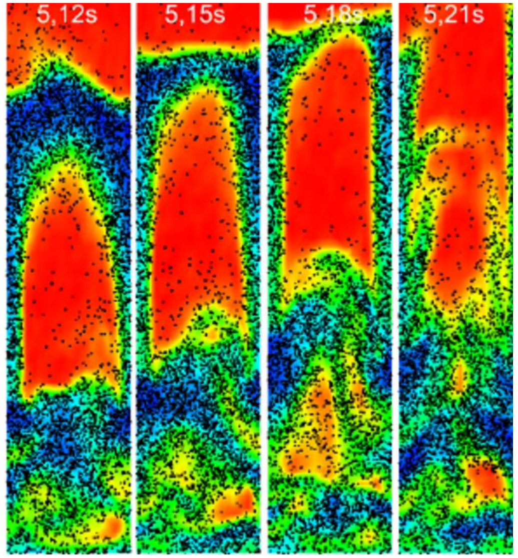
Multiphase

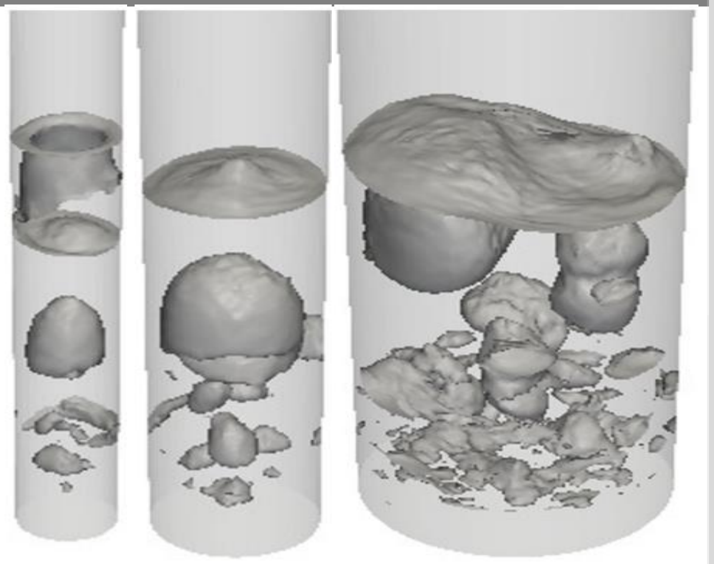
Multiscale

Hydrodynamics

Heat-/mass transfer

Reaction kinetics





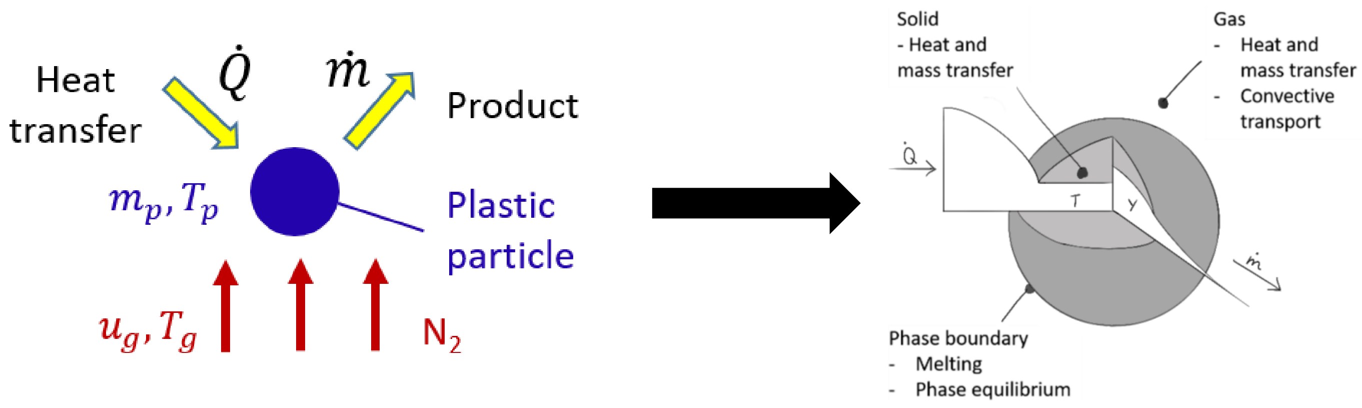
Motivation

- ~350 Mt plastic waste per year worldwide
  - 9% recycled, 22% mismanaged
- Advantages
  - Contaminated/mixed plastics
  - Significant reduction of CO_2 emission
- Challenges
  - Process design, efficiency, product yield, scale-up, economic viability
- Design and optimization of pyrolysis process via numerical simulation

Objectives

- Effect of particle morphology
- Heat transfer vs. pyrolysis reaction
- Lagrangian vs. Eulerian modeling

Homogeneous/thermally thin — Resolved



https://www.oecd.org/environment/plastic-pollution-is-growing-relentlessly-as-waste-management-and-recycling-fall-short.htm

Mismanaged 22%	Landfilled 49%	Incinerated 19%	Rec. 9%

Simulation of multiphase flows

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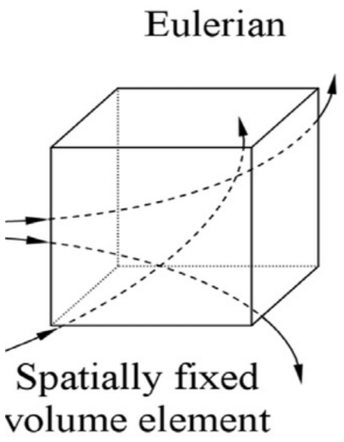
Multiphase Flow

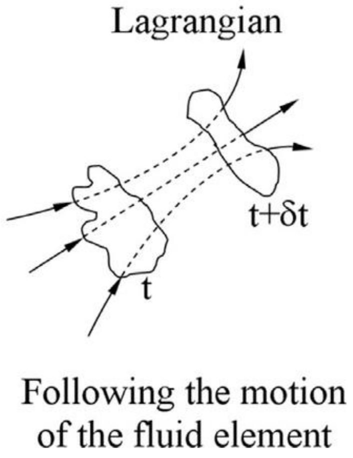
- **Euler-Lagrange**
  - **DPM/CFD-DEM**
    (discrete-particle method)

    Particle properties such as temperature and velocity are updated along the path of the individual particle.
- **Euler-Euler**
  - **TFM**
    (Two-Fluid model)

    Continuum description of the solid in which the particle properties are averaged in the computational domain
  - **VOF**
    (Volume of Fluid)

    Dispersed and continous phase combined to form a single continous phase.





