Virtual functional product development of a micro steam methane reformer

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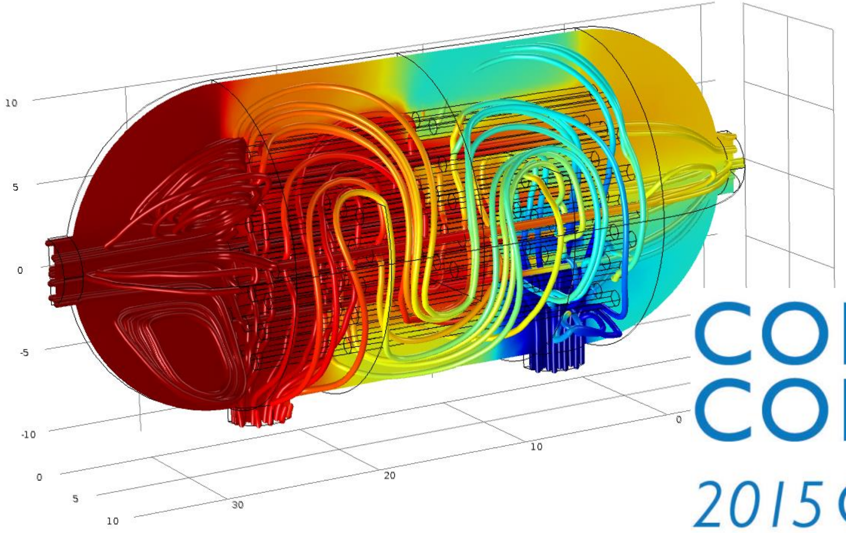
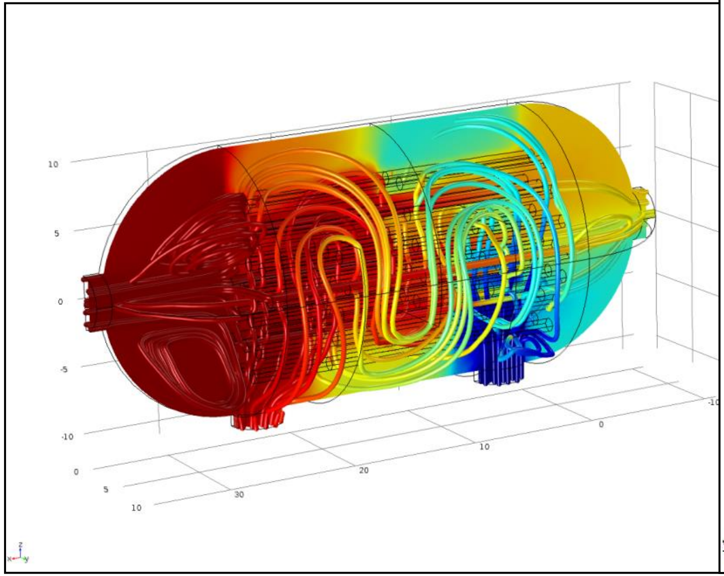
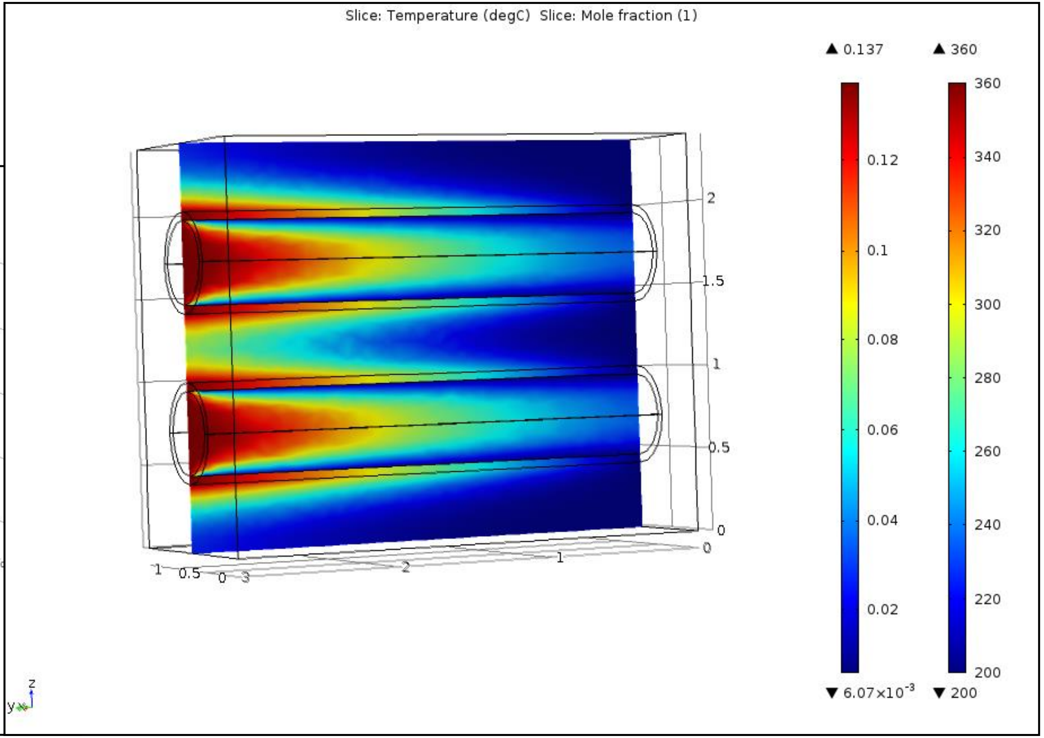


