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# Interaction between kinetics, mass and heat transfer in a catalytic plate reactor. Experiments and CFD modeling

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## 1. Introduction

Designing chemical reactors for heterogeneous reactions is challenging due to the coexistence and interplay of multiple phenomena like reactions, local flow dynamics, interfacial mass and heat transfer. The knowledge of the reaction mechanism with their corresponding kinetic description is of primary importance. Traditionally, kinetic data are experimentally gather using small laboratory packed bed reactors with end-of-pipe measurements only. These reactors provide limited scale-up insights as non-uniform catalyst mass distribution as well as concentration and temperature gradients along with the axial and radial directions are not considered. Moreover, these reactors are usually operated with highly diluted gas and/or catalysts to avoid possible temperature hot-spots due to exo- and/or endothermicity nature for some reactions. Utilizing an integral reactor like our recently developed optically accessible catalytic plate reactor (CPR) with spatially resolved measurement capability allows for collecting high-resolution gas composition and catalyst surface temperature profiles along the reactor axis via a small movable sampling capillary and short-wave infrared camera, respectively [1]. This is a great advantage compared to standard packed bed reactors. The CPR represents a reactive flow between two parallel plates (i.e., catalyst coated bottom plate and quartz glass top plate) that has a 0.5 mm inserted capillary. The goal of this work is to understand the hydrodynamic, and mass and heat transfer effects on the kinetic data generated, through computational fluid dynamics (CFD) modeling and experiments, in order to develop a robust reactor model for kinetic parameter estimation. The reactor domain flow profiles generated using the above model include the effects of reaction and heat transfer on the fluid flow. These results are compared with the profiles from the earlier non-reactive CFD modeling studies. This enables us to quantitatively compare and isolate their effect heat transfer on the flow.

## 2. Methods

Geometric features that can potentially impact the flow phenomena in the CPR with the channel dimensions of 40 x 100 x 5 mm are the gas inlet, sampling capillary and the suction from the sampling capillary nozzle as well as the orientation of the capillary nozzle (downward or sideward facing). The effect of each is independently investigated using the catalyticFOAM[2] framework; a CFD numerical solver based on OpenFOAM able to couple the solution of Navier-Stokes with energy and mass balances and detailed modeling of heterogenous chemistry. A full feature CFD model of the CPR reactor with $CO_2$ methanation kinetics is ultimately developed and used to establish the flow phenomena and compare with a comprehensive set of experimental data was collected over a broad range of operational conditions (280-420 °C, 1.2-7.3 $bar_{abs}$, 50-150 ml(STP)/min). The temperatures on the catalyst surface and on quartz glass surface were measured.

## 3. Results and discussion

The flow phenomena in the CPR reactor is affected by the rapid change in cross sectional area in the inlet and the outlet regions. The three channels present at the either end that connect the CPR reactor with the inlet/outlet manifold contributes to this change in cross-sectional area. The rapid increase in area at the end of the inlet channel results in recirculation of flow in this region (shown as rotating red arrows in Figure 1(a)). This secondary flow is present at all the investigated flowrates and it dissipates in the initial 20 mm into the reactor for the 150 ml(STP)/min case. Within the operating range (<250 ml(STP)/min) of CPR reactor, the flow gets fully developed before reaching the catalyst coated region and hence the need of flow straightener can be ruled out Further, a reactive CFD model of CPR is developed and validated for a feed flowrate of 150 ml(STP)/min with a $H_2/CO_2$ molar ratio of 5 at 360 °C and a pressure of 1.2 $bar_{abs}$. The mesh independent CFD model predictions for $CO_2$ conversion compare against experimental data with <1% error. The validated CPR model is used to perform sensitivity study over a range of temperature (300 to 400 °C) and pressure of (1.2 to 7 $bar_{abs}$). Figure 1(b) shows, the axial gas composition profiles over the catalyst coated area (starting at length=0). Here, $H_2$ and $CO_2$ decreased from 53 to 43 mol% and from 11.5 to 8 mol%, respectively, while $CH_4$ is increased to 0 and 4 mol%.

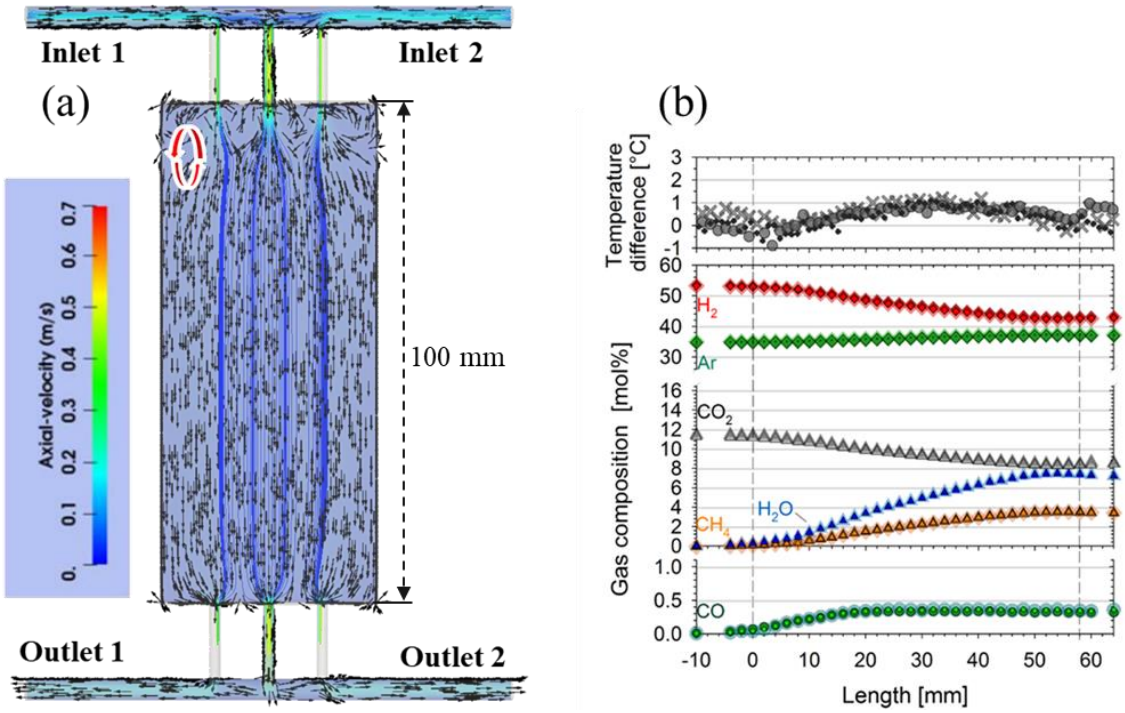


Figure 1 (a) velocity vectors on a horizontal plane in the CPR reactor. (non-reactive CFD model-150$ml_N$/min) (b) Measured axial gas composition profiles and catalyst surface temperatures. (CPR experiments-100 $ml_N$/min, 340°C, 1.1 bar and $H_2$/C=5)

## 4. Conclusions

A comprehensive experimental and CFD model-based study has been performed on the CPR for the $CO_2$ methanation. The influence of the inlet flowrates and capillary suction on the conversion obtained in the reactor have been quantified. The influence of capillary suction is determined by comparing the local species concentration at the sampling location below the capillary pore with the suction active/inactive. This knowledge has been used to determine the optimum location of flow straightener and orientation of the capillary nozzle. The validated reactive CFD model of the CPR reactor is used to come up with the optimum operating conditions for the kinetic experiments including the feed flowrate and capillary suction rate.

## References

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