

Revisiting homogeneous modeling with volume averaging theory: structured catalysts for steam reforming and CO₂ methanation

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Abstract. We discuss the fluid mechanics modeling of structured catalysts for use on steam reforming (SR) and carbon dioxide (CO₂) methanation (MT). Results of the study should allow better informed modeling decisions. As an example, we do not find significant differences among the choice of available gas or homogeneous surface kinetics models. For homogeneous models, we verify assumptions that prioritize appropriate modeling of thermodynamic dispersion tensors over the modeling of hydrodynamic dispersion (drag).

Keywords: Combustion, reactive flows, porous flows, homogeneous modeling, structured catalysts, steam reforming, CO₂ methanation.

1. Context of the research

Utilizing hydrogen (H₂) as an alternative fuel can contribute to industrial decarbonization. A large part of H₂ production is achieved via SR of natural gas, a relatively high efficiency process (80 – 85%, [1]). When compared to natural gas (methane CH₄), H₂ has a lower energy density (≈ 11 MJ/m³ versus ≈ 36 MJ/m³). This poses technical storage and transport challenges, especially in terms of existing infrastructure. To alleviate the shortcoming, one may produce CH₄ from H₂ (during excess H₂ production) for transport, storage or utilization (CO₂-MT). Both SR and MT processes require catalysts, given their hindered kinetics at typical operating conditions [2]. Advancements in structured catalysts are crucial for enhancing efficiency and scalability in industrial applications [3]. Studies have extensively explored reactive flows over catalyst surfaces, covering chemical kinetics analysis [4], as well as porosity and dispersion analysis for porous media flow simulations [5]. The focus of this contribution is on modeling strategies favouring the use of homogeneous models, due to the complexities of large scale H₂ production, either related to turbulence, or complex porous structures. Both situations may hinder the application of otherwise more reliable direct numerical simulations (DNS).

2. Modeling strategies and most relevant results

2.1. Zero-dimensional (0-D) homogeneous modeling

We formulate a 0-D homogeneous modeling strategy to assess the influence of simplified gas chemical kinetics versus detailed surface chemistry. Figure 1a) illustrates the 0-D model results for CO₂ conversion in a MT process under conditions similar to [3]. The choice between available gas or detailed surface chemistry has a minimal impact on the MT modeling outcome. Figure 1b) shows the 0-D model results for temperature-dependent concentrations obtained from the SR process simulated by [6]. As seen, 0-D models deliver reasonable results.

2.2. Three-dimensional (3-D) modeling

We also formulate a 3-D homogeneous model employing volume averaging theory (VAT). To compare the results of the 3-D homogeneous model, we conduct 3-D inhomogeneous simulations (implicit large eddy simulations with a deliberate choice of no sub-grid stress modeling). Figure 2a) shows the model results for H₂ concentration and velocity field magnitude for the selected SR process in 2.1. Figure 2b) shows a cross-sectional view of the detailed simulation results. The results and key implications will be discussed and analyzed in detail in the full paper.

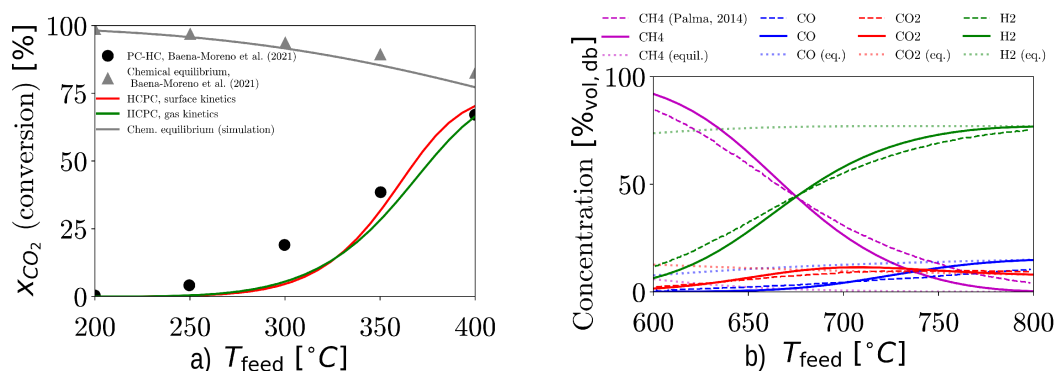


Figure 1. a) CO₂ conversion in a MT process and b) concentration in a SR process (0-D model)

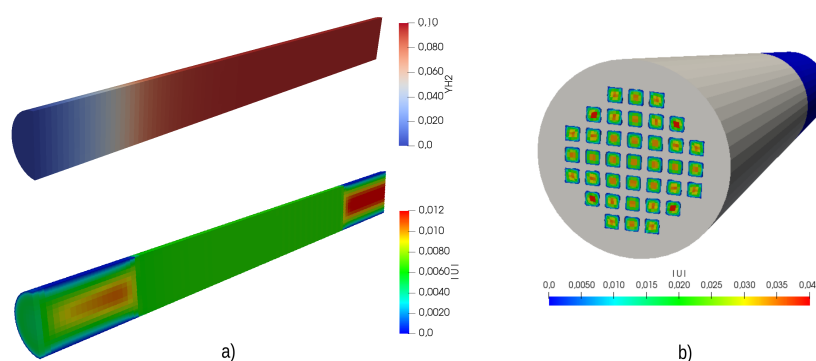


Figure 2. 3-D model for SR process as in [6]

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