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Highly resolved temperature measurements in slender fixed beds for validation of heat transport in particle-resolved CFD simulations

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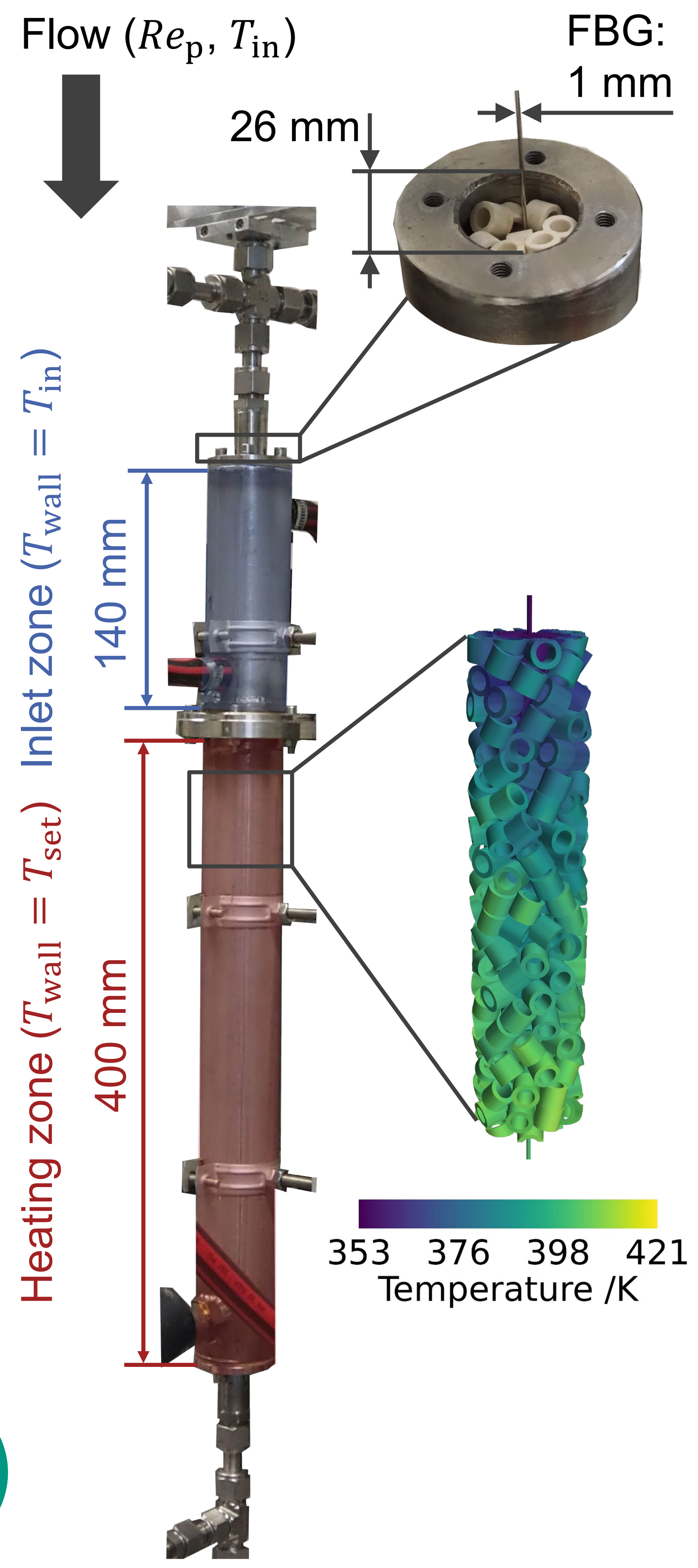
Motivation

In the chemical industry, highly exothermic or endothermic catalytic reactions are commonly carried out in slender fixed bed reactors ($D/d_\mathrm{p} < 7$). Due to the application of questionable correlations for effective heat transport parameters, pseudo-continuum models fail to describe the heat transport and consequently the performance of such reactors. Particle-resolved CFD (PRCFD) simulations overcome this issue by considering particles explicitly within the bed. In this work, an experimental setup for validating the PRCFD is presented. Finally, the validated PRCFD is used to determine detailed temperature fields, which can be used for estimating effective heat transport parameters applied in a pseudo-continuum model

Methodology

Experimental methods

- Two sectioned, double-tube heat exchanger loaded with a fixed bed based on the setup of Stegehake et al. [1].
- Two thermostats guaranteeing **defined temperatures at the wall** of the inlet (353.15 K) and the heating (353.15 to 473.15 K) zone.
- Fiber Bragg Granting (FBG) sensor protected by a stainless-steel capillary is axially centered in the fixed bed to **measure temperature simultaneously at 30 individual points**.
- Differential pressure sensor to record pressure drop during temperature profile measurements.