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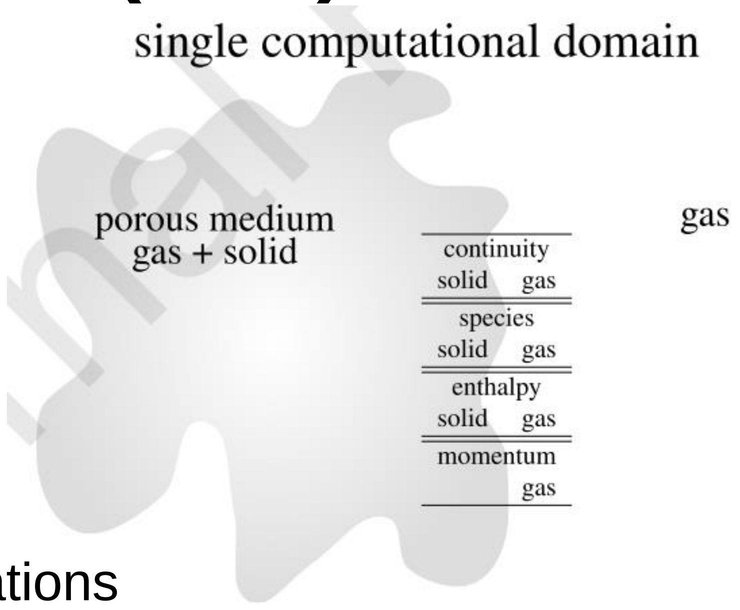
Two-fluid model (TFM)



- OpenFOAM for multiphase flow simulation
- Two sets of balance equations for gas and solid phases in Eulerian framework
- Heterogeneous reactions (pyrolysis)

ϵ – porosity

Energy equations

Gas phase

$$\frac{\partial}{\partial t}\epsilon\rho^f c_p^f\langle T\rangle^f + \nabla\cdot\left(\rho^f c_p^f\langle T\rangle^f\langle \boldsymbol{u}\rangle\right) = \nabla\cdot\nabla\left(\epsilon k_{eff}^f\langle T\rangle^f\right) - \epsilon\sum_i h_{f0,i}\langle\dot{\omega}_i\rangle^f \boxed{- h_{conv}\Sigma_{conv}\left(\langle T\rangle^f - \langle T\rangle^s\right)} + \boxed{(1-\epsilon)\sum_i h_i\langle R_i\rangle^s} + \left\langle S^{f,radiation}\right\rangle$$

Heat exchange

Solid phase

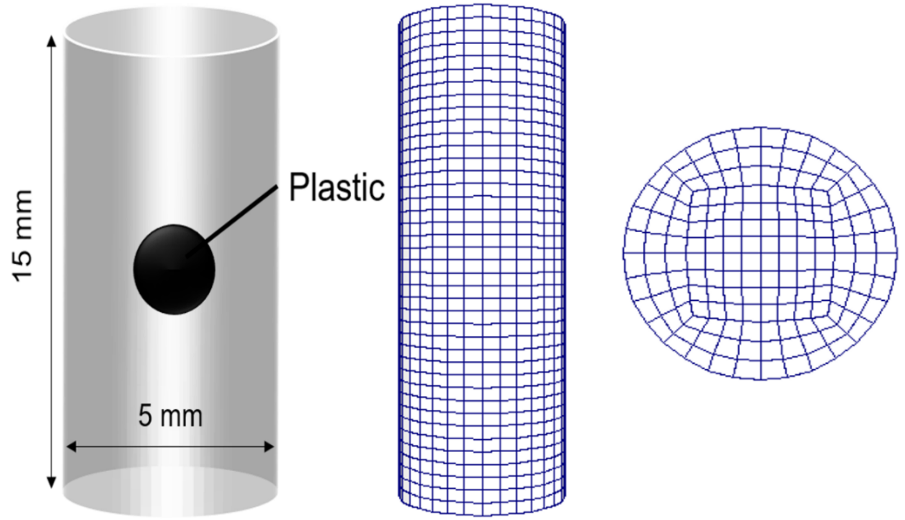
$$\frac{\partial}{\partial t}(1-\epsilon)\rho^s c_p^s\langle T\rangle^s = \nabla\cdot\left((1-\epsilon)\mathbb{K}k_{eff}^s\cdot\nabla\langle T\rangle^s\right) - (1-\epsilon)\sum_k h_{f0,i}\langle R_k\rangle^s \boxed{+ h_{conv}\Sigma_{conv}\left(\langle T\rangle^f - \langle T\rangle^s\right)} - \boxed{(1-\epsilon)\sum_i h_i\langle R_i\rangle^s} + \left\langle S^{s,radiation}\right\rangle$$

