

# Impact of Intra-Particle Heat Conduction on Waste Plastic Pyrolysis

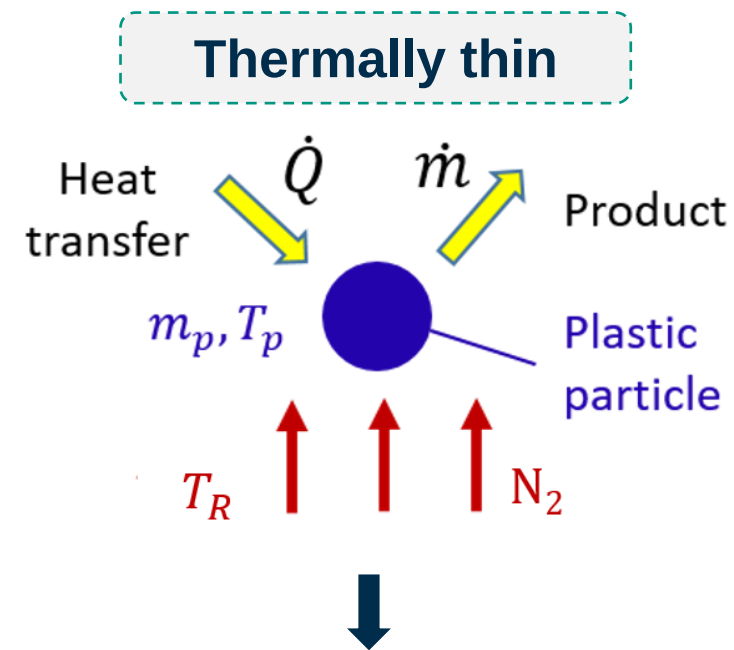
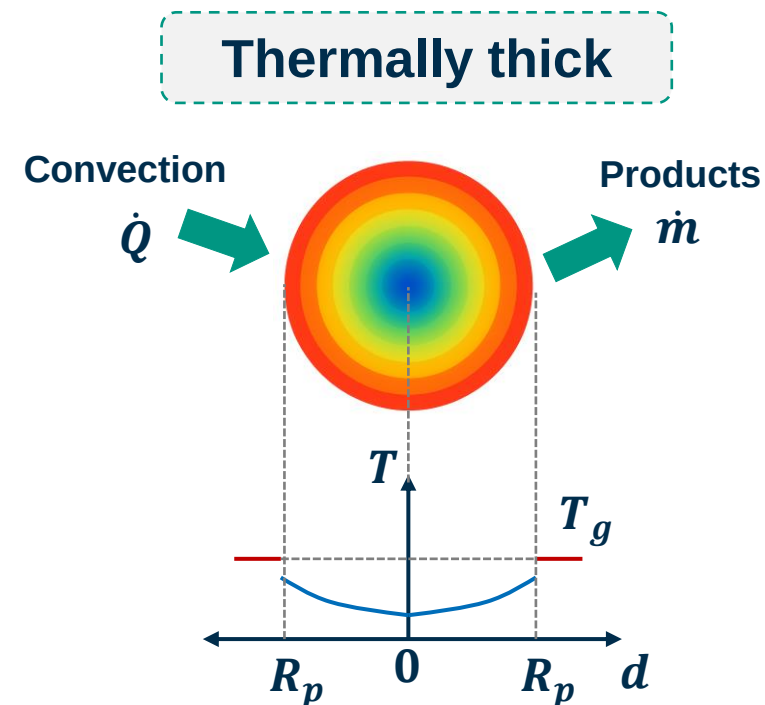
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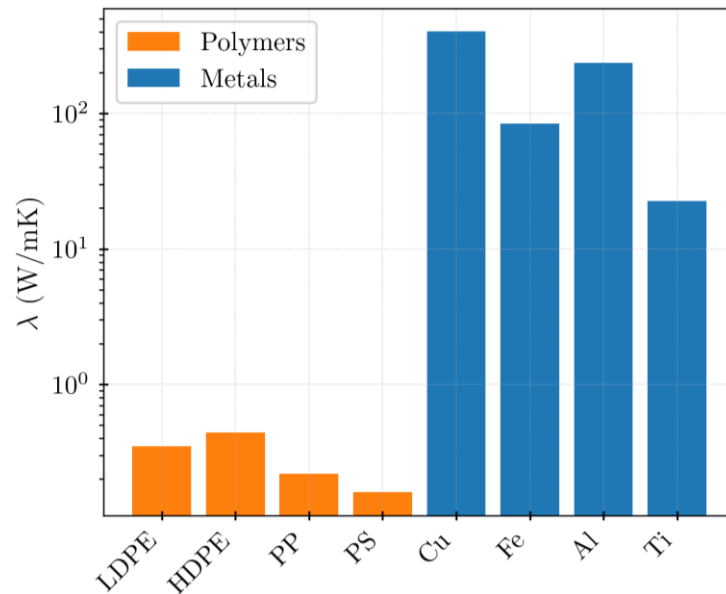
**PYRO2026**  
 25<sup>th</sup> International Symposium on  
 Analytical and Applied Pyrolysis  
 7-11 June 2026, Pisa, Italy

**PYRO2026**



# Motivation

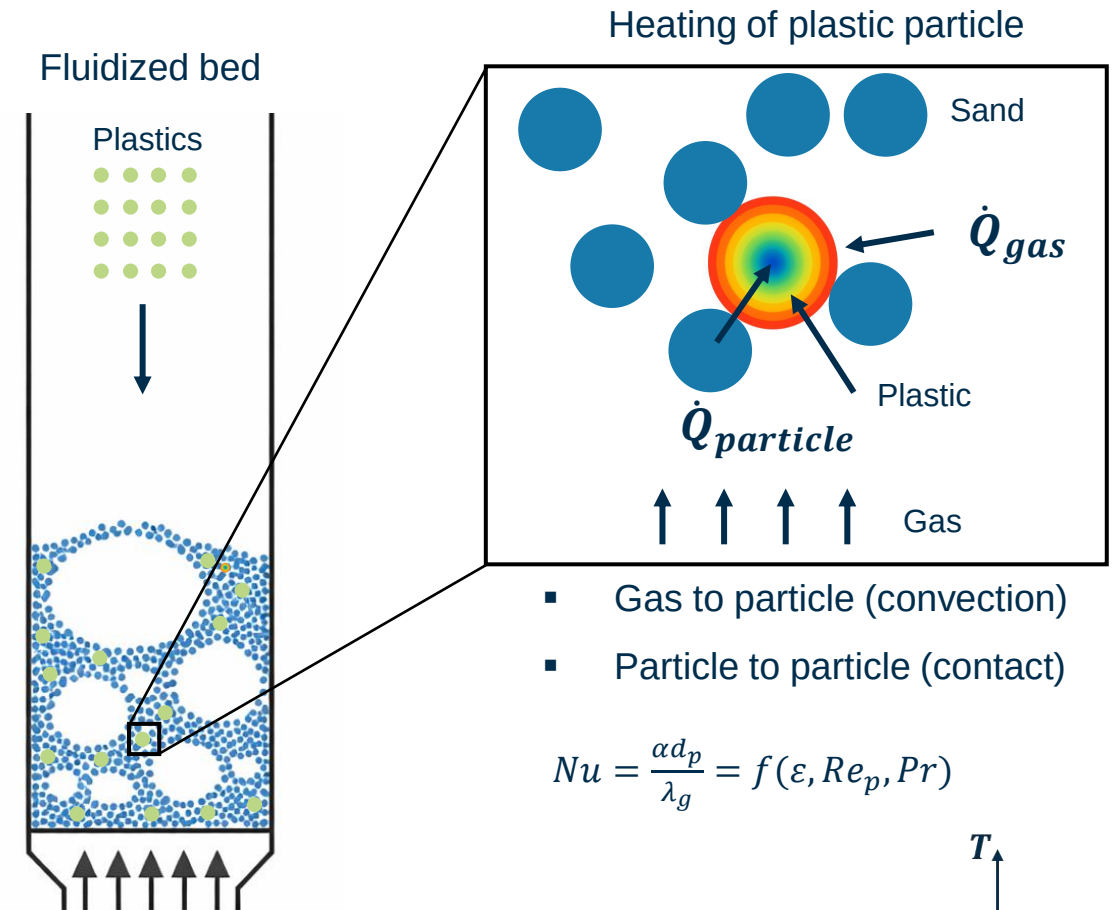
- ❑ Plastic wastes: ~ 400 Mt/a, ~10% recycled [1]
- ❑ Chemical recycling via pyrolysis
  - Converting plastic waste into secondary raw materials
  - Capable of mixed/contaminated plastics
- ❑ **Simulation of plastic pyrolysis process**



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

[2] Thermal conductivity of different metals and polymers at 0°C

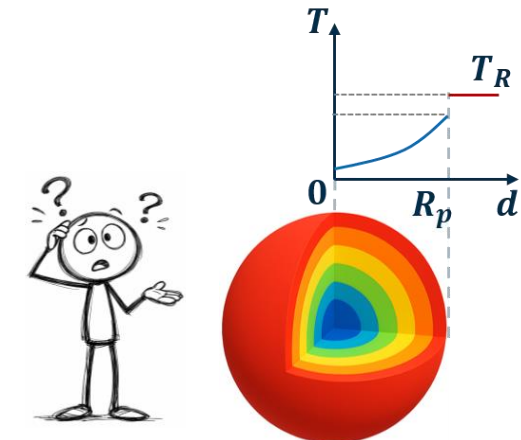
Data source: VDI-Wärmeatlas (12th edition), Springer, Berlin/Heidelberg, 2019.



