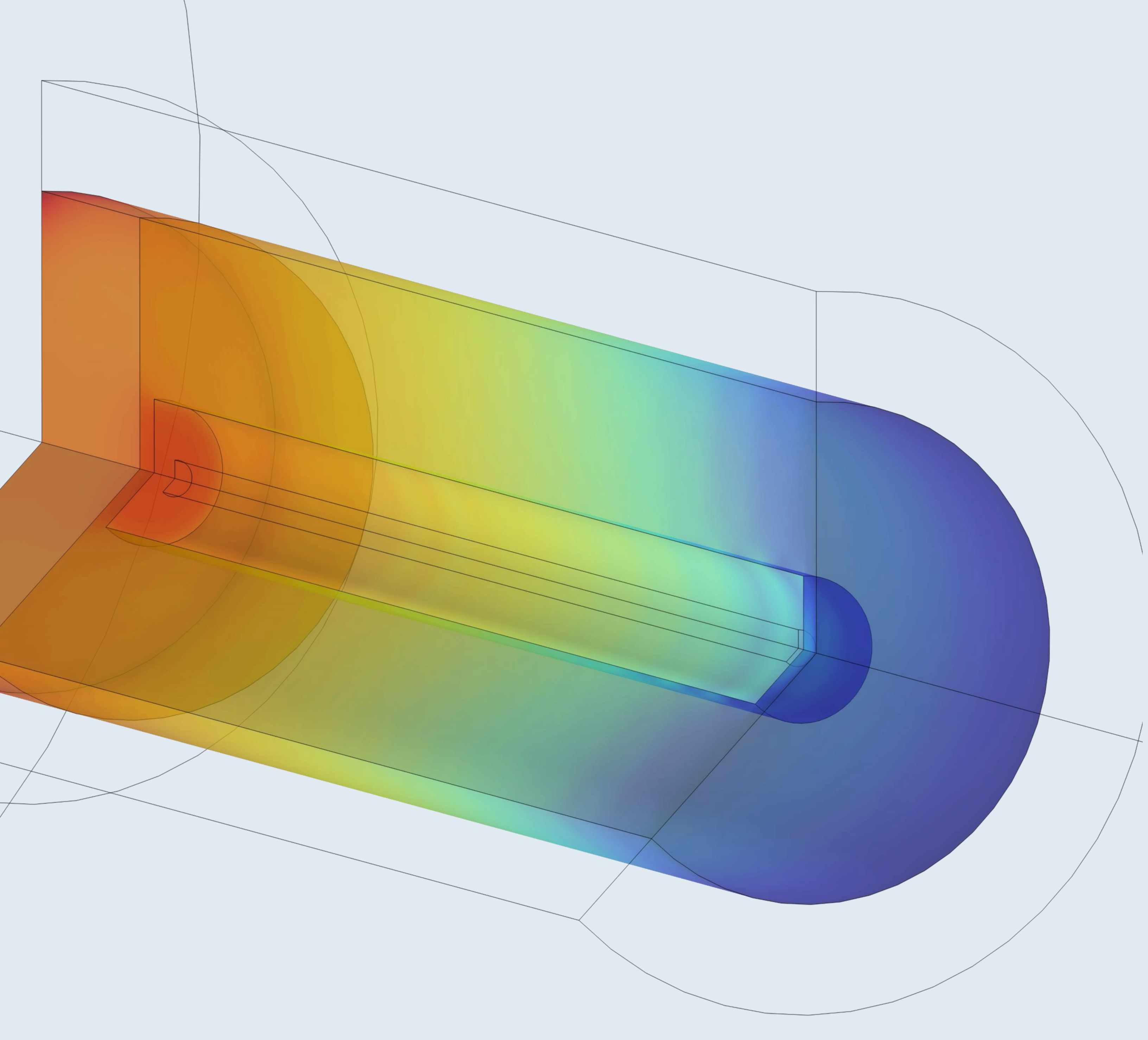

Methanation in catalytic reactor

Synthetic methane is produced using a catalytic reactor. Optimisation of the variable parameters has a significant impact on conversion efficiency.

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Introduction & Goals

Power-to-gas is an important area of research for reducing greenhouse gases and for seasonal energy storage. Methane, with a Lower Heating Value (LHV) of 50 MJ/kg, is a commonly used gas, and its synthesis using green hydrogen (generated by electrolysis based on renewable energy) is a remarkable way to break the carbon cycle.