COMSOL CONFERENCE
2015 GRENOBLE

Air cooled exothermal micro reactor

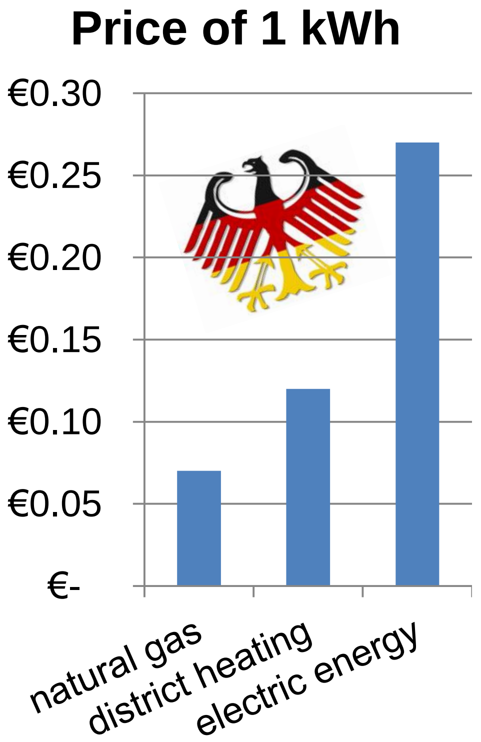




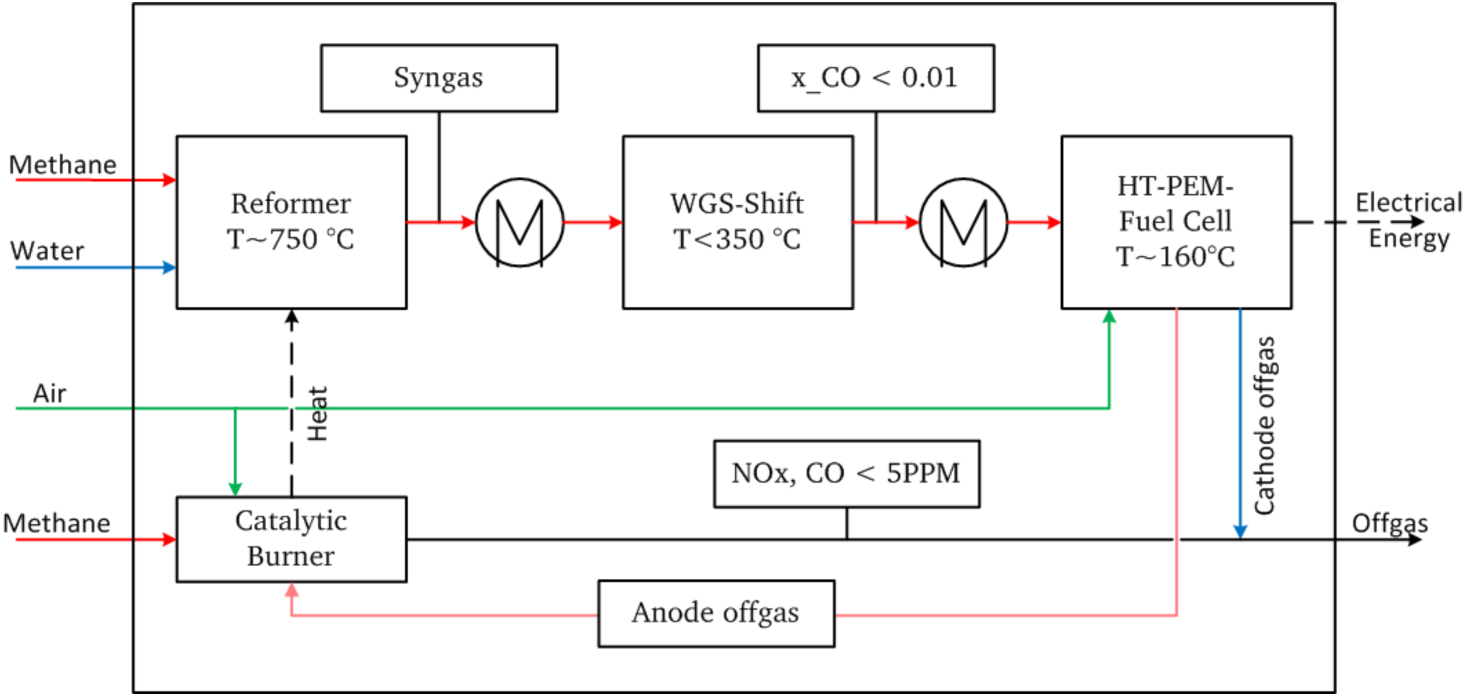