## Intra-particle heat conduction

- Neglected for Lagrangian simulation

→ How important, how to model?



# Numerical method

## Homogeneous particle (0D)

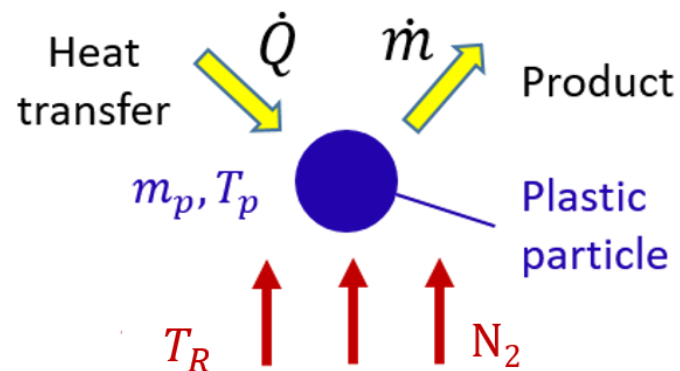
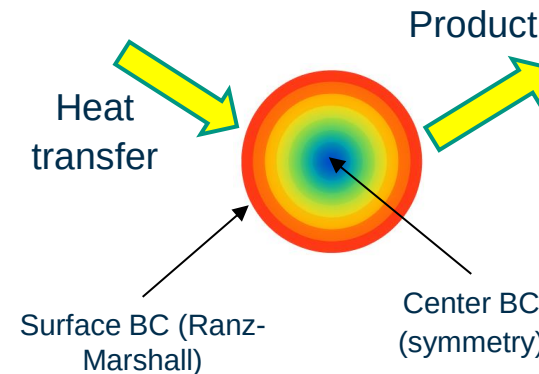
$$\frac{\partial m_p}{\partial t} = \dot{r}(t) = -A \cdot \exp\left(-\frac{E_a}{RT_p}\right) m_{p,0}^{(1-n)} m_p^n$$

$$m_p c_p \frac{\partial T_p}{\partial t} = \frac{Nu \lambda_g}{d_p} (T_G - T_p) - \Delta H_R \cdot \dot{r}(t)$$

## Resolved particle (1D, with N shells)

$$\frac{\partial \tilde{m}_p}{\partial t} = \dot{\tilde{r}}(r_p, t) = -A \cdot \exp\left(-\frac{E_a}{R\tilde{T}_p}\right) \cdot \tilde{m}_{p,0}^{(1-n)} \tilde{m}_p^n$$

$$\rho_P \tilde{c}_P \frac{\partial \tilde{T}_p}{\partial t} = \frac{1}{r_p^2} \frac{\partial}{\partial r_p} \left( \lambda_p r_p^2 \frac{\partial \tilde{T}_p}{\partial r_p} \right) - \frac{\Delta H_R \cdot \dot{\tilde{r}}(t, r_p)}{\tilde{V}_p}$$



## Boundary conditions (BC)

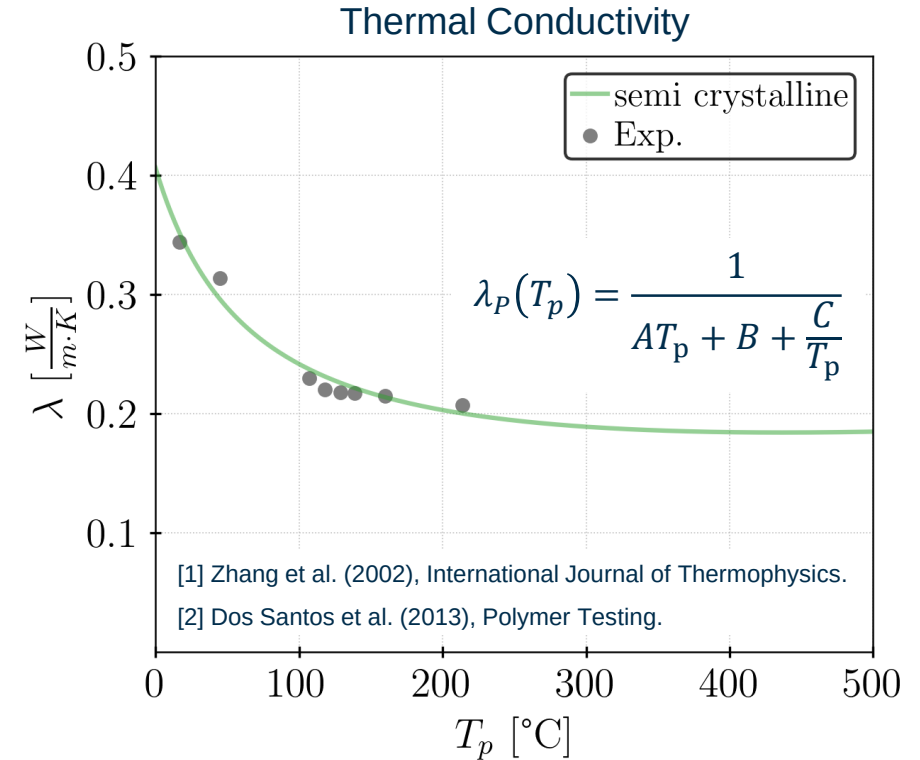
Particle surface  $\lambda_p \frac{\partial T}{\partial r_p} = \frac{Nu \lambda_g}{d_p} (T_R - T_p)$

Particle center  $\frac{\partial T}{\partial r_p} = 0$

# Simulation plan

- LDPE particle with varied particle size  $d_{p0}$ , reactor temperature  $T_R$  and Nusselt number  $Nu$

|      | $T_R [^{\circ}C]$ | $d_{p0} [mm]$ | $Nu [-]$ | $Bi [-]$ | $Py [-]$ |
|------|-------------------|---------------|----------|----------|----------|
| LDPE | 500               | 4             | 4        | 1.20     | 0.082    |
| LDPE | 450               | 4             | 4        | 1.14     | 1.75     |
| LDPE | 550               | 4             | 4        | 1.26     | 0.01     |
| LDPE | 500               | 2             | 4        | 1.20     | 0.327    |
| LDPE | 500               | 6             | 4        | 1.20     | 0.036    |
| LDPE | 500               | 4             | 2        | 0.60     | 0.082    |
| LDPE | 500               | 4             | 6        | 1.80     | 0.082    |



