Brandenburgische Technische Universität Cottbus - Senftenberg

Possible Topic for a MASTER THESIS OR STUDY PROJECT

at Brandenburg University of Technology (BTU) in Cottbus, Germany

Modeling of structured catalysts for CO_2 methanation

Synopsis – Within the widespread field of applications for structured catalysts, one application with current strategic importance is that of emissions control. The CO or CO_2 methanation has some fundamental significance, since it is associated both to natural gas production, as well as CO and CO_2 emissions removal [1]. For the optimization of the process of natural gas production,the development of selective, reliable and efficient catalysts is required. Although structured catalysts have been received with initial skepticism due to their poor performance in comparison to pellet beds, as well as their virtual adiabatic character, specific requirements for structured catalysts can be met with dedicated designs [2]. One example of such dedicated design is the gyroid 3-D printed catalyst presented by [3]. Preliminary evaluations of this catalyst have already demonstrated a reliable and highly efficient CO2 conversion. However, the optimization of the design is complicated due to the multitude of factors playing a role in the catalytic efficiency: from the chemical kinetics taking place, all the way to the catalyst-enhanced flow drag, and the associated heat and mass transfer. Desired for this work is a focus on the evaluation of the recently introduced Ru-Ni/$MgAl_2O_4$ structured catalysts [3] from the numerical fluid-dynamic point of view. To that extent, fluid dynamic treatment of structured catalysts is generally conceived within the framework of porous media flows, specifically, the most widely used closure model for the upscaling of the momentum balance using volume-averaging theory (VAT) is the Darcy- Forchheimer equation [4]. A research path is suggested as follows:

- **a) Master Thesis (1 semester):** The student should focus on an overall validation of the implementation of the chemical kinetics obtained by the OpenFOAM and Cantera libraries using a pre-specified chemical mechanism for CO_2 methanation. Previous work did not manage consistency between both libraries results or calculation methods [5]. A verification of the hydrodynamics produced by the OpenFOAM solver for a laminar flow is also expected.
- **b) Study Project (2 semesters):** In this case, the student should compare the previous results obtained with the OpenFOAM simulations for laminar flow, now considering the additional implementation of a typical turbulence model (e.g., LES), which should emulate the residual stress tensor obtained by the application of volume averaging to the governing equations, see [4].
- **c) Study Project and Master Thesis (3 semesters):** Same as b). Additionally, the student will evaluate cold flow (isothermal and non-reactive) in the catalyst using OpenFOAM and a stochastic reduced order turbulence model (in-house developed software library).

[1] Gao and Goodman (2012), *Annu. Rev. Phys. Chem.* **63**, 265–286 — [2] Tronconi *et al.* (2014), *Curr. Opin. Chem. Eng.* **5**, 55–67 — [3] Baena-Moreno *et al.* (2021), *ACS Sustainable Chem. Eng.* **9**, 8198–8206 — [4] Whitaker (1996), *Transp. Porous Media* **25**, 27-61 — [5] Medina Méndez *et al.* (2022), *J. Phys.: Conf. Ser.*, accepted for publication —

Tasks

- Review of relevant literature and theoretical foundations
- Code development, compilation and testing
- Visualization, post-processing, and data analysis of numerical simulation data
- Comparison of simulation results with relevant reference data

Desired skills and requisites

- Solid knowledge of fundamentals of fluid mechanics and combustion
- Affinity to programming (preferably Python and C/C++)
- Scientific attitude (curiosity, self-motivation, and critical reasoning)
- Experience with data analysis, numerical simulation and modeling, or CFD is an asset
- **For the intended take of the Master Thesis:** The student must have approved the modules of Turbulence Modeling and CFD 1.
- **For the intended take of the Study Project:** The student is required to take the modules of Turbulence Modeling and CFD 1 in parallel to the project time frame.

Contact information:

Dr.-Ing. Juan Medina E: `medinjua@b-tu.de` T: +49-355-69-6033

Chair of Numerical Fluid and Gas Dynamics, Brandenburg University of Technology (BTU)
Siemens-Halske-Ring 15A, D-03046 Cottbus, Germany

URL: `https://www.b-tu.de/en/fg-stroemungsmodellierung`