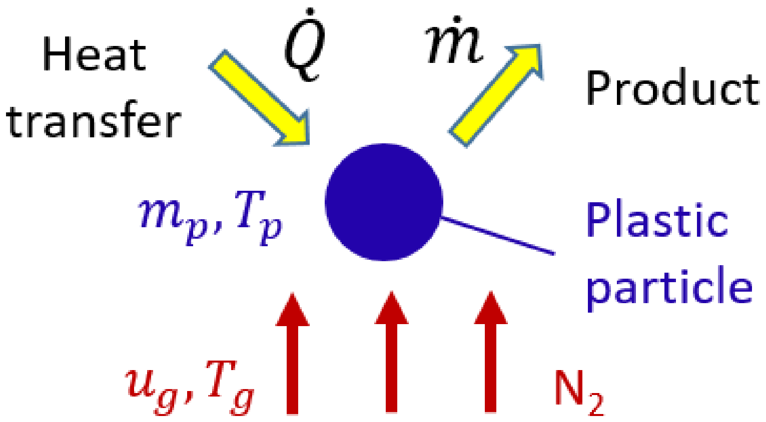
Heat transfer

Heating source due to heterogeneous reaction

Simulation setups

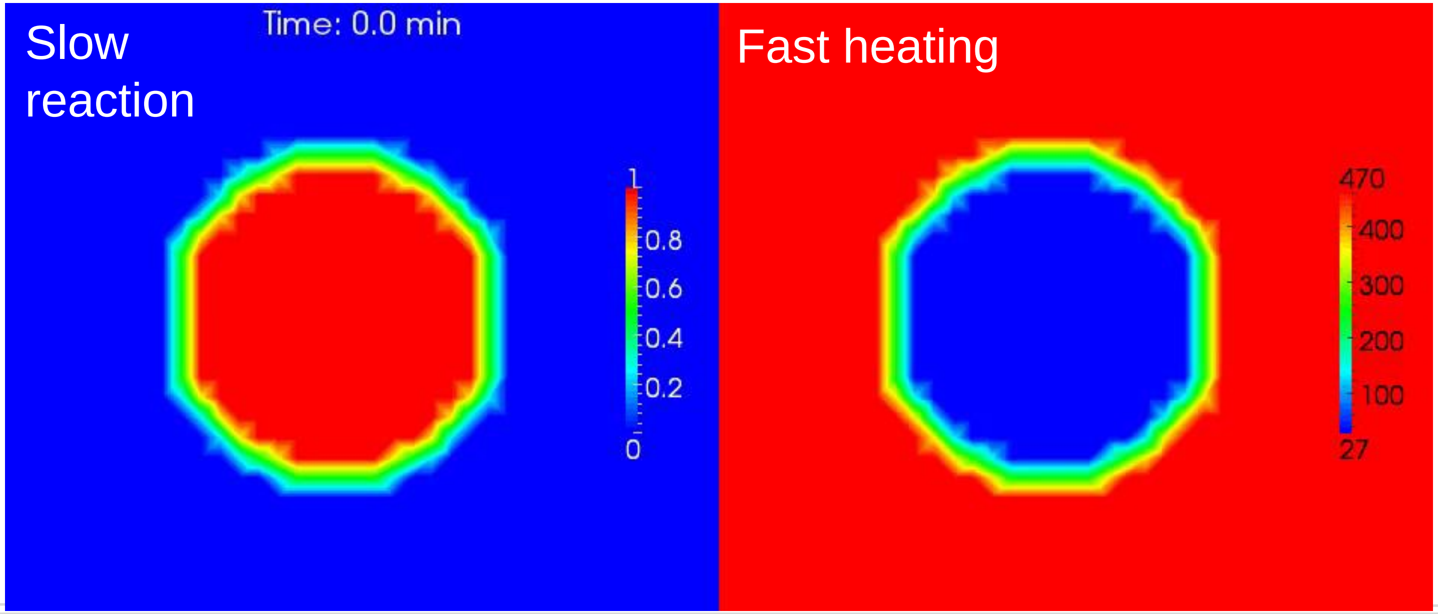
- ❑ Single PE plastic particle
  - 2 mm – 6 mm
  - Sphere, cylinder, shell
- ❑ 3D with ca. 400,000 cells / Δ = 0.35 mm
- ❑ Objectives
  - Heat transfer vs. pyrolysis reaction
  - Development of sub-models
- ❑ Challenges:
  - Resolution of boundary layers
  - Physical simulation time up to 40 min
- ❑ Computing time
  - HPC with 320 cores for 3 days





Sphere: d_P = 6 mm, T_G = 470 °C

Particle volume fraction **Particle temperature**



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Overview of simulation cases

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Morpholoy	d [mm]	Mass [mg]	Re [-]	Bi [-]	Py^I [-]
Sphere	1.8	3	0.56	0.31	3.47
	2.7 at **450, 470** and **490** ℃	10	0.83	0.33	1.54
	4	32	1.24	0.34	0.70
	6	107	1.85	0.36	0.31
Cylinder	3.2/ AR0.5	10	0.97	0.13	1.12
	2.4/ AR1	10	0.74	0.11	1.95
	2/ AR2	10	0.62	0.20	2.81
	2.4/ AR1 **Vertical**	10	0.37	0.09	0.33
Shell	Inner: 2 Outer: 2.9	10	0.83	0.33	1.47

$$Re = \frac{\rho V d_p}{\mu_g}$$

$$Bi = \frac{\alpha \cdot d_p}{\lambda_p}$$

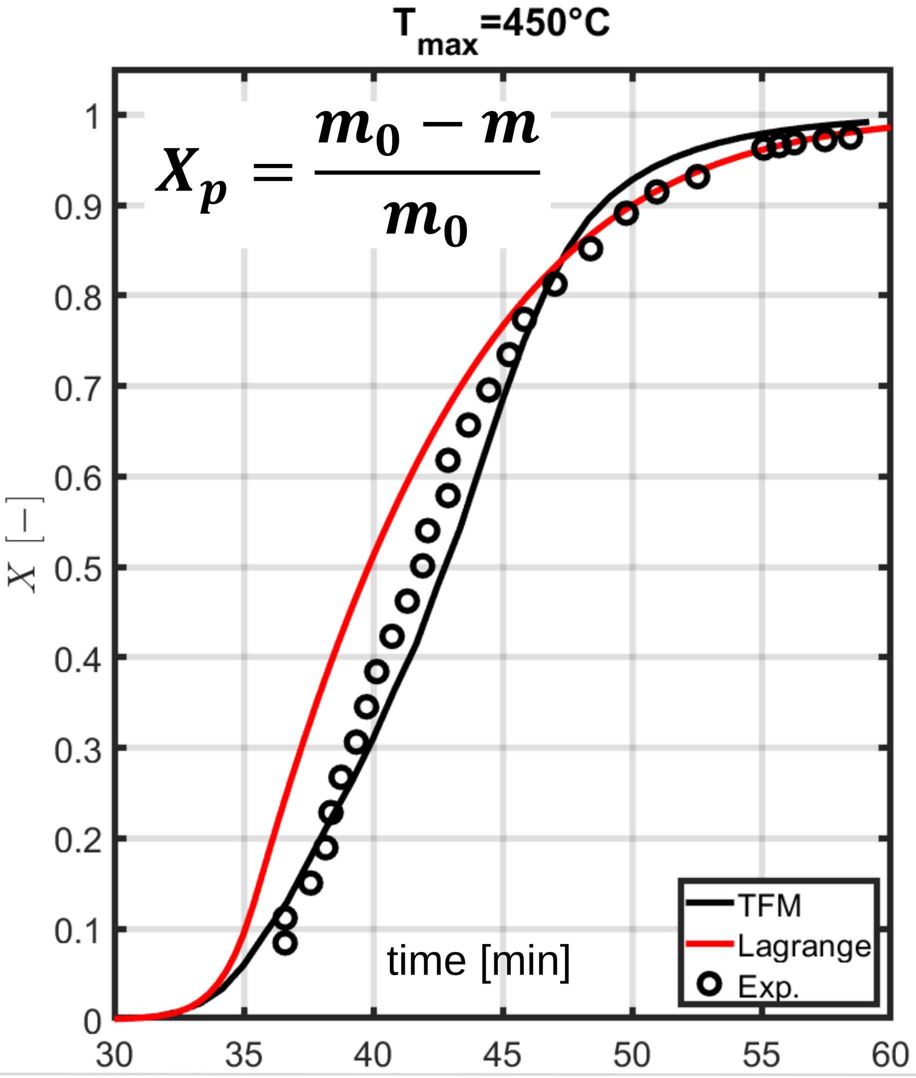
$$Py^I = \frac{\lambda_p}{k \cdot \rho_p \cdot c_{p,p} \cdot d_p^2}$$