- Biot number  $Bi$  and pyrolysis number  $Py$

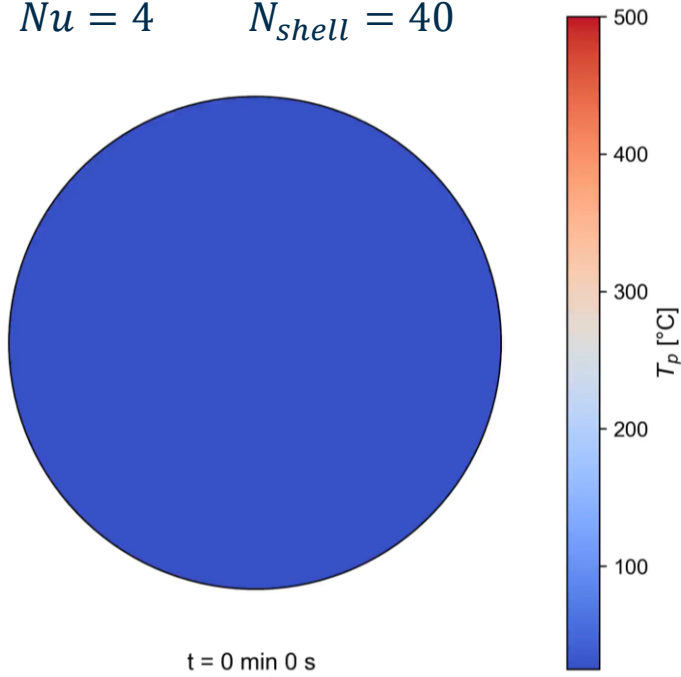
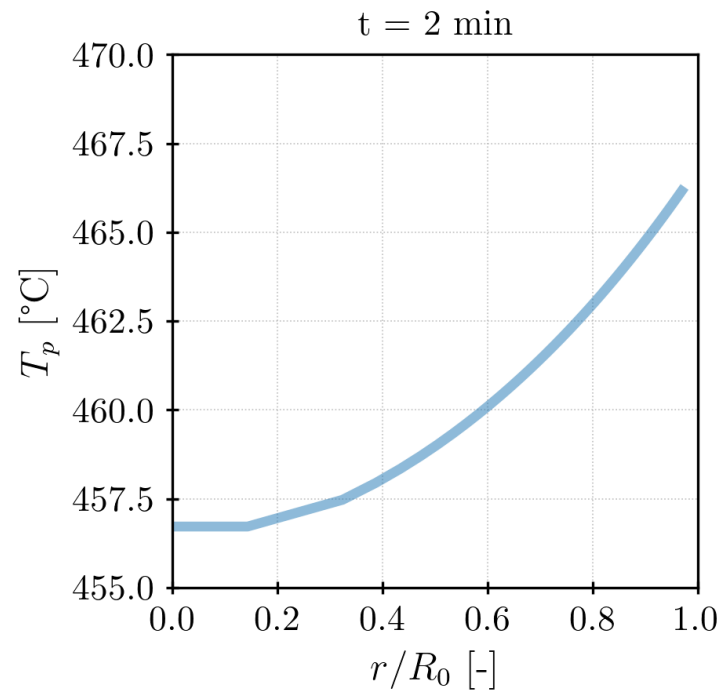
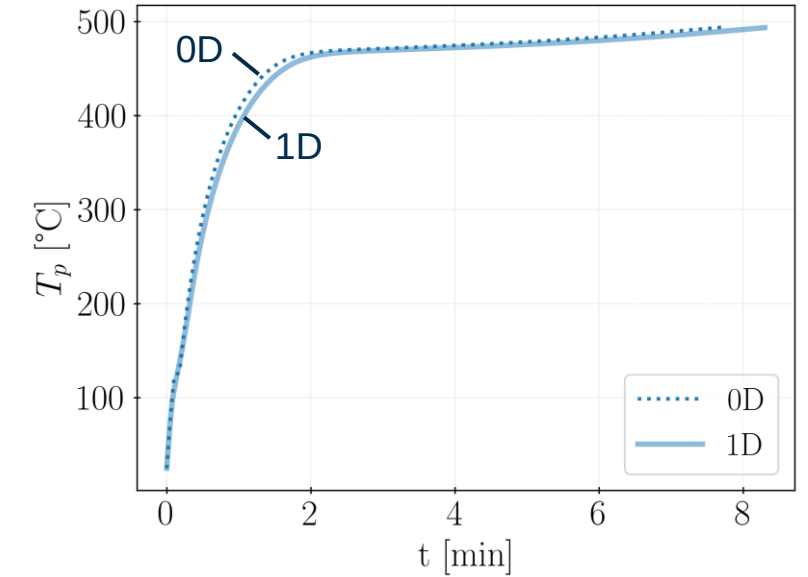
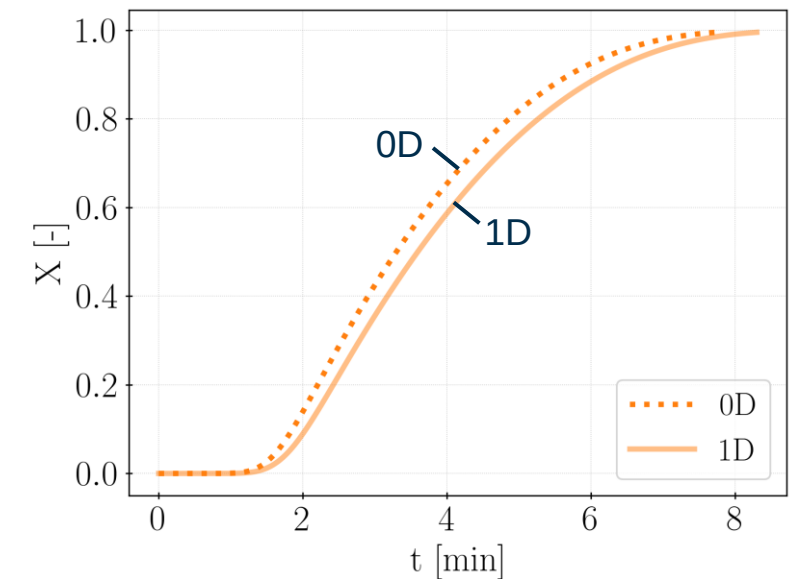
$$Bi = \frac{\tau_\lambda}{\tau_\alpha} = \frac{\alpha d_{p0}}{\lambda_p} = \frac{Nu \lambda_g}{\lambda_p} \quad Py = \frac{\tau_c}{\tau_\lambda} = \frac{\lambda_p}{k_r \rho_P c_{p,P} d_p^2}$$

# General behavior

- ❑ Smaller temperature at the center than at the boundary
- ❑ Slower heating and conversion for 1D simulation

$$T_R = 500\text{ }^{\circ}\text{C} \quad d_{p0} = 4\text{ mm}$$

$$Nu = 4 \quad N_{shell} = 40$$



# Effect of particle diameter

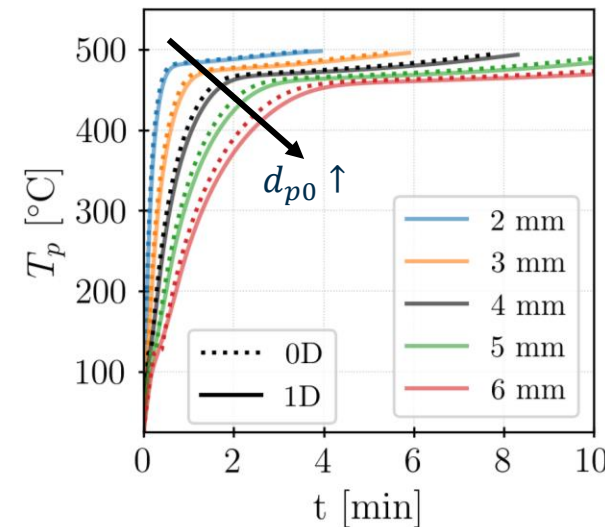
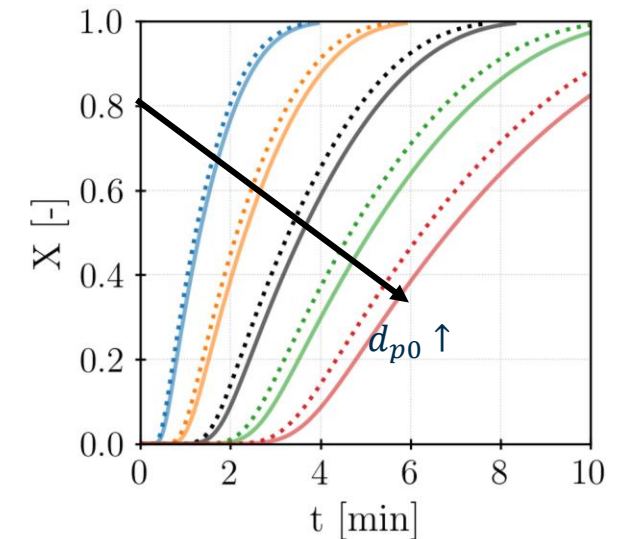
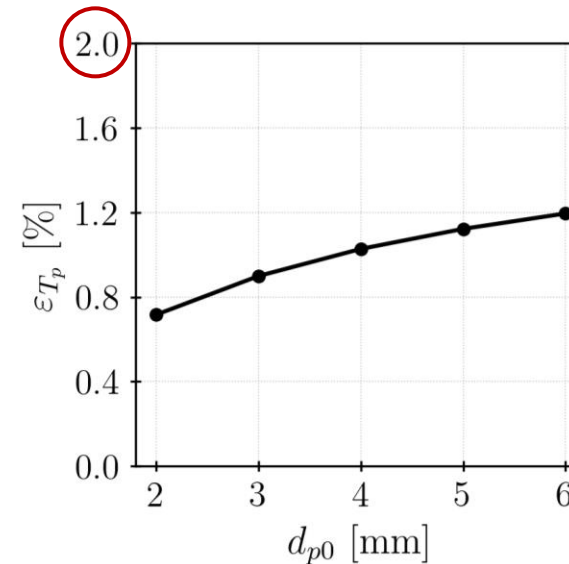
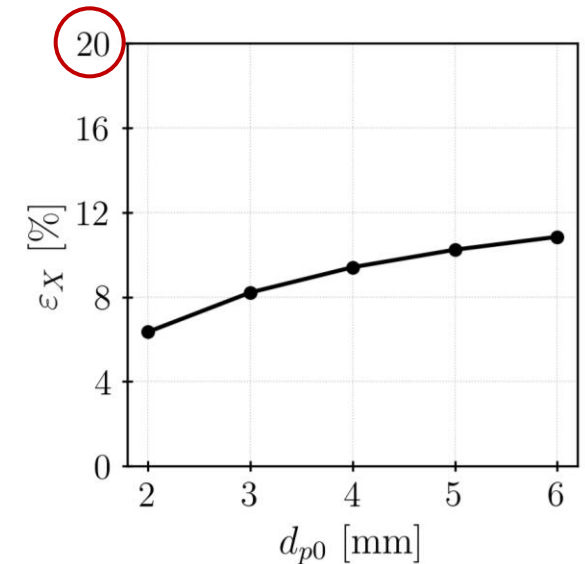
- Increasing  $d_{p0}$  leads to
  - Slower heating and conversion
  - Larger error for 0D simulations
- Larger error for conversion

