Modeling transient CO_2-methanation in single catalyst particles with CFD and continuum models

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Motivation

The dynamic operation of catalytic gas-solid reactors has gained attention in recent years with special emphasis put on load-flexibility and periodic feed perturbations. Fixed-bed reactors for transient methanation (Sabatier reaction) have predominantly been described with 1D heterogeneous models, however, it is not clear as to whether these models can capture the propagation of the underlying feed perturbations through the packed bed reactor. Despite recent advances in particle-resolved computational fluid dynamics (PRCFD) of entire fixed beds, dynamic simulations of such are still infeasible due to the high computational cost. In previous work, steady-state flow around a single ring-shaped pellet has been modeled with a 3D PRCFD simulation and a 1D pellet model [1]. The results showed that the 1D model can capture integral quantities such as the mean pellet temperature and catalyst effectiveness factor. However, it has not yet been verified for transient cases. To close this knowledge gap, dynamic 2D PRCFD simulations of a single catalytic pellet are performed and compared to 1D pseudo-continuum simulations, see Fig. 1. The results further give valuable insight into the single pellet dynamics itself, which is a crucial aspect for operando measurements in single pellet profile reactors and the respective experimental design [2,3].

Methods and outlook

In this work, the transient 2D PRCFD model of a cylindrical catalyst pellet for the CO_2-methanation is developed based on an existent workflow for conjugated heat and mass transfer formulations [4]. The effects of feed perturbation, by concentration and temperature forcing, as well as of flow instabilities on the reaction-diffusion processes within the pellet are evaluated across a relevant range of particle Reynolds numbers. In a similar way, the 1D pseudo-continuum model is subjected to

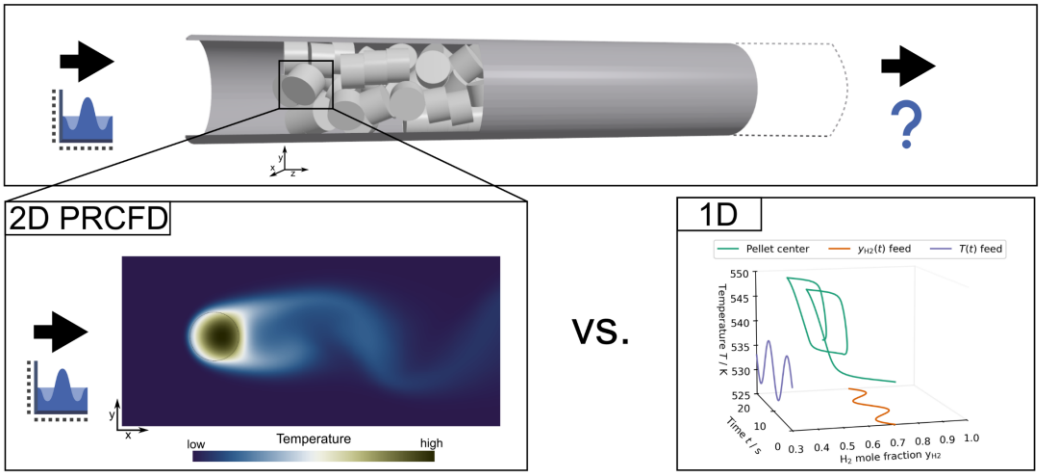

Figure 1: Schematic of different modeling approaches including the 2D PRCFD and 1D model.

transient boundary conditions. Finally, the two approaches are compared against each other with respect to limitations in describing pellet dynamics under locally variant boundary conditions, which are imposed on pellets in catalytic packed beds or single pellet profiling reactors. This may serve as a decision tool for a computationally efficient model and can prospectively be extended by system identification studies to delve into the description of the dynamics by surrogate models.

References

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