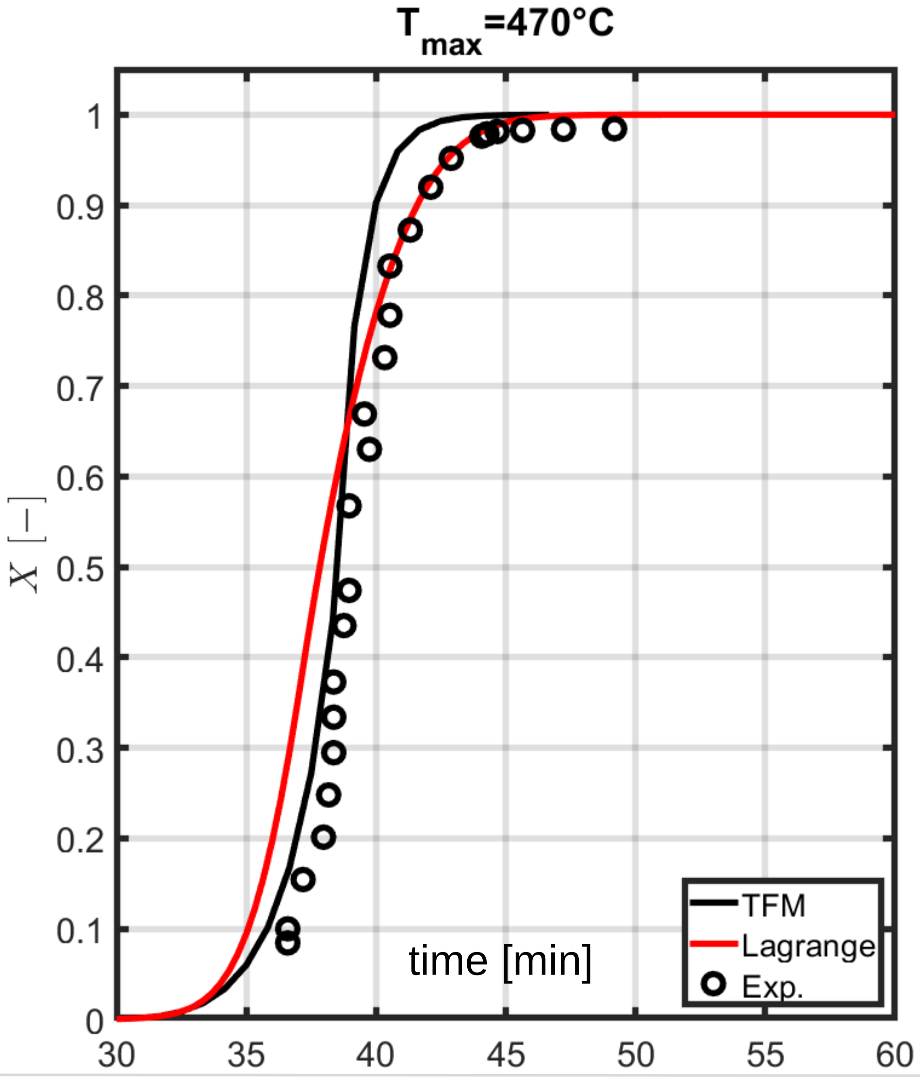
Comparison with TG experiments

TG experiment by [1]

- d_p = 1.82 mm
- <u>m_p = 3 mg</u>
- v_{gas} = 2.5 cm/s
- T_0 = 300 K
- p_0 = 1 bar
- β = 12 K/min