Sabatier's methanation process combines hydrogen and CO_2 in a catalytic reactor at 250-350°C to produce CH_4:

$$CO_2 + 4H_2 \xrightarrow{catalyst} CH_4 + 2H_2O$$

Several constraints influence the efficiency of the reaction: temperature (exo-thermal), pressure (concentration), flow rates (ratio), cooling (insulation) and the uniformity within the reactor. The target is to maximize CO_2 conversion to obtain a complete reaction and high-purity CH_4 production (after water removal).

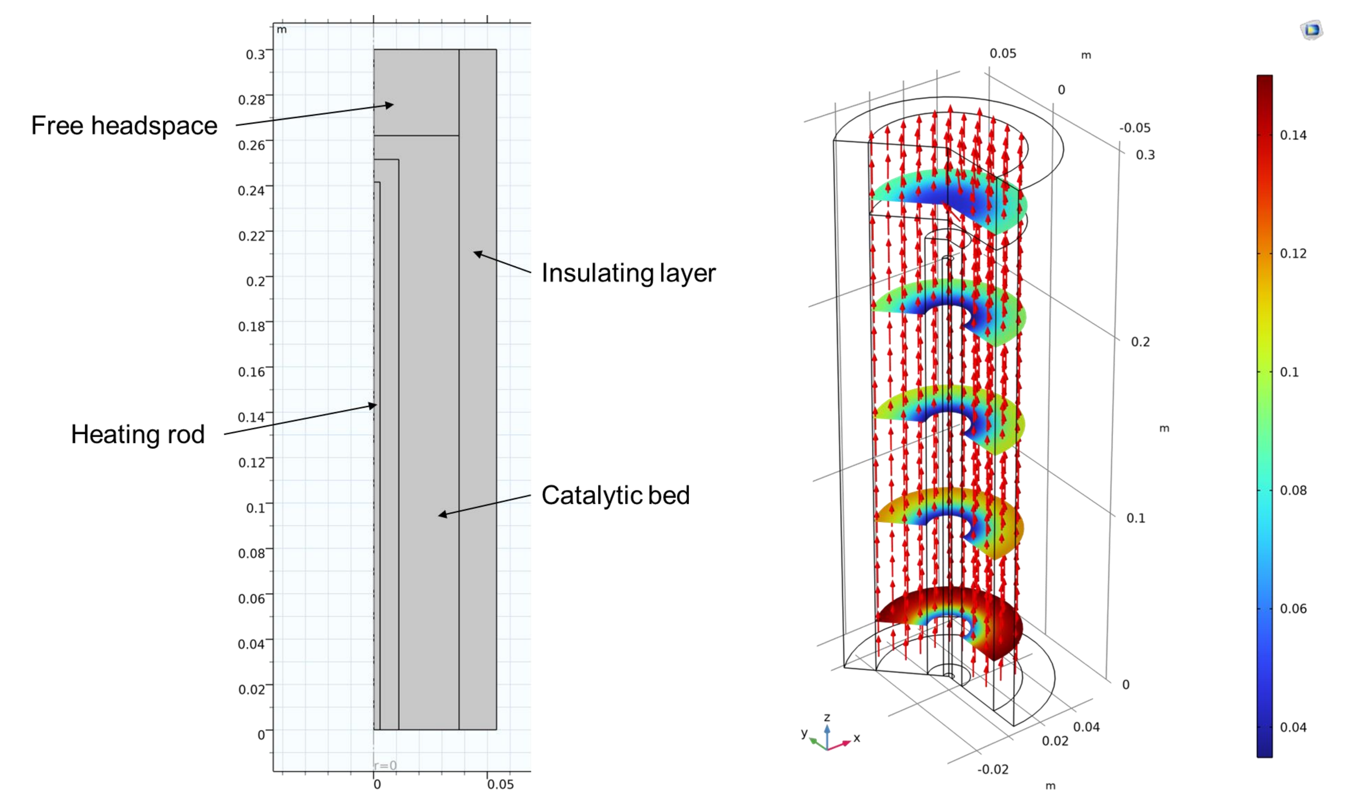

FIGURE 1. Left: 2D geometry of the existing reactor in the laboratory used for modeling. Right: 3D view of the reactor, with the gas flow (arrows) and CO_2 concentrations at different planes

Methodology

The Chemical Reaction Engineering, Heat Transfer, Porous Media Flow and Transport of Concentrated Species modules were used to model the existing reactor in our laboratory. The aim is to create a digital twin of this reactor, in order to understand the thermal behavior in particular. The volume of the reactor is 1.2 L and contains small cylinders of Al_2O_3 covered by catalysts. The temperature distribution in the catalytic bed, the heat generated by the reaction and the gas pressure are obtained, giving a better understanding of how and where the CH_4 conversion works to improve the geometrical arrangement to design a new reactor with an optimized thermal management and a full CO_2 conversion.

