Design Simulations of a General Purpose Research Micro Reactor for Methane Conversion to Syngas.

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Introduction

A general purpose stainless steel micro reactor setup for methane conversion is being designed for research purposes. We intend to design and build a modular device that would be able to manage different types of reactions depending on the installed modules. The device should be able to allow the study of gas phase reactions at low (atmospheric) and high pressures (up to 20 MPa), with the possibility of testing different catalysts.

The device is particularly oriented towards production of synthesis gas (H_2/CO) by means of catalytic partial oxidation: $CH_4 + ½\ O_2 \rightarrow CO + 2H_2$, ΔH^0_{298K}= -44 kJ/mol

and CO_2 reforming: $CH_4 + CO_2 \rightarrow 2H_2 + 2CO$, ΔH^0_{298K}= +261kJ/mol

A three module micro reactor, subject of this study, is shown in Figure 1. It includes a mixing, homogenizing and preconditioning module with 20 µm square shaped channels, a catalytic module with 1000 µm x 500 µm rectangular shaped channels intended as coated nickel catalyst support.

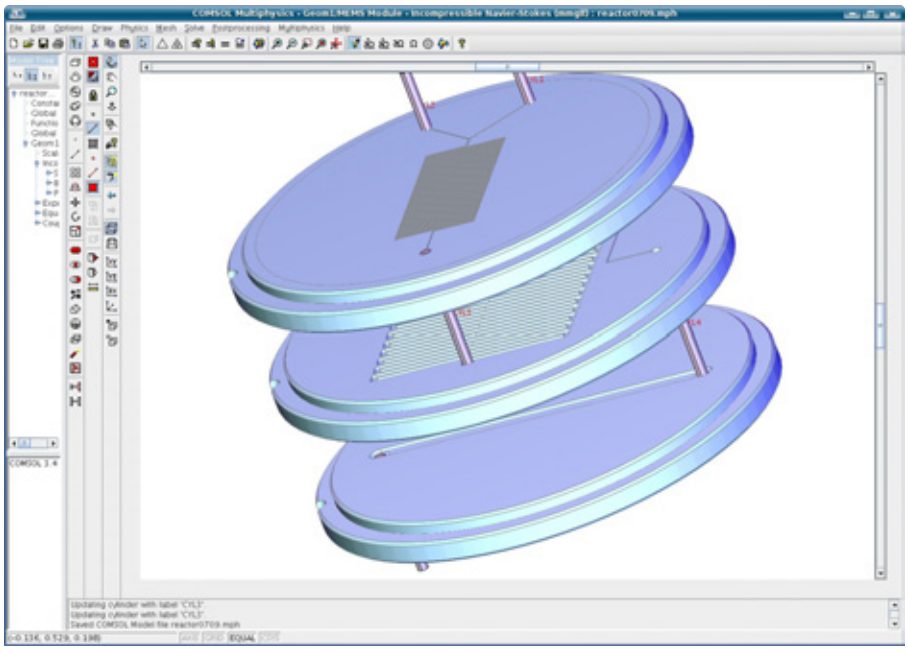

Figure 1: A three module reactor design for methane conversion.

The third module is merely a quenching step, and may be optional or adapted to act as a filter depending on the structure of the catalyst.

The fabrication of such a device is still very costly for an academic institution due to the precision required in micro machining, the involved technology and unitary production. It is thus quite important to be able to perform realistic simulations of its behavior in various situations, prior to its fabrication.

The simulations are performed with the aim to optimize in some extent the basic design, for instance in terms of the length of the micro channels that would allow to reach a specific pressure drop in the device. Within the catalytic module, the hydrodynamics of the reacting flow and the residence time of the gas mixture on the surface of the catalysts have to be considered to give information about the necessary extent and shape of the micro channels.

Use of COMSOL Multiphysics

The use of a framework like COMSOL for the above mentioned purposes thus comes straightforward. In this study we will lay basically on the quality of the Fluid – Chemical reaction interaction models available in the Chemical Engineering module of the simulation program, with the possibility of allowing for weakly compressible flows in the Navier-Stokes equations.

Due to the relatively high temperatures involved in the adiabatic working regime of the device for the considered reactions and the nature of these reactions, heat transfer (conductive and convective) have to be coupled to the flow equations. For this purpose the respective equations in the energy transport mode of the chemical engineering module will be employed.

We expect CONSOL, to provide answers about the flow regime and initial mixing, so that the length of an optimal reactor can be obtained. We also expect to obtain information on the feasibility of the mentioned reactions within the reactor path, and especially about the temperature distribution within the reactor.