$$X_p = \frac{m_0 - m}{m_0}$$

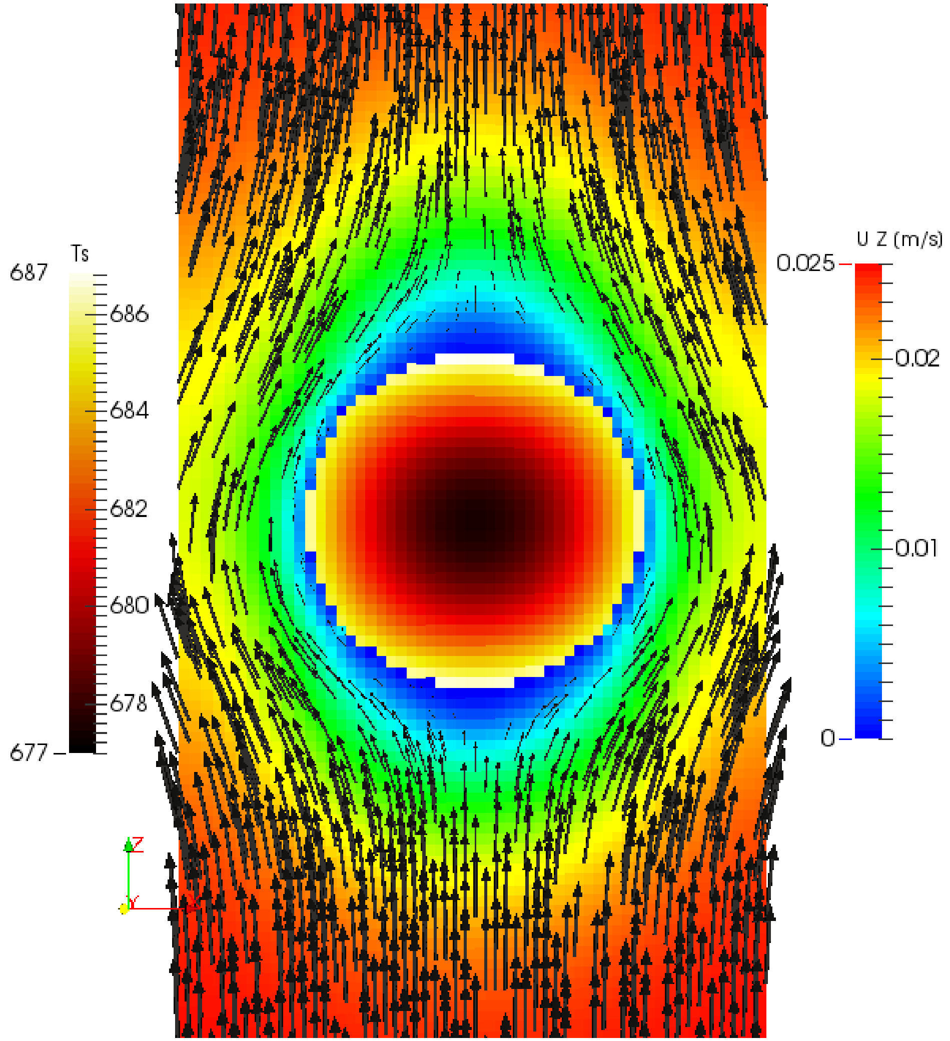




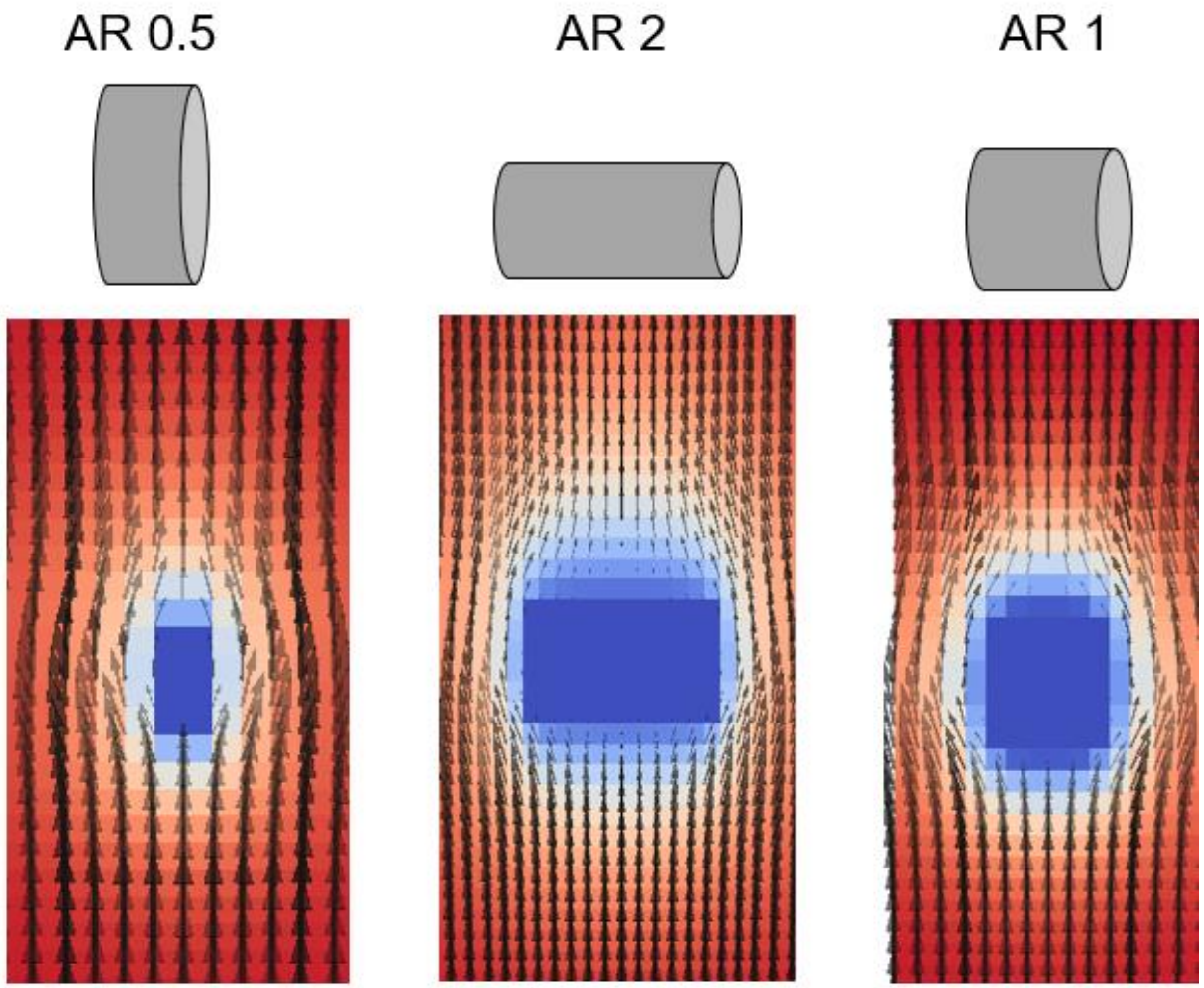
Ceamanos et al. Journal of Analytical and Applied Pyrolysis 65, 93110, 2002.