Modeling approach

- Fixed beds for PRCFD simulation are generated synthetically using the Rigid body approach within the open-source software Blender [2] and **validated with experimental void fraction**.
- PRCFD simulation resolved packed bed structure and do **not require semi-empirical correlations** to describe fluid flow and heat transport.[3]

Validating PRCFD with measurements
Simulations reflecting experimental boundary condition and including the stainless-steel capillary [4]

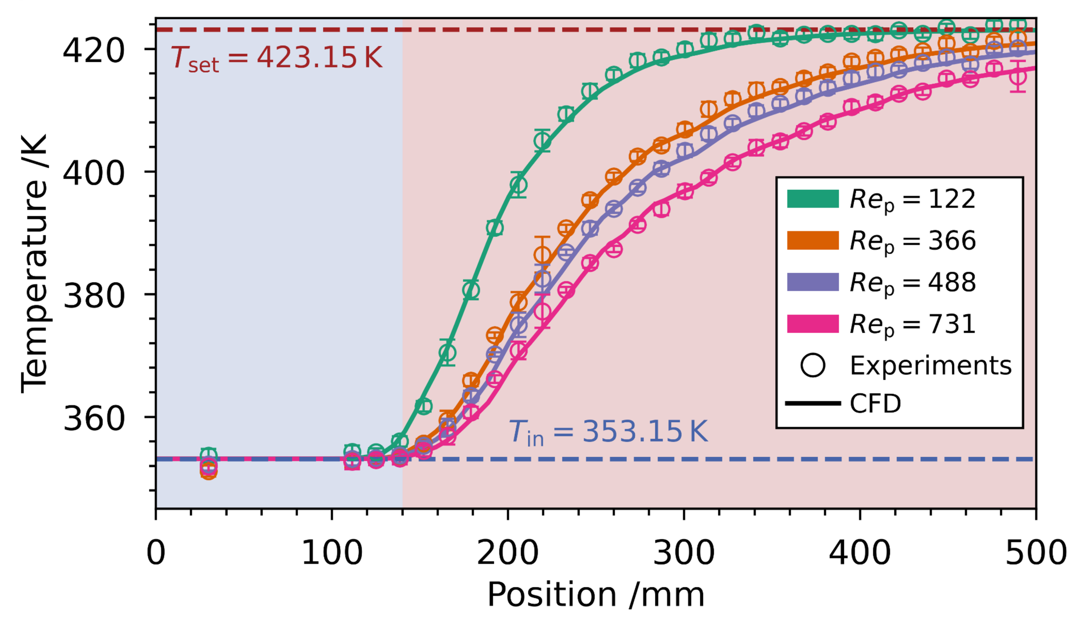
Extracting 2D temperature fields from PRCFD
PRCFD simulations without capillary, extracting circumferentially averaged 2D temperature fields

Determining effective heat transport parameters
2D pseudo-continuum model to estimate the wall heat transfer coefficient (α_wall) and the effective thermal conductivity (λ_eff) with 2D temperature fields using the Maximum-Likelihood-Method.