Situation in Germany

Energiewende

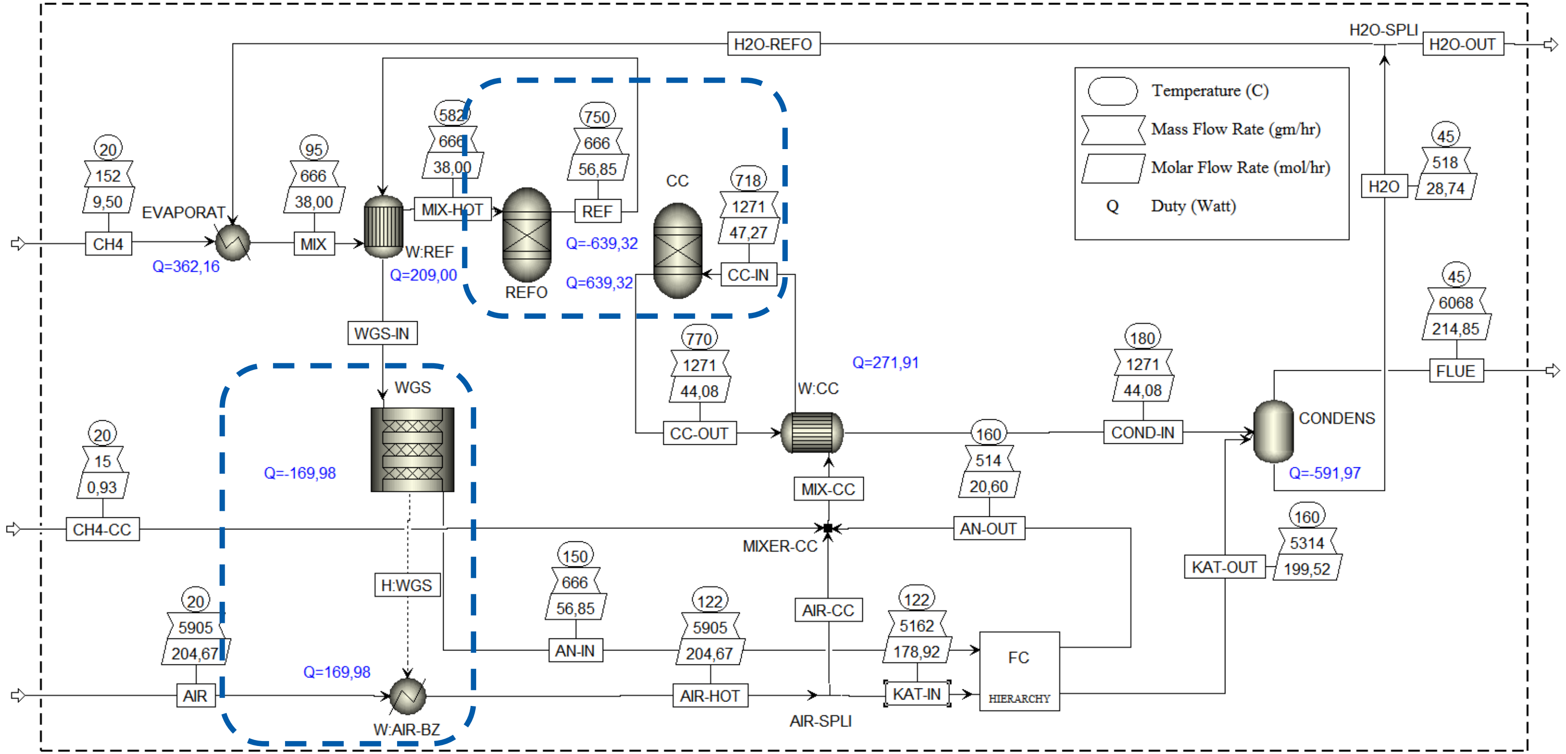
energy efficiency	renewable energy	energy saving