Flow fields around particles

Sphere: d_P = 6 mm



Effect of aspect ratio



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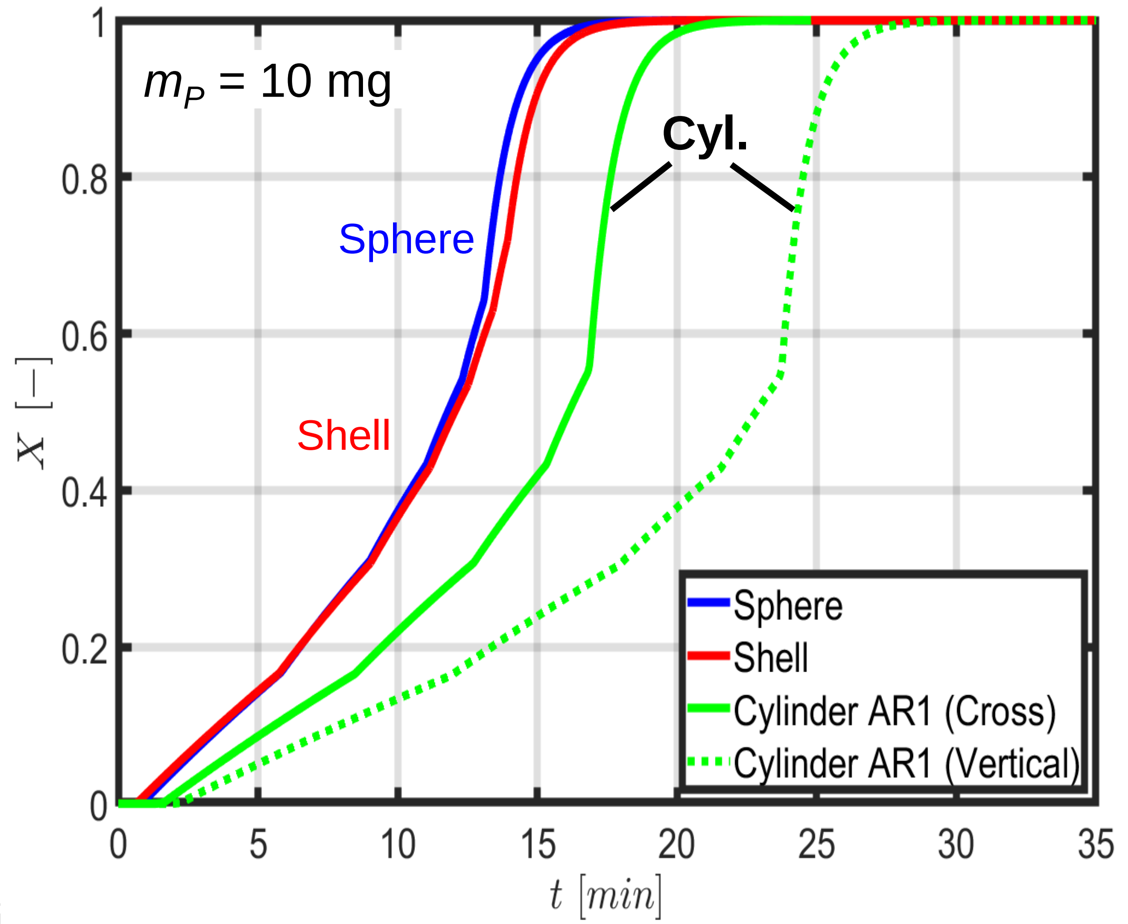
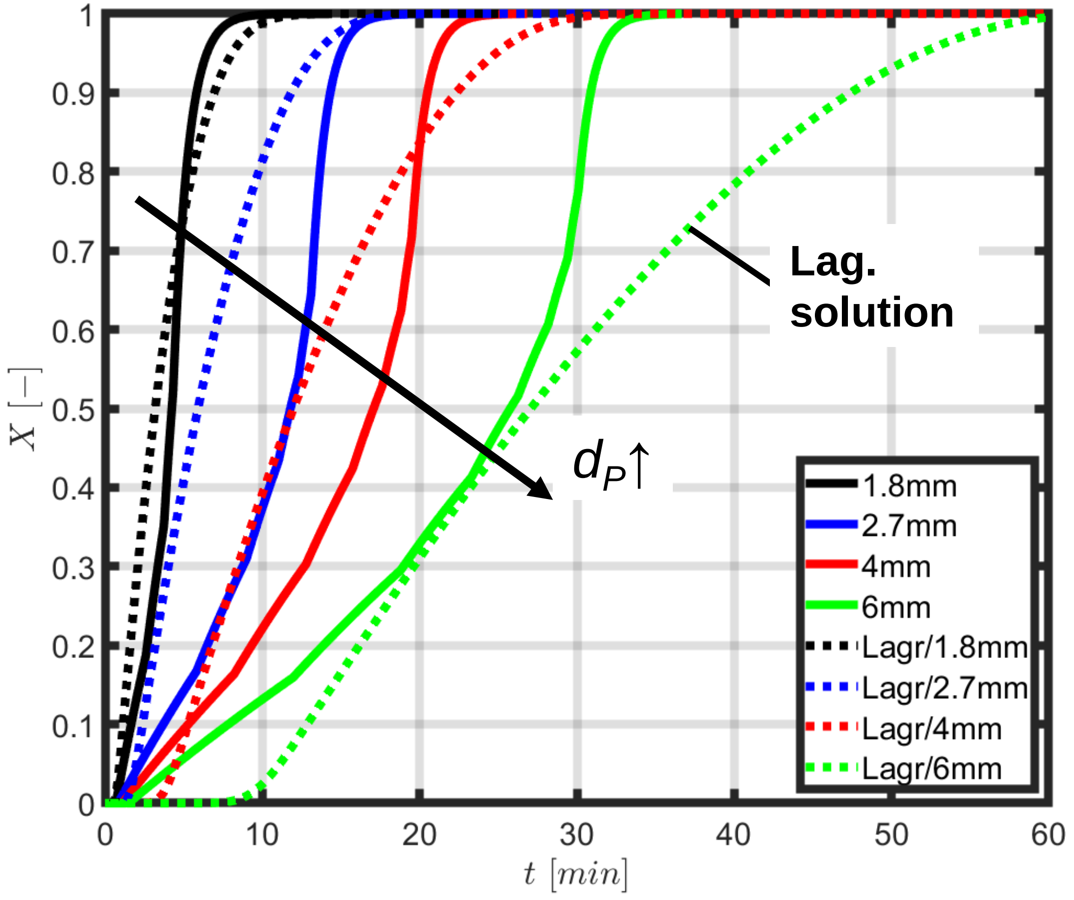
Effect of particle morphology