Conversion progress:  $X = \frac{m_{p,0} - m_p}{m_{p,0}}$

Difference between 0D/1D solutions

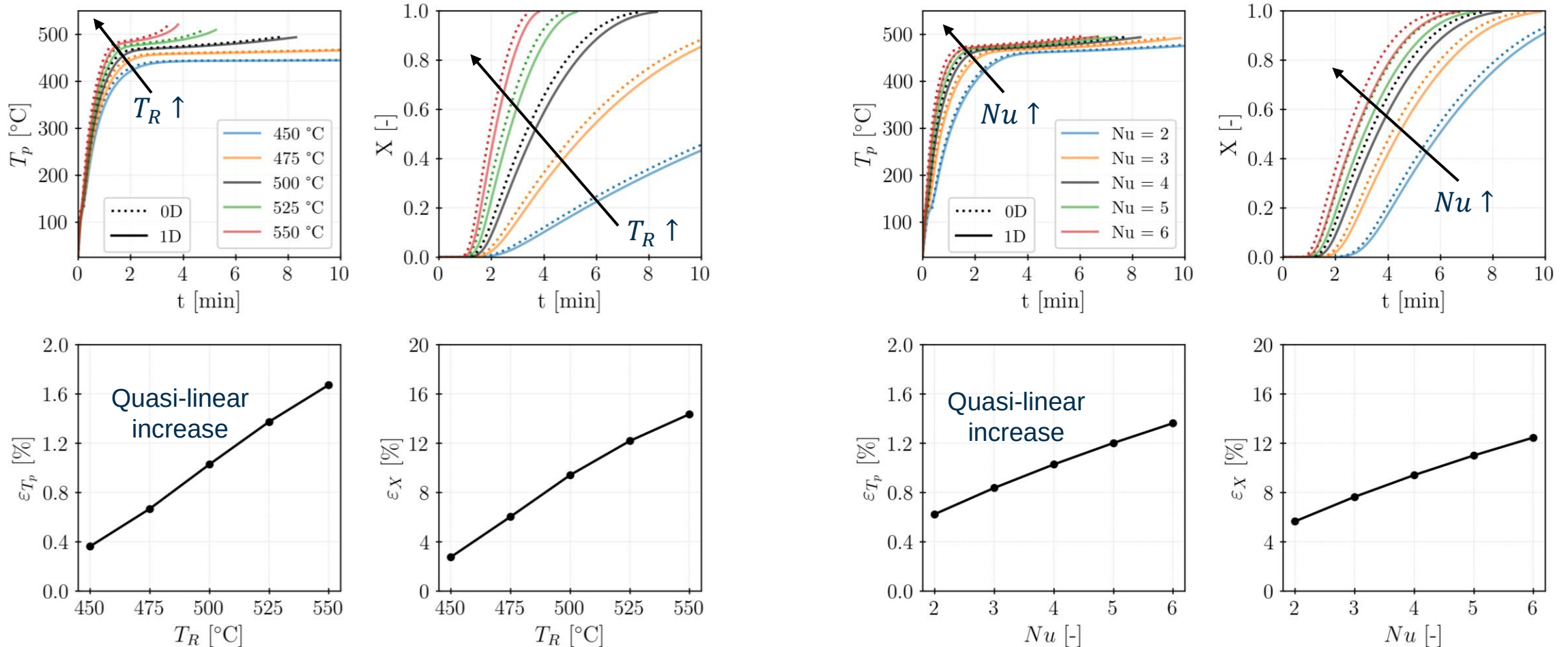
$$\varepsilon = \text{RMS} \left( \frac{\varphi_{0D} - \varphi_{1D}}{\bar{\varphi}_{0D}} \right)$$

Time evolution of  $T_p$  and  $X$



# Effect of reactor temperature and Nusselt number

- ❑ Faster heating and conversion at larger  $T_R$  and  $Nu$
- ❑ Quasi-linear increase of error with  $T_R$  and  $Nu$



# Corrected 0D model

$$\frac{dT_p^{0D}}{dt}_{orig} = \frac{\alpha A_p (T_p - T_R) - \dot{m} \Delta h_r}{m_p c_{p,p}}$$

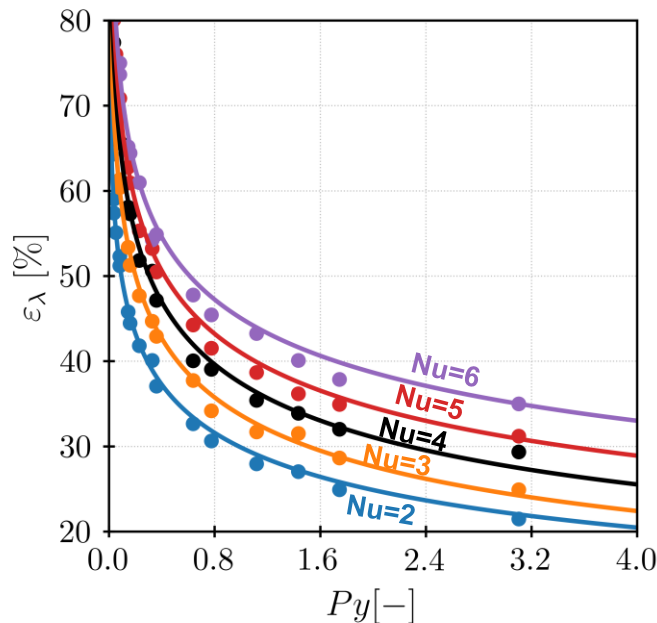
❑ Heating rate in 0D model is larger

→ Correction/reduction based on differences between 0D/1D simulations  $\epsilon_\lambda$