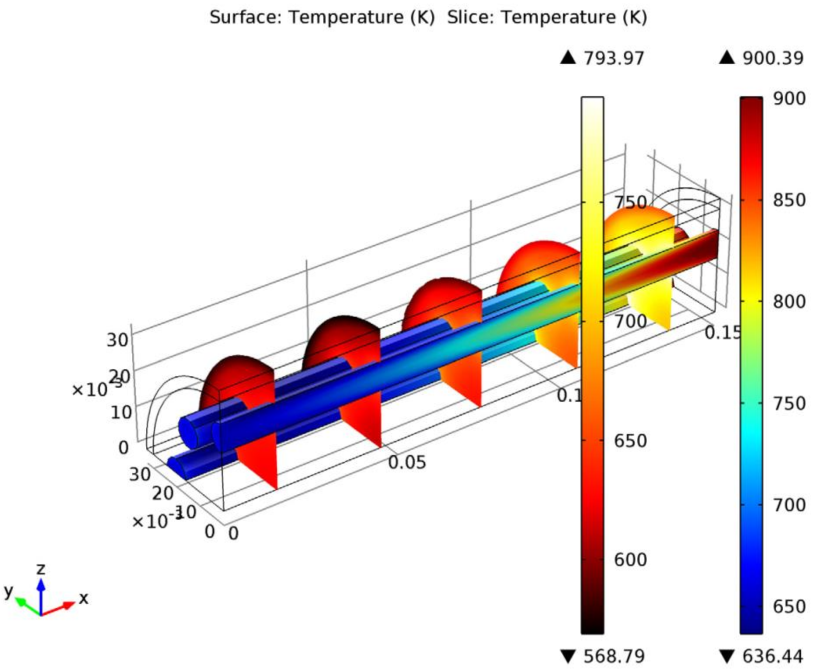
Steam Methane Reformer Fuel Cell Process



Process simulation with Aspen Plus for a 1kWh$_{el}$ µ-SMR-FC plant



COMSOL model library: Steam reformer

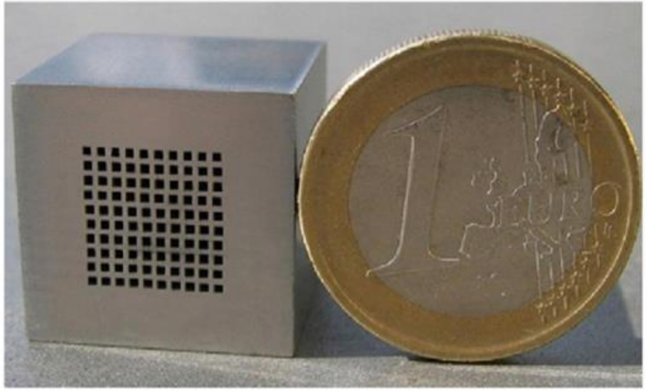


COMSOL (2010): Chemical Reaction Engineering Module Model Library. Steam Reformer (models.chem.steam_reformer).

Micro Structured Catalytic Reactors (MSR)

heat & mass transport:

- transfer capacities increase by several magnitudes
- homogenous ignition can be avoided
- less catalyst is needed, due to increased catalyst utilisation
- no runaway, hot spot, cold spot formation



S. Cruz, O. Sanz, R. Poyato, O.H. Laguna, F.J. Echave, L.C. Almeida, M.A. Centeno, G. Arzamendi, L.M. Gandia, E.F. Souza-Aguiar, M. Montes, J.A. Odriozola, Design and testing of a microchannel reactor for the PROX reaction, Chemical Engineering Journal 167 (2011) 634–642.