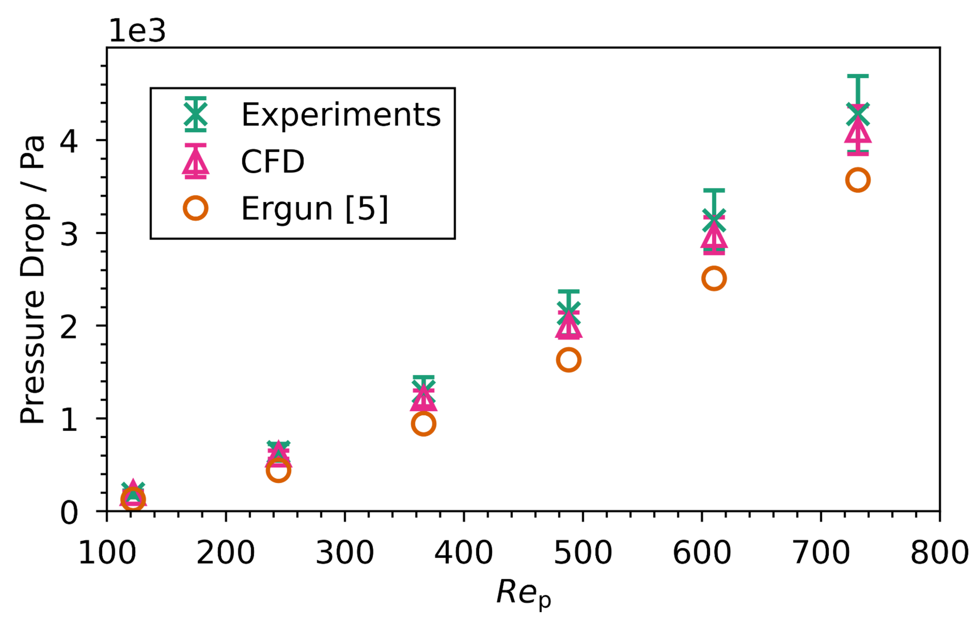
Results

Experiments and simulations are preformed with ring shaped particles ($d_\mathrm{p,o} = 6\ \mathrm{mm}$, $d_\mathrm{p,i} = 4\ \mathrm{mm}$, $h_\mathrm{p} = 5\ \mathrm{mm}$) and for various flowrates at $T_\mathrm{set} = 423.15\ \mathrm{K}$, and $T_\mathrm{in} = 353.15\ \mathrm{K}$.

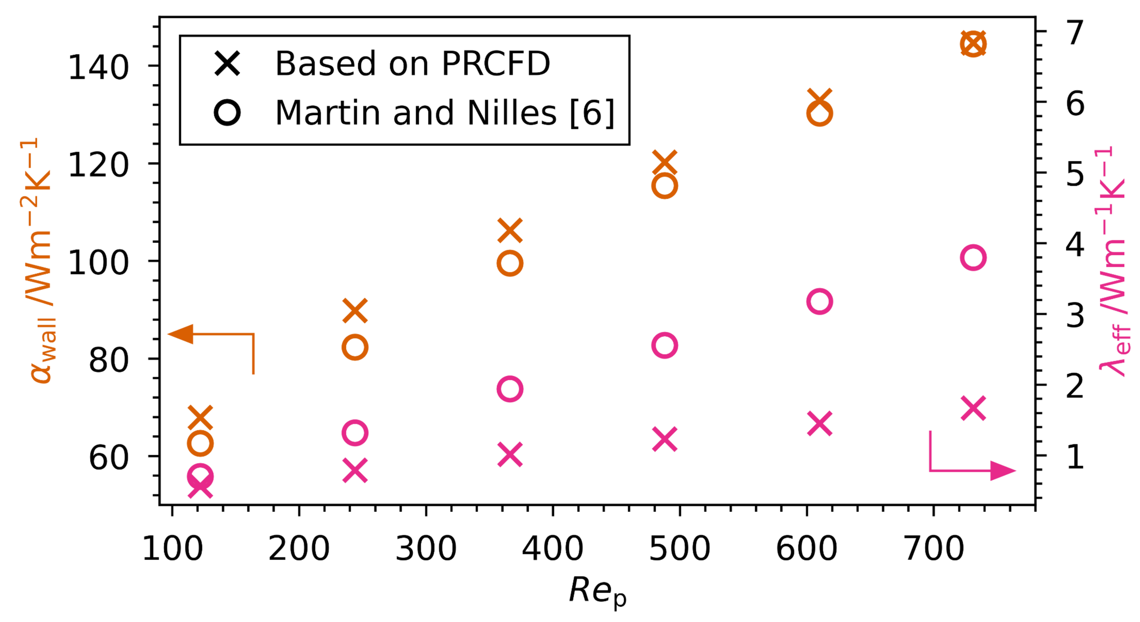
Experimental vs. simulated axial temperature profiles:



Experimental vs. simulated pressure drop:



Effective heat transport parameters based on PRCFD and according the correlation of Martin and Nilles [5]:



Conclusion and outlook

The PRCFD simulations can be validated with highly resolved measurements of the axial temperature profile within a fixed bed. The validated PRCFD approach is used to determine effective heat transport parameters applied in a pseudo-continuum model of an undisturbed fixed bed. In future work, the presented setup will be employed to resolve temperature gradients in catalytic packed beds with strong heat effects.

References

[1] Stegehake, Grünewald (2017), Chem. Ing. Tech., 89 (4), 480-485.
[2] Partopour, Dixon (2017) *Powder Technol.*, 322, 258-272.
[3] Dixon, Partopour (2020) *Annu. Rev. Chem. Biomol. Eng.*, 11, 109-130.
[4] Kutscherauer et al. (2022) *ACS Engineering Au.*, 3(1), 45-58.
[5] Ergun (1952) *Chem. Eng. Prog.*, 48(2), 89-94.
[6] Martin and Nilles (1993), *Chem. Ing. Tech.* 65(12), 1468-1477.

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