Reactor and process design for hydrogen production in liquid metal bubble columns

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Simulation of methane pyrolysis

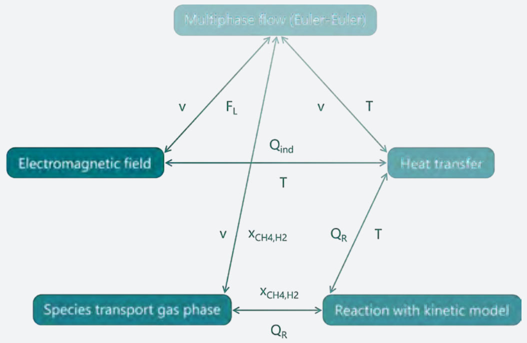


Figure 1: Illustration of the included physics in Comsol Multiphysics and their coupling

Bubble column reactors with molten metals are a promising concept for methane pyrolysis. However, the processes in the reactor are difficult to access, making simulations helpful to obtain insights. In the reactor to be simulated (shown schematically in the centre), methane is introduced into the inductively heated molten metal, where it is decomposed. Simulations are performed in Comsol Multiphysics and include conservation equations for the physics shown in Figure 1. An axisymmetric 2D approach is applied to reduce the required computational capacity. Due to the different processes, the validation is carried out by using two setups, one for the reactive flow and one for the magnetically induced flow.

Reactive bubbly flow

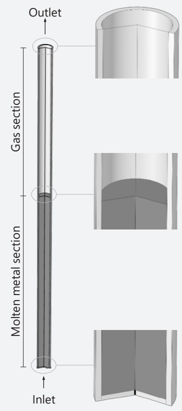


Figure 2: Geometry of the reactor for validation [1,2]

To validate the reactive bubbly flow without inductive heating, two publications of the KIT [1,2] are used. The aim is to find a suitable non-catalytic kinetic model as tin is used as the molten metal. Between the models, large differences in the conversion rates occurred, which can be seen in figure 3a and 3c. Besides the kinetic model, the Euler-Euler model requires the input of the bubble size and a model for the drag coefficient, the calculation of which has not yet been resolved in molten metals. Therefore, their influence on the conversion was determined and found to be minor compared to the impact of the kinetic model (see figure 3b).

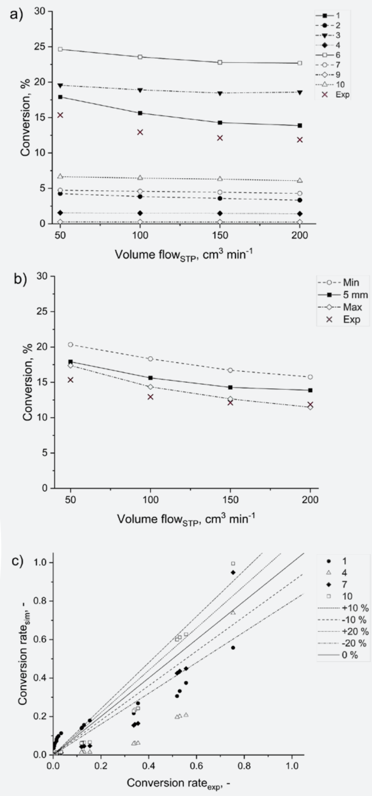
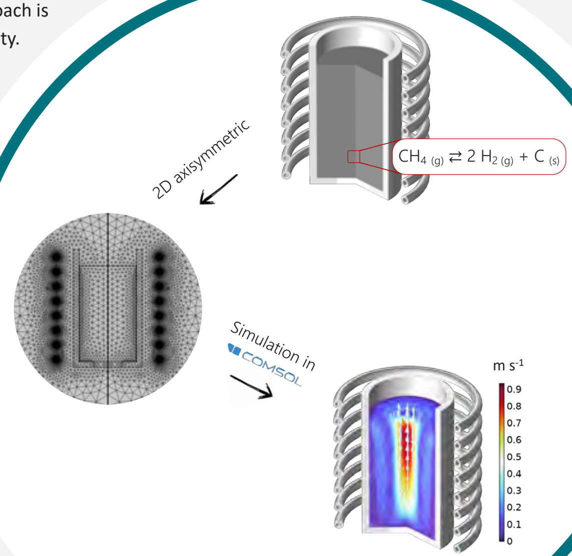


Figure 3: a) Conversion at 1000 °C for different kinetic models, b) conversion at 1000 °C for different bubble diameters, c) Parity plot at 850 - 1175 °C for four kinetic models



Magnetically induced flow

In order to examine the simulation of the flow induced by the magnetic field in the molten metal separately from the multiphase flow and the methane pyrolysis reaction, only the movement of the molten metal and the electromagnetic field of the inductive heating are included. Validation is carried out through comparison with simulation results from the pilot plant manufacturer. When the reactor is in operation and thus also in the simulation, it is possible to set varying phase shifts between the two coils. This makes it possible to change both the size and position of the vortices that form as well as the velocity of the melt.

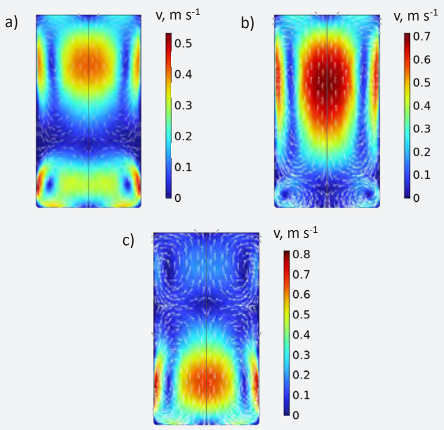


Figure 4: Velocity field of the molten metal induced by the magnetic field at different phase shifts of a) 0 °, b) 90 °, c) -90 °

Outlook

The results show that the flow induced by the magnetic field can be well represented. However, it is difficult to draw a reliable conclusion about the kinetic models, as no clearly suitable kinetic model can be determined. Therefore, the most suitable kinetic models will be used and compared in further simulations of experiments at the Chair of Nonferrous Metallurgy with an inductively heated bubble column reactor. In this reactor, the gas is introduced with a lance from the top. An exemplary simulation of the flow in the reactor can be seen in Figure 5. With these simulations, the suitability of the simulation for the methane pyrolysis reactor including all relevant processes can be examined and more information about the applicability of the kinetic models is obtained.

In order to extend the residence time in the molten metal, the insert of plates into the melt is currently being investigated at the Chair of Nonferrous Metallurgy. It is planned to simulate only the fluid flow within this setup in order to evaluate the effects on the gas flow.

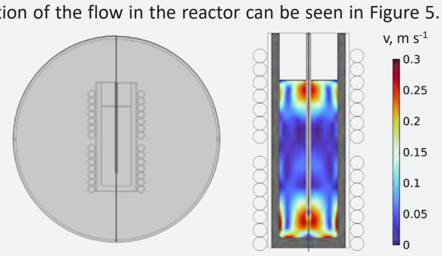


Figure 5: Geometry and velocity field of the molten metal in the methane pyrolysis reactor

[1] Plevan, M., et al. (2015): Thermal cracking of methane in a liquid metal bubble column reactor: Experiments and kinetic analysis. *International Journal of Hydrogen Energy* 40(25)
[2] Uhlenbruck, N., et al. (2022): Methane Pyrolysis in a Liquid Metal Bubble Column Reactor: A Model Approach Combining Bubble Dynamics with Byproduct and Soot Formation. *Energy Tech* 10(11)

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