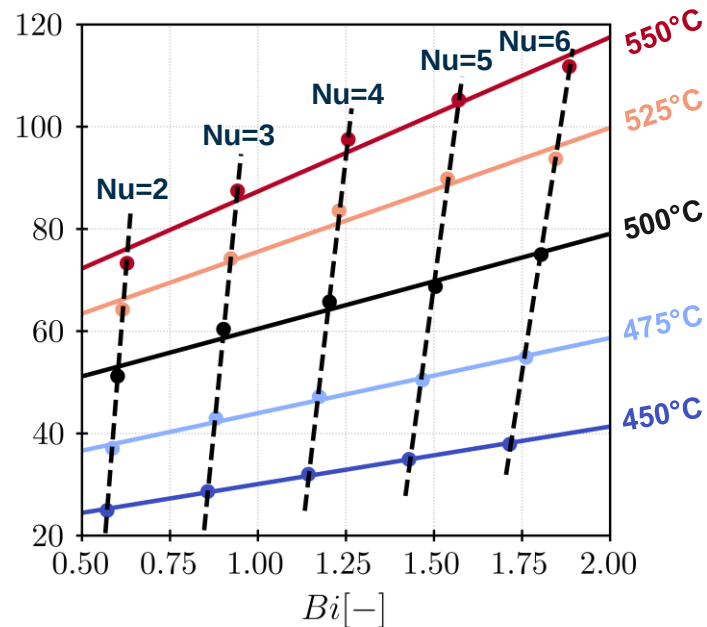
$$\frac{dT_p^{0D}}{dt}_{corr} = (1 - \epsilon_\lambda) \frac{dT_p^{0D}}{dt}_{orig} \quad \epsilon_\lambda = \text{RMS} \left( \frac{\frac{dT_p^{0D}}{dt} - \frac{dT_p^{1D}}{dt}}{\frac{dT_p^{0D}}{dt}} \right)$$

❑ Correlation with dimensionless metrics

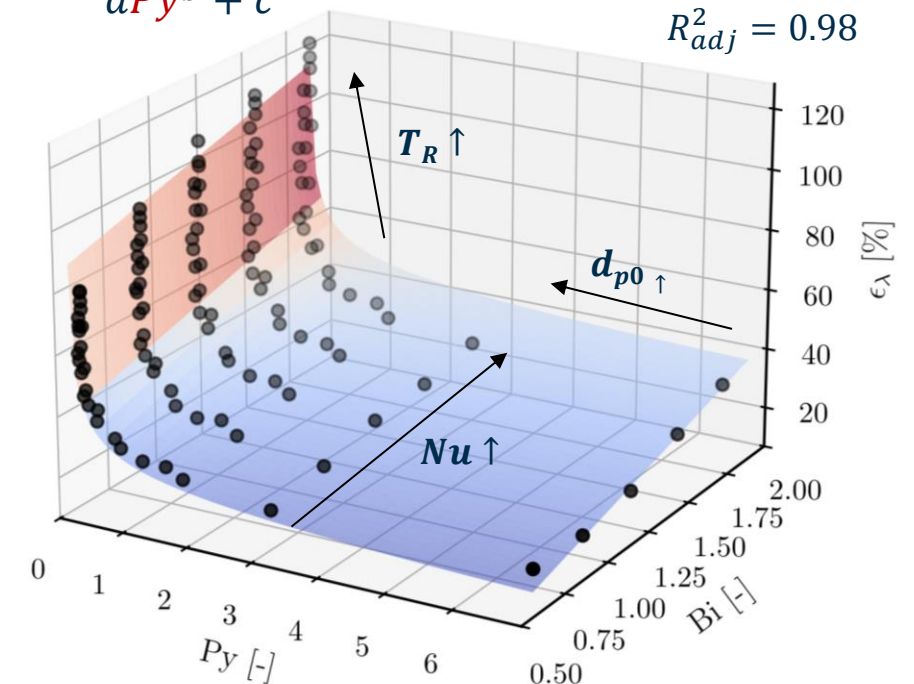
$$\epsilon_\lambda = \frac{1}{a \cdot Py^b + c}$$



$$\epsilon_\lambda = a \cdot Bi + b$$

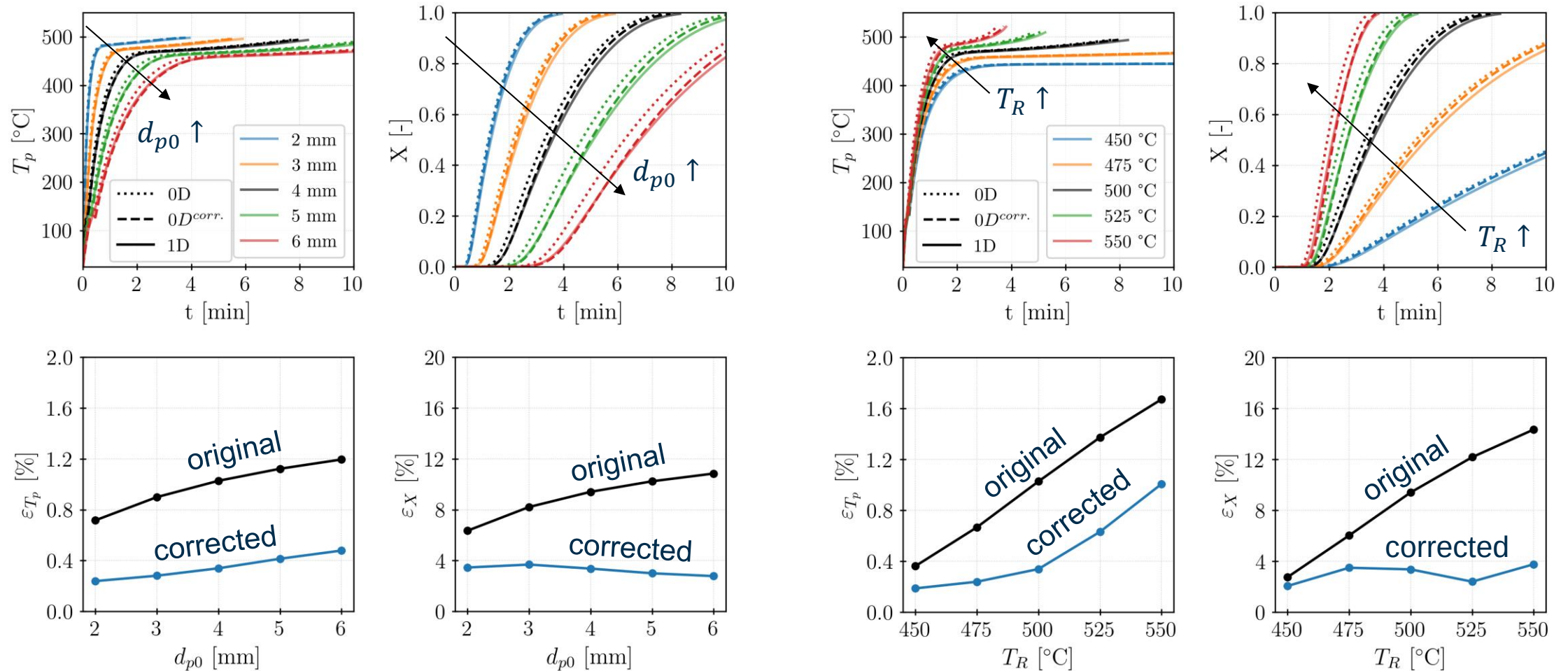


$$\epsilon_\lambda = \frac{1}{a Py^b + c} + d Bi + e$$



# Validation of corrected 0D model

- Significantly improved accuracy by using corrected model



# Summary

## Conclusion

- ❑ Quantitative analysis of intra-particle heat transfer during plastic pyrolysis
  - Slower heating and conversion for finite-rate heating
  - Intensified effects with larger particles, higher temperatures, and stronger external heating
- ❑ Physics-based closure using dimensionless groups

## Outlook

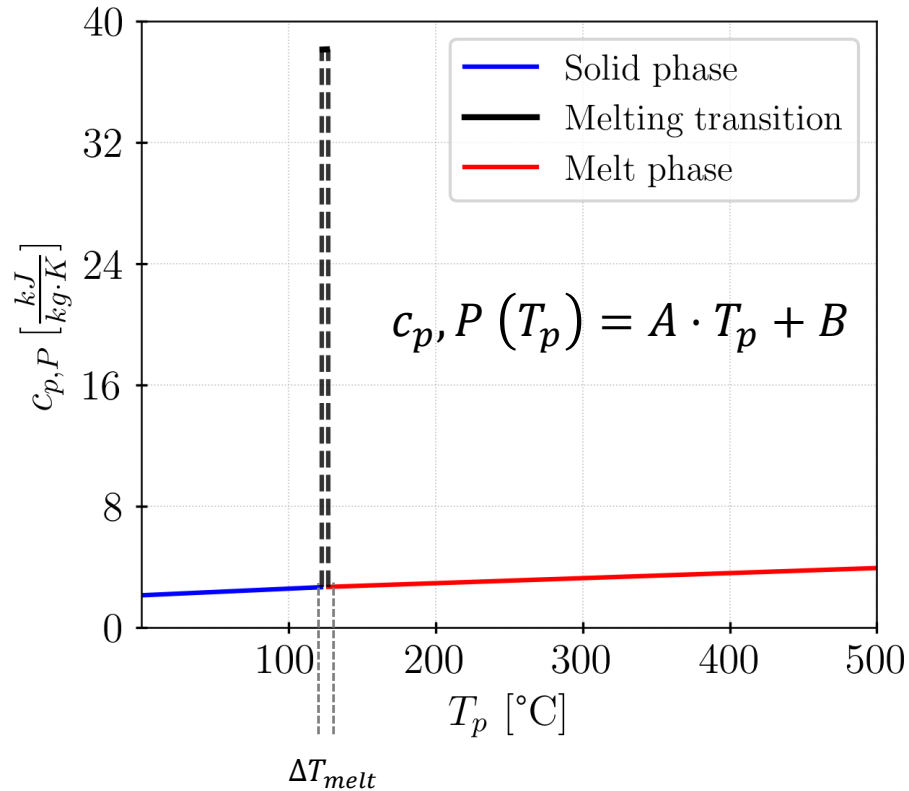
- ❑ Extended parameter range: different plastics, larger particles ...
- ❑ ML surrogate model for closure