Results

The results of the simulations are presented in Figure 2. The mole fractions of the gas along the reactor, the temperature distribution and the heat source are presented for a total gas flow of 2.5 slm and a heater temperature of 300°C. H_2 and CO_2 are converted into methane and water in the first couple of centimeters of the catalytic bed. The heat is generated in this tiny part, which causes a huge temperature inhomogeneity in the reactor.

Thermal management is a crucial goal in order to avoid a runaway effect, causing catalyst and/or reactor damages.

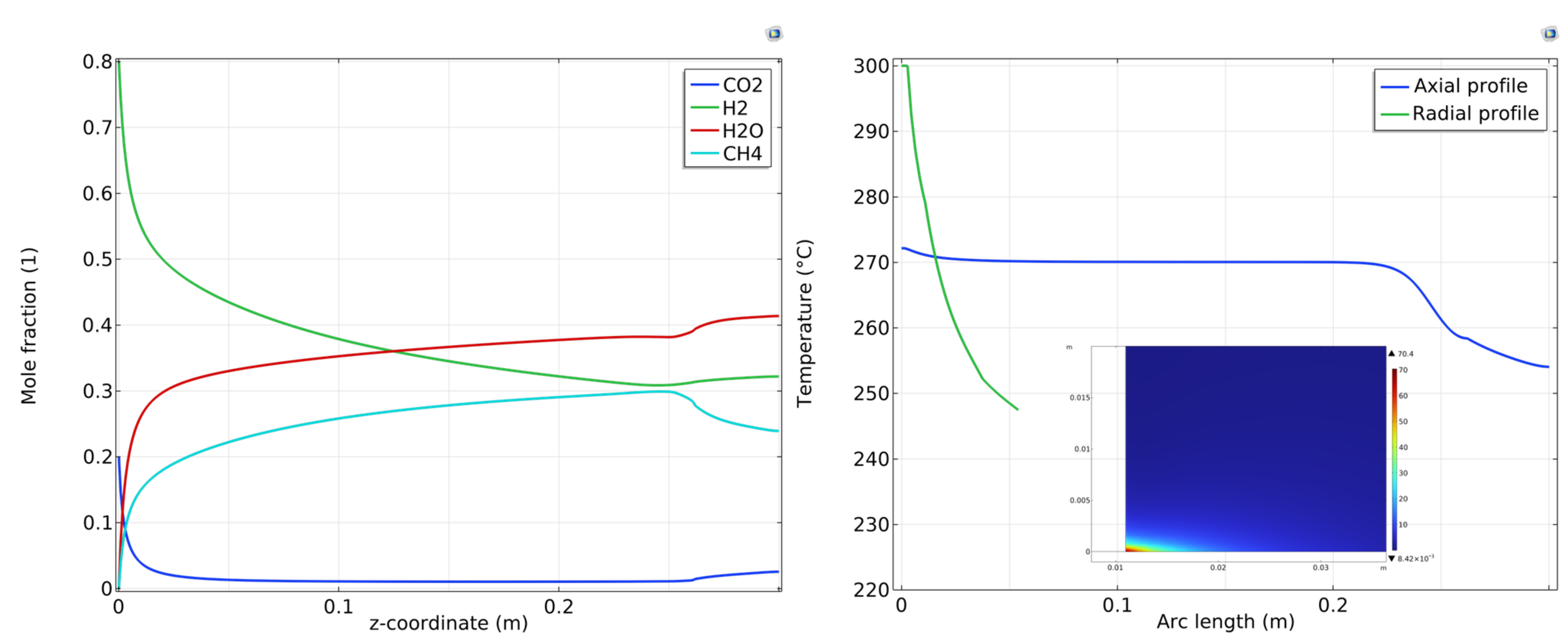

FIGURE 2. Left: Gas mole fractions in the axial direction. Right: Temperature profiles in axial and radial directions, with the inset being heat generated by the reaction in the lower part of the reactor, explaining the temperature inhomogeneity.

REFERENCES

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