Catalytic combustion

- Stability over wide concentration ranges
- High selectivity → No NO_x formation
- lower temperature
- total conversion

Kinetic data for the heterogeneous oxidation of H_2 and CH_4

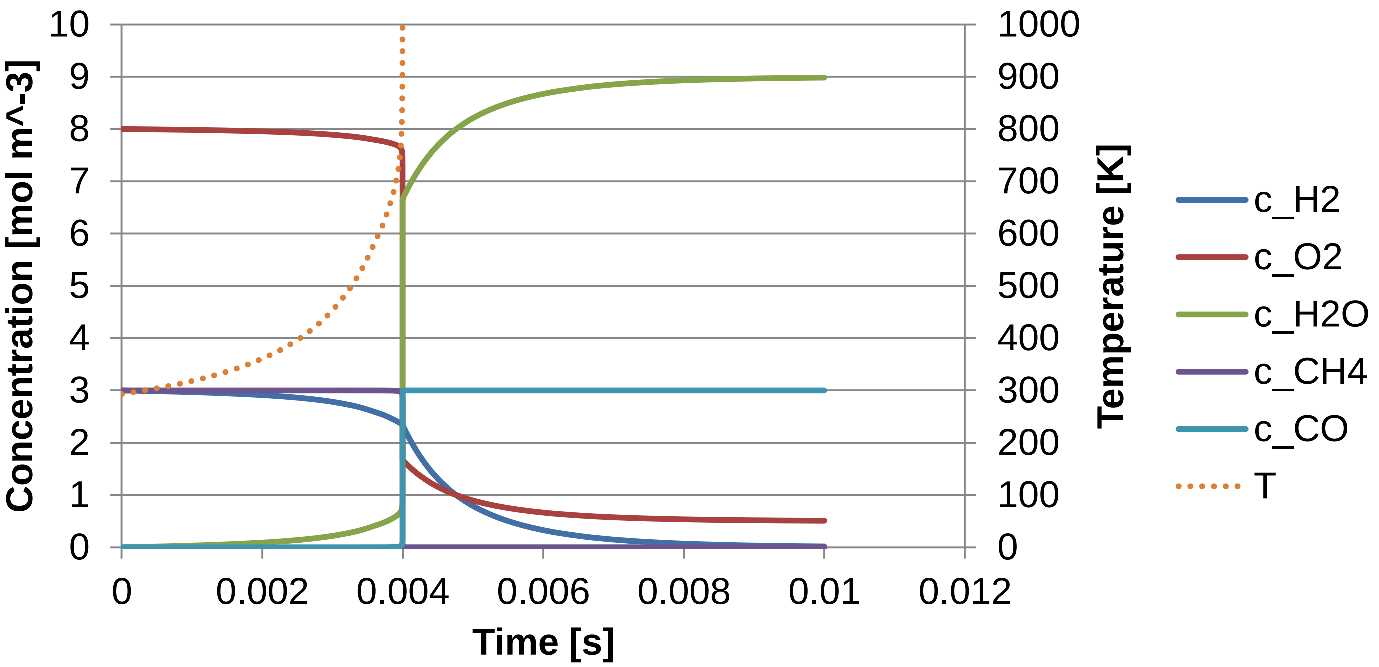
Song, X.; Williams, W. R.; Schmidt, L. D.; Aris, R. (1991): Ignition and extinction of homogeneous-heterogeneous combustion: CH4 and C3H8 oxidation on PT.

In: *Symposium (International) on Combustion* 23 (1), S. 1129–1137. DOI: 10.1016/S0082-0784(06)80372-3.

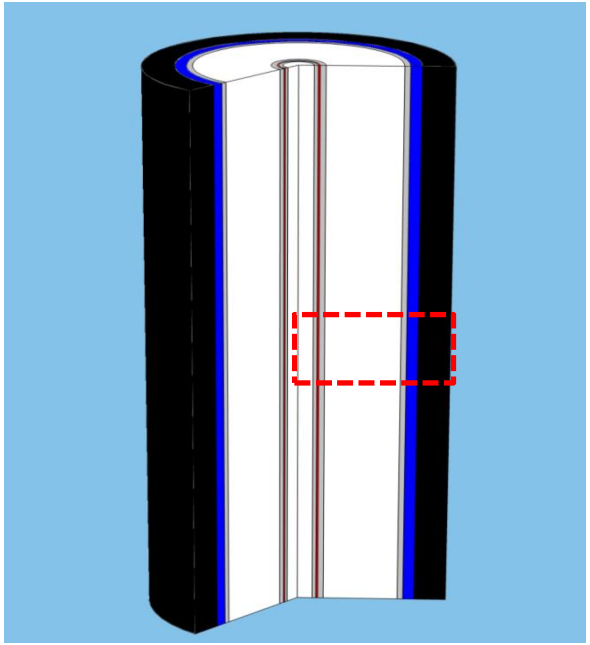
Schefer, R. W. (1982):Catalyzed combustion of H2/air mixtures in a flat plate boundary layer: II. Numerical model.