- Significant influences of particle shape and flow direction



- Strong increase of pyrolysis time with particle size



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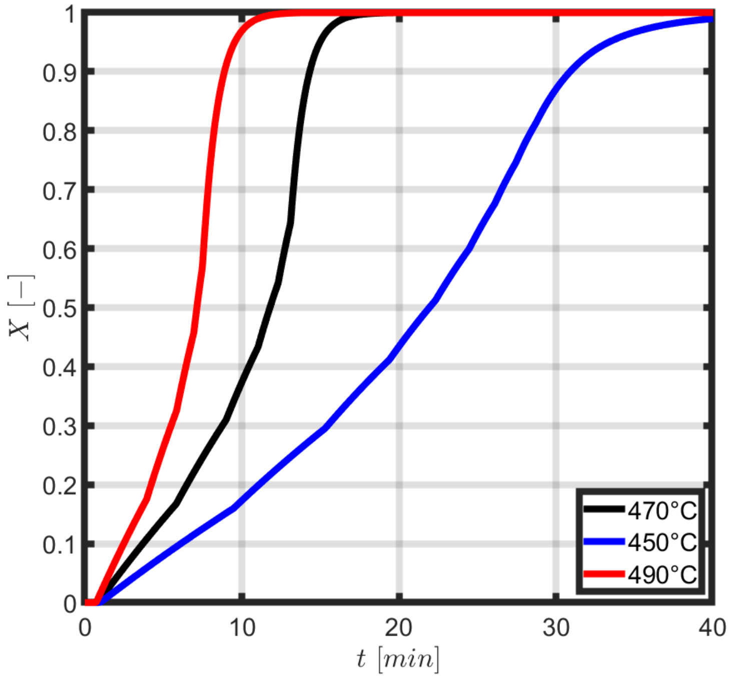
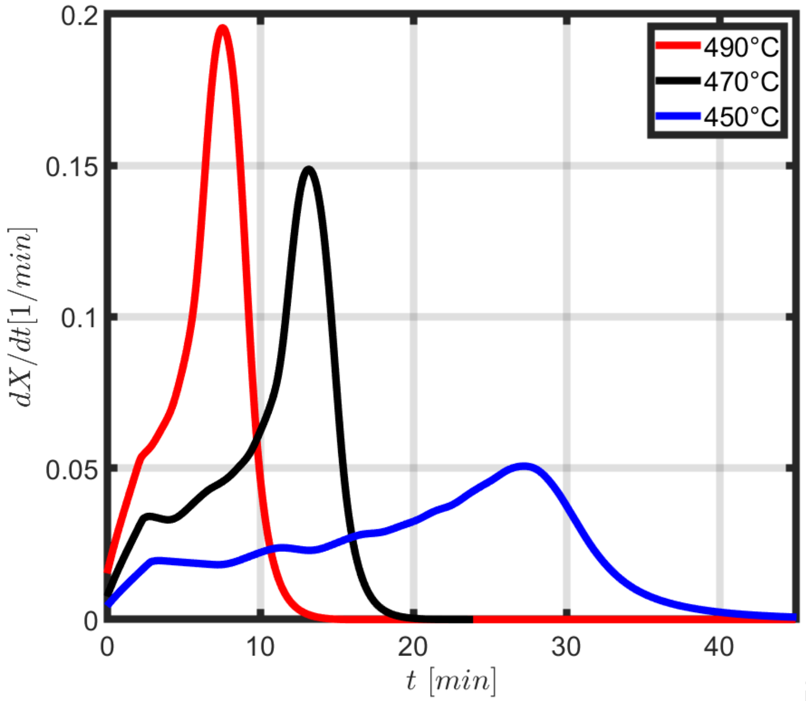
Effect of reactor temperature

- Faster conversion at increased ambient temperature due to
  - Increased reaction rate
  - Increased pyrolysis temperature

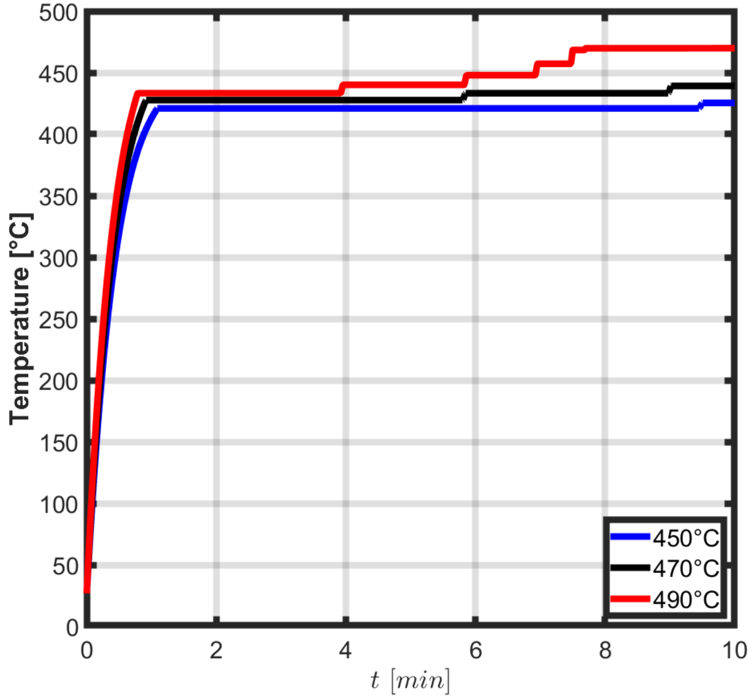
Reaction progress



Conversion rate



Particle temperature



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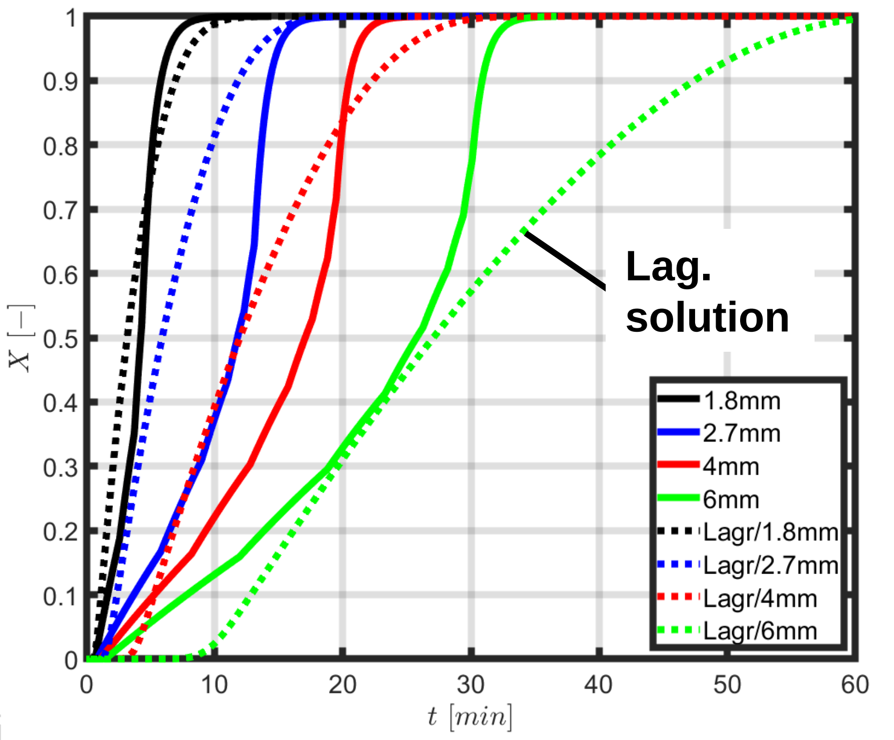
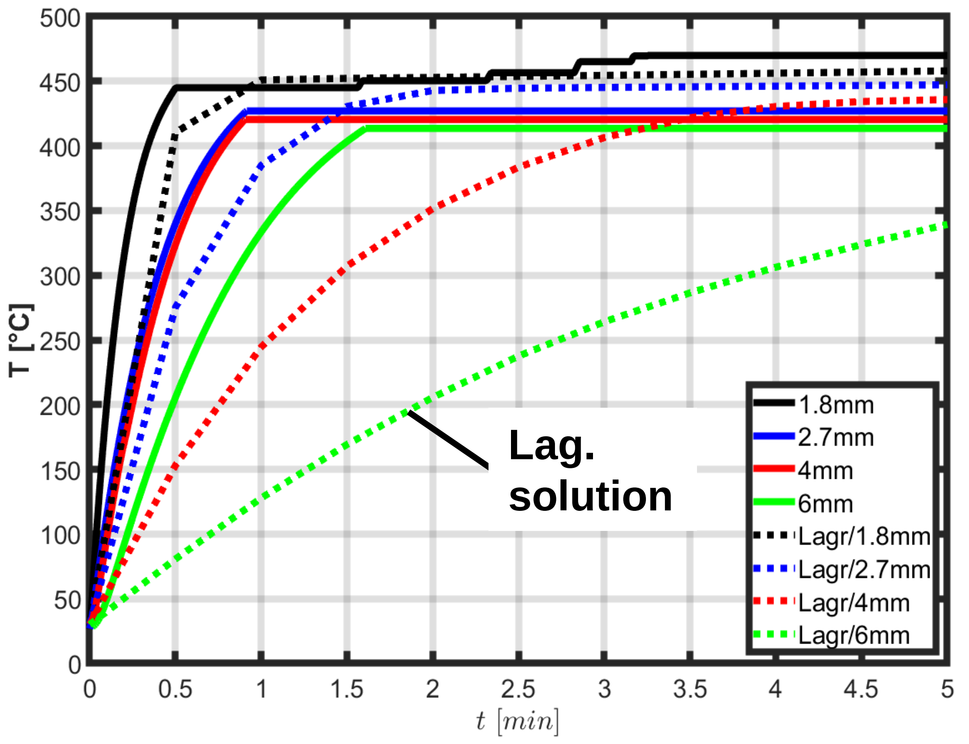
Particle-resolved vs. Lagrangian simulation