**Thank you for  
your attention!**



# Thermal properties of LDPE

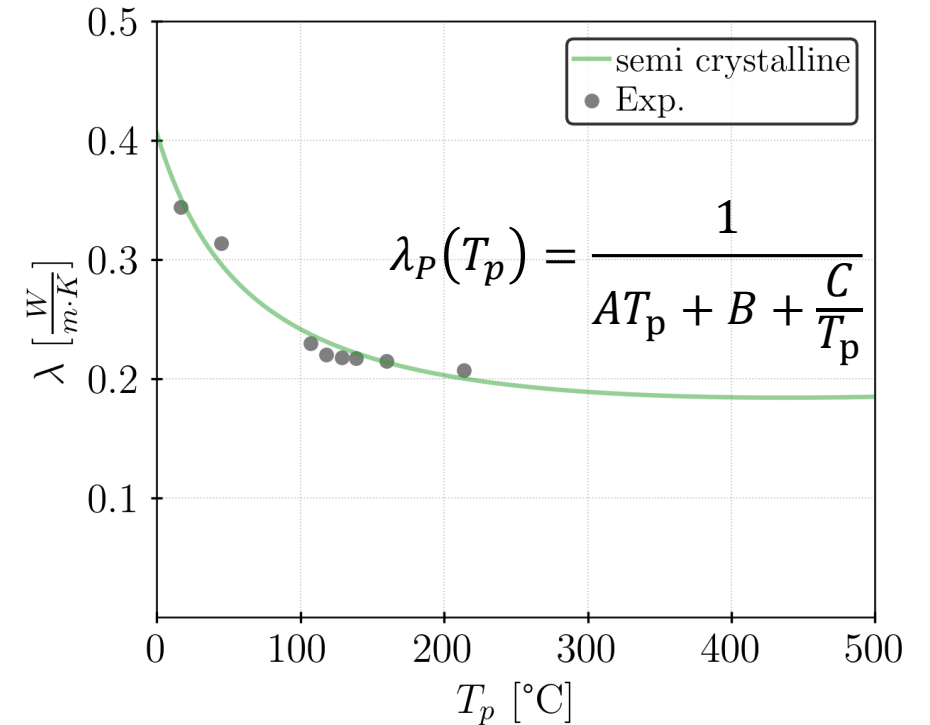
Heat capacity



Netsch et al. (2024) Thermogravimetric study on thermal degradation kinetics and polymer interactions in mixed thermoplastics. *Journal of Thermal Analysis and Calorimetry*

| $T_m^* \text{ [}^\circ\text{C}\text{]}$ | $h_f \text{ [J/g]}$ | $c_{p,\text{postGT}} \text{ [J/(kg} \cdot \text{K)]}$ | $c_{p,m} \text{ [J/(kg} \cdot \text{K)]}$ |
|-----------------------------------------|---------------------|-------------------------------------------------------|-------------------------------------------|
| 125                                     | 235                 | $4.376 \cdot T_p + 2106$                              | $3.336 \cdot T_p + 2238$                  |

Thermal Conductivity



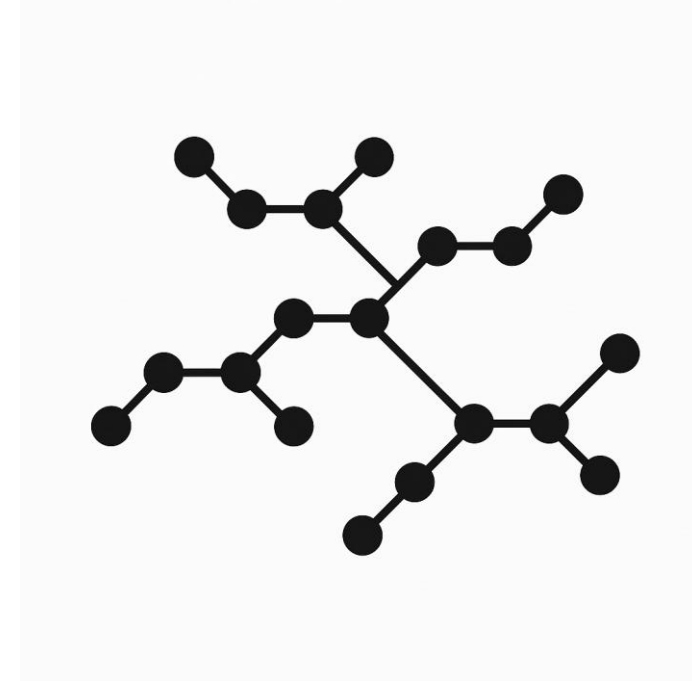
- 1) Zhang et al. (2002) Measurements of the thermal conductivity and thermal diffusivity of polymer melts with the short-hot-wire method. *International Journal of Thermophysics*
- 2) Dos Santos et al. (2013) Thermal Conductivity Behaviour of Polymers around Glass Transition and Crystalline Melting Temperatures

# Thermal conductivity Inside a Polymer

- ❑ Heat is transported primarily by phonons.
  - ❑ Relatively low compared to metals.
- ❑ Phonon scattering increases at higher temperatures.
  - ❑ Reduction in thermal conductivity
  - ❑ Thermal conductivity dependency on phonon

scattering:

$$\lambda_p = \frac{1}{3} C_p v l$$

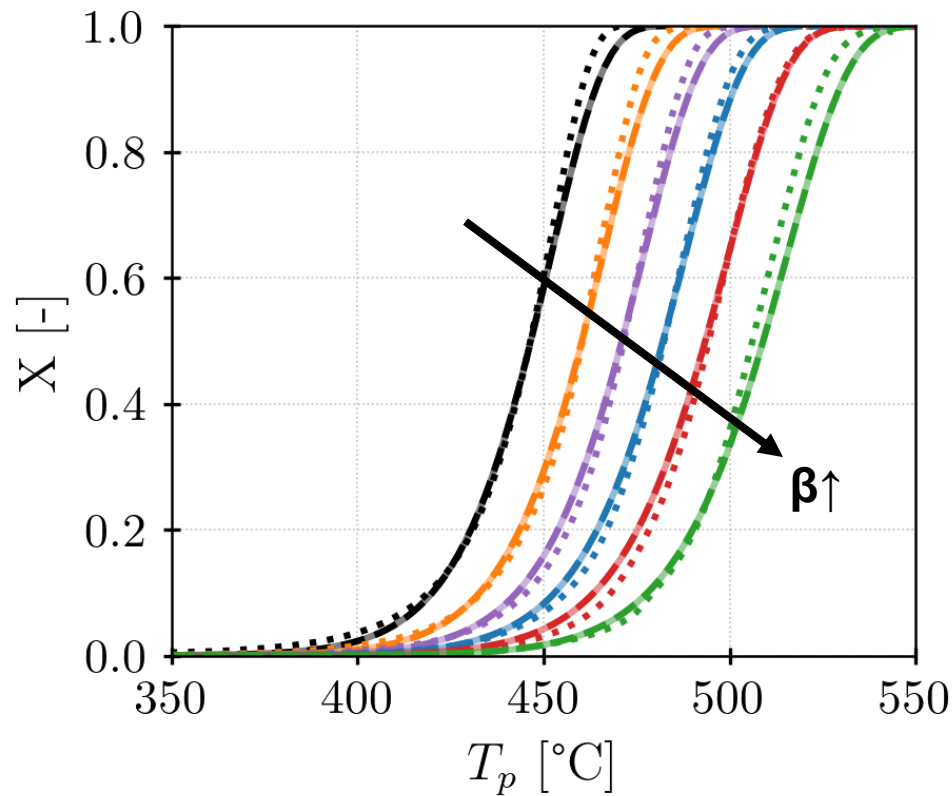
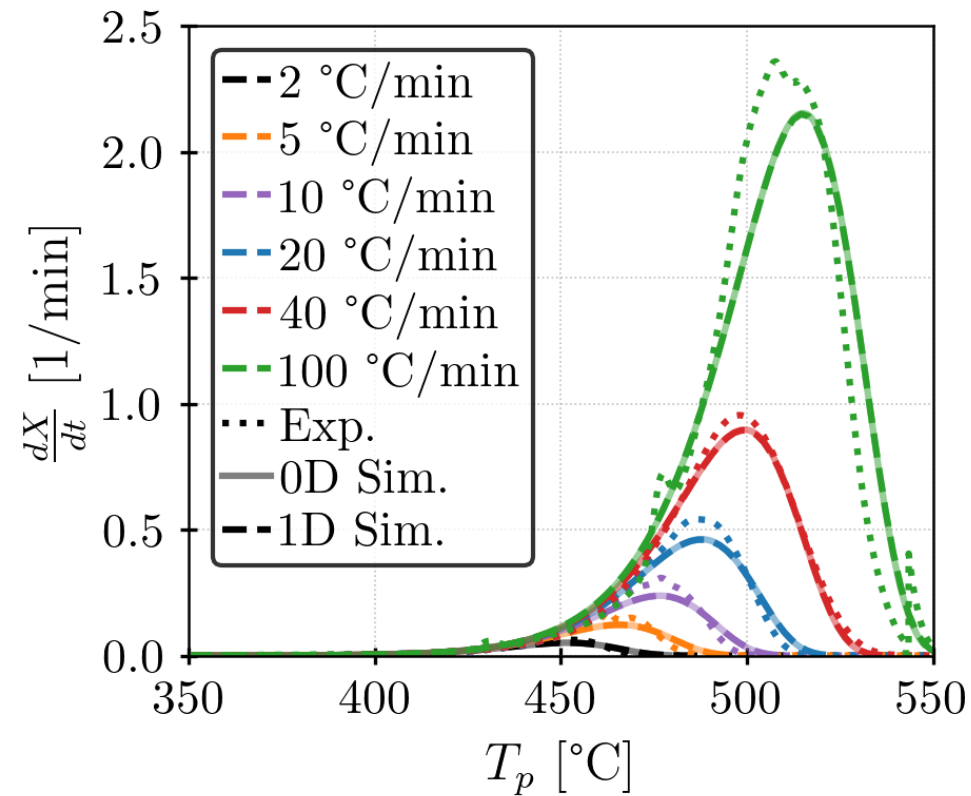


Polymer Chain LDPE

# Comparison with TG experiments

$$X(t) = \frac{m_{p,0} - m_p(t)}{m_{p,0}}$$

- ❑ Identical results for 0D and 1D simulations
- ❑ Higher heating rate leads to larger reaction rate and conversion at higher temperature



Netsch, et al. Thermogravimetric Study on Thermal Degradation Kinetics and Polymer Interactions in Mixed Thermoplastics. *Journal of Thermal Analysis and Calorimetry* 150, no. 1 (2025): 211–29.

# Grid-independence study

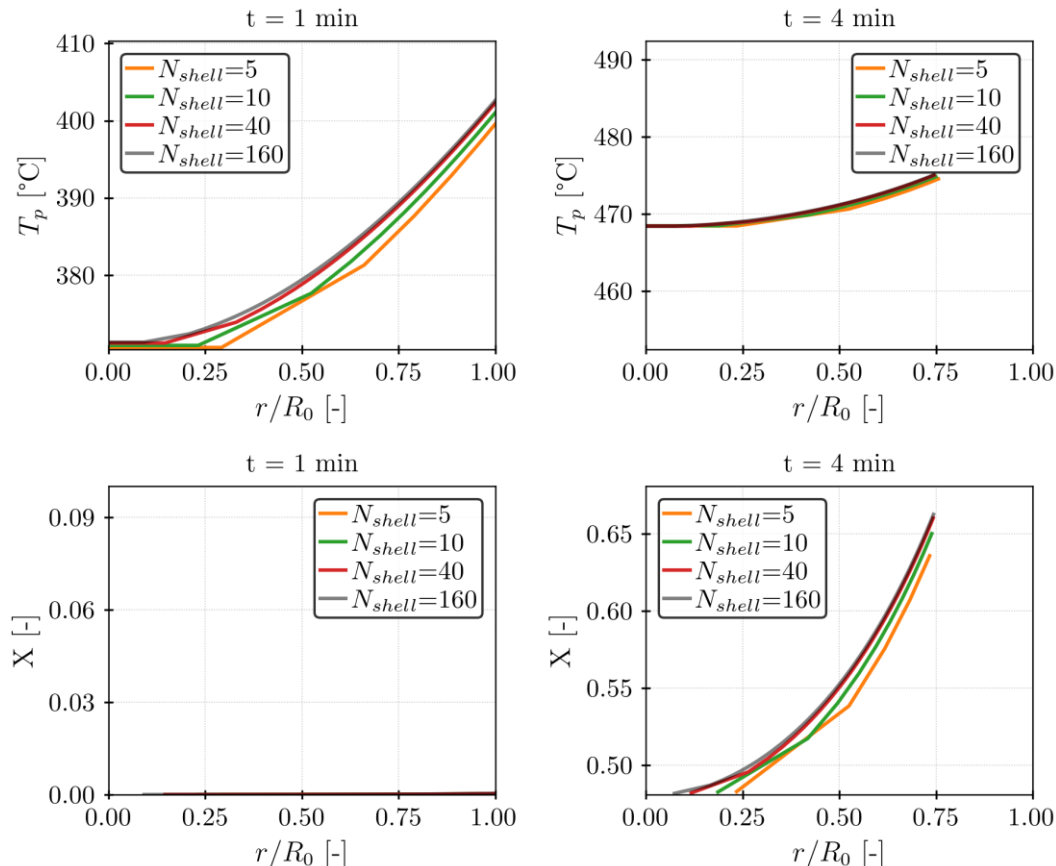
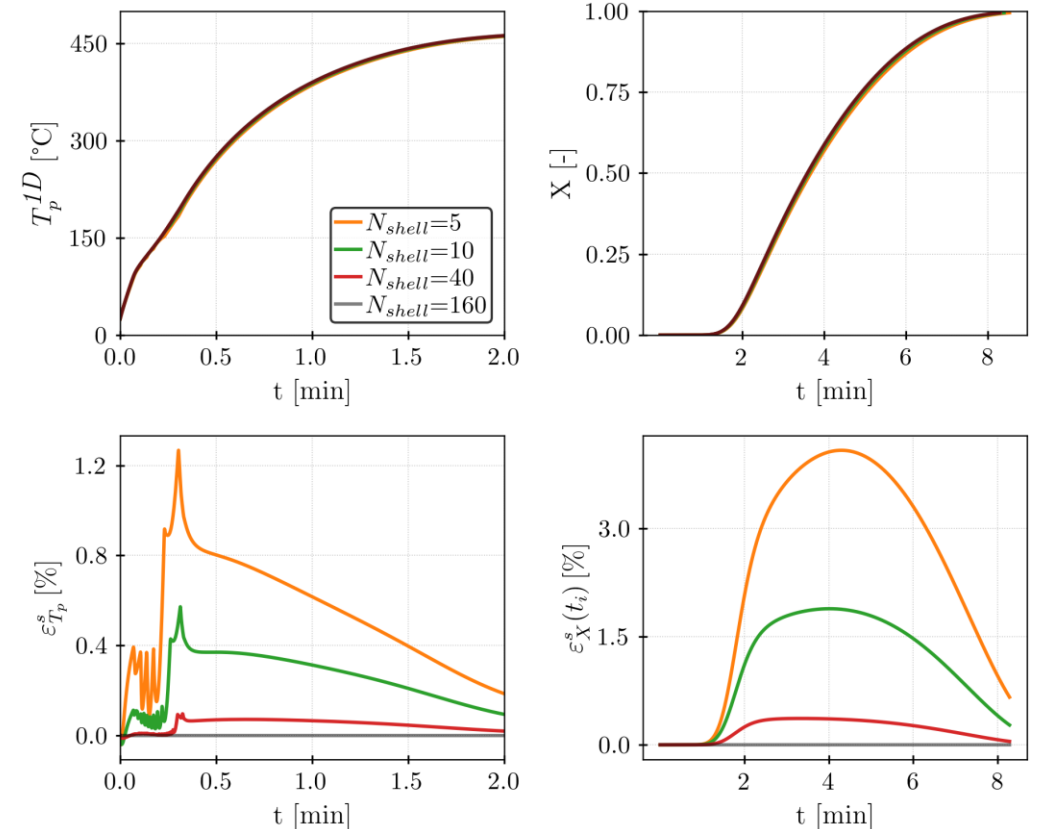
Reference Case:

$$T_R = 500\text{ }^{\circ}\text{C}, d_{p0} = 4\text{ mm}, Nu = 4, N_{shell} = 160$$