- Faster heating and conversion for particle-resolved simulation
- Larger difference for larger particle
  - Velocity/temperature boundary layers are not resolved for Lagrangian approach
  - Lagrangian method assumes homogeneity

Conversion progress



Core particle temperature



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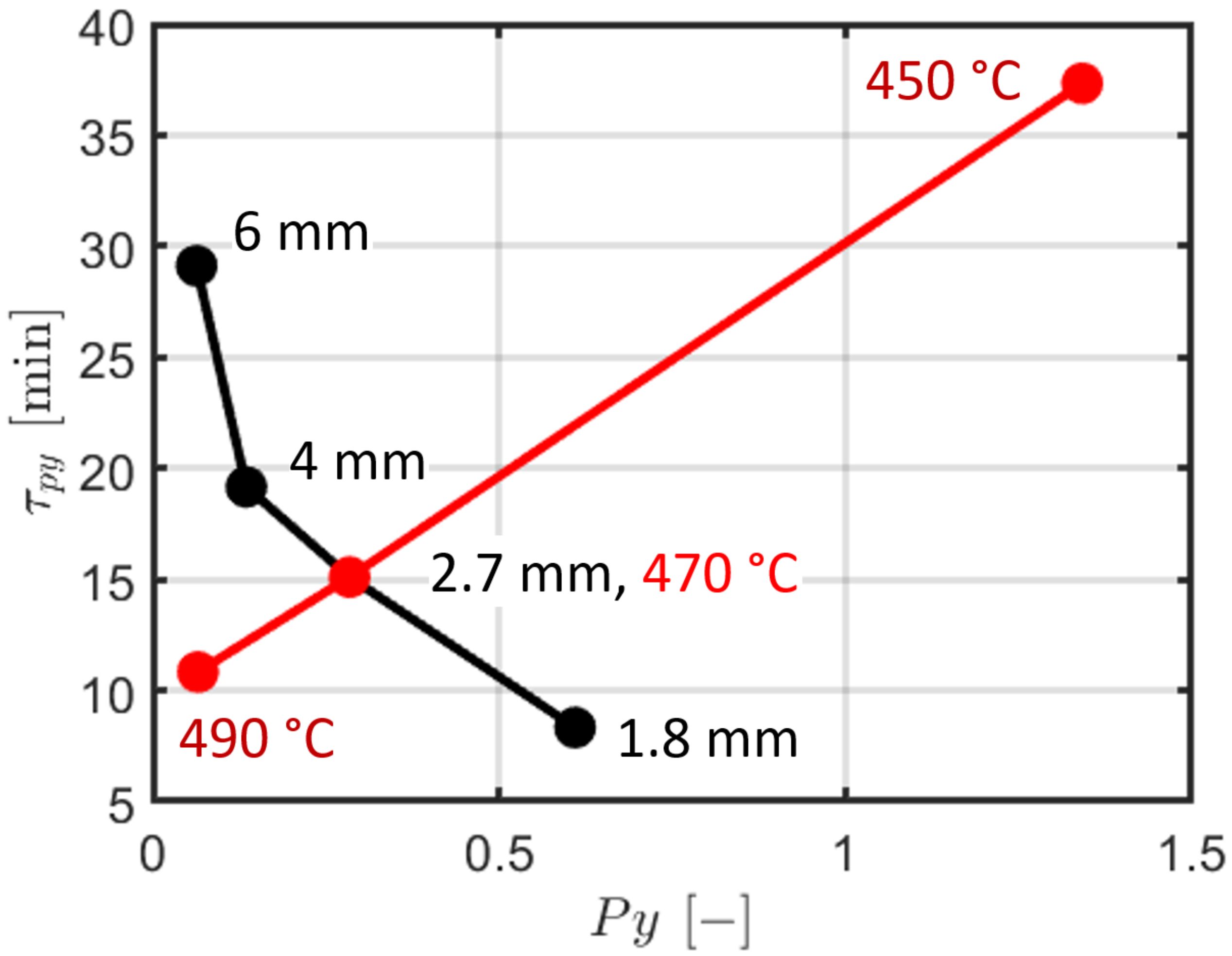
Pyrolysis reaction vs. heat transfer

- Pyrolysis number: ratio of time scales between chemical reaction and convective heat transfer

$$Py = \frac{\tau_c}{\tau_h} = \frac{\alpha}{k_r \rho_p c_p d_p}$$

- Decrease of τ_Py with Py at constant reactor temperature

- Quasi-linear increase of τ_Py with Py at constant particle diameter



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Conclusion

- Significantly influence of particle shape and flow direction
- Slower pyrolysis for larger particle
- Quasi-linear increase of pyrolysis time with increasing gas temperature
- Strong deviations betw. Lagrangian and Eulerian methods for large particles
- Enhanced heat results in a higher pyrolysis temperature and faster conversion
- Strong correlations betw. pyrolysis time and pyrolysis number

Thank You