Comparison of simulations with different grid resolutions

→  $N_{shell}=40$  selected as compromise between computational accuracy and cost

$$\varepsilon^S(t_i) = \frac{y_{160}(t_i) - y_{N_{shells}}(t_i)}{\bar{y}_{160}}$$

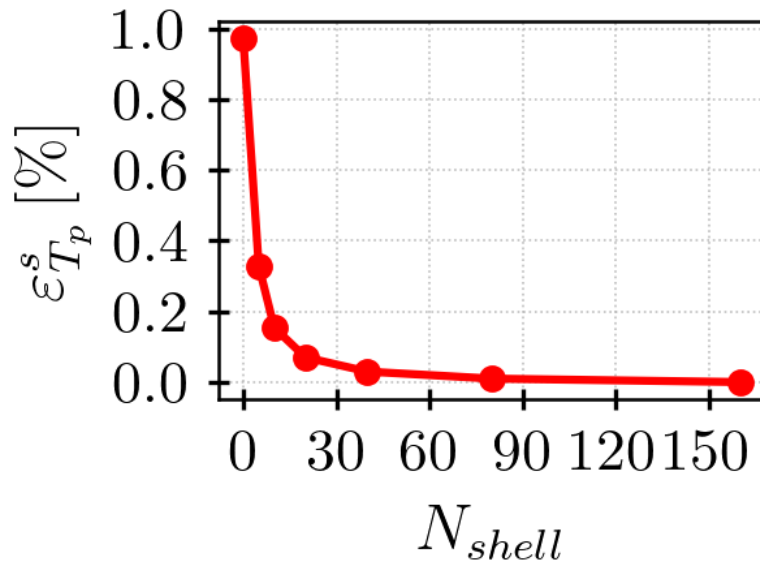


# Grid-independence study

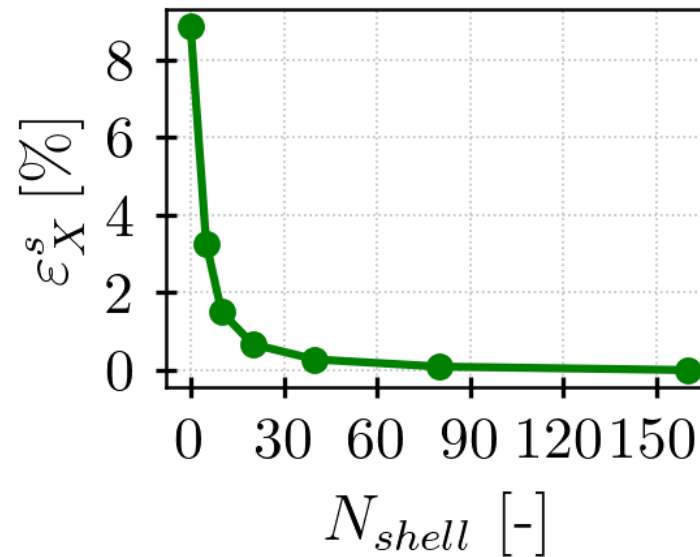
Reference Case:  $T_R = 500\text{ }^{\circ}\text{C}$ ,  $d_{p0} = 4\text{ mm}$ ,  $Nu = 4$

$$\varepsilon^S = RMS\left(\frac{y_{160} - y_{N_{shells}}}{\bar{y}_{160}}\right)$$

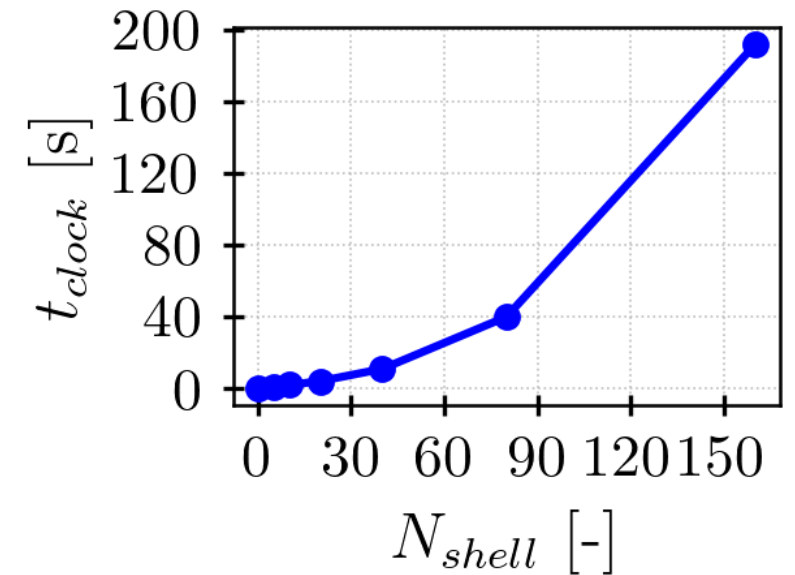
Averaged error over time



Averaged error over time

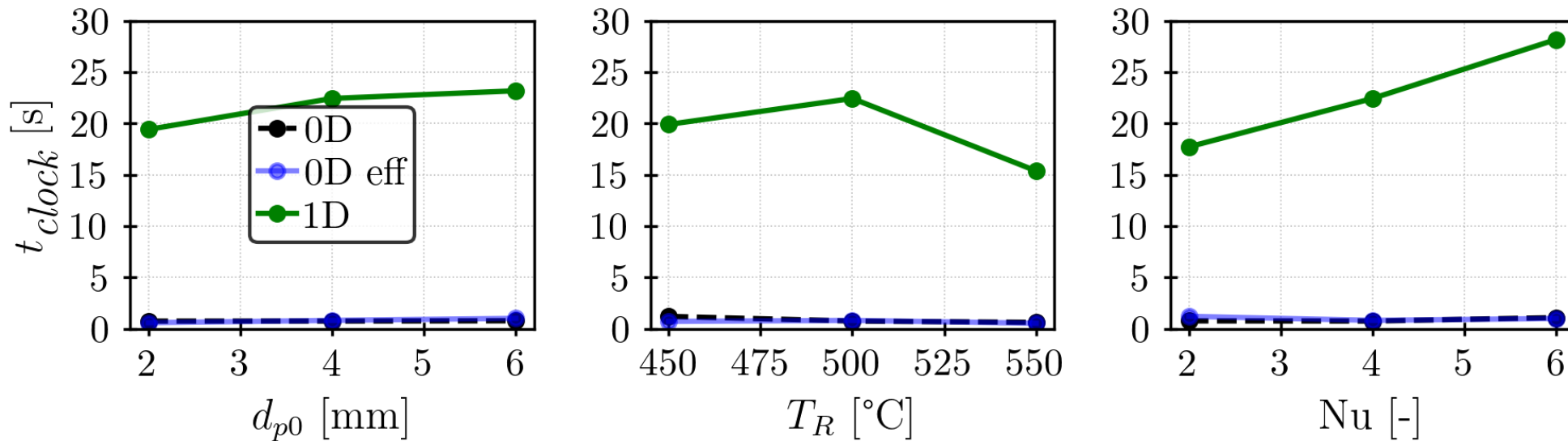


Computing time



# Computational Cost

- ❑ 0D → 1D : Computational cost increase of  $\approx 3,000$  % (reference case)
- ❑ 0D → 0D-eff : Computational cost increase of  $\approx 8$  %.
  - ❑ Improved accuracy by  $\approx 60$  % (for X).
- ❑ Minimal computational cost increase while gaining substantial accuracy.



Comparison of computational time for 1D, 0D, and 0D-eff models in a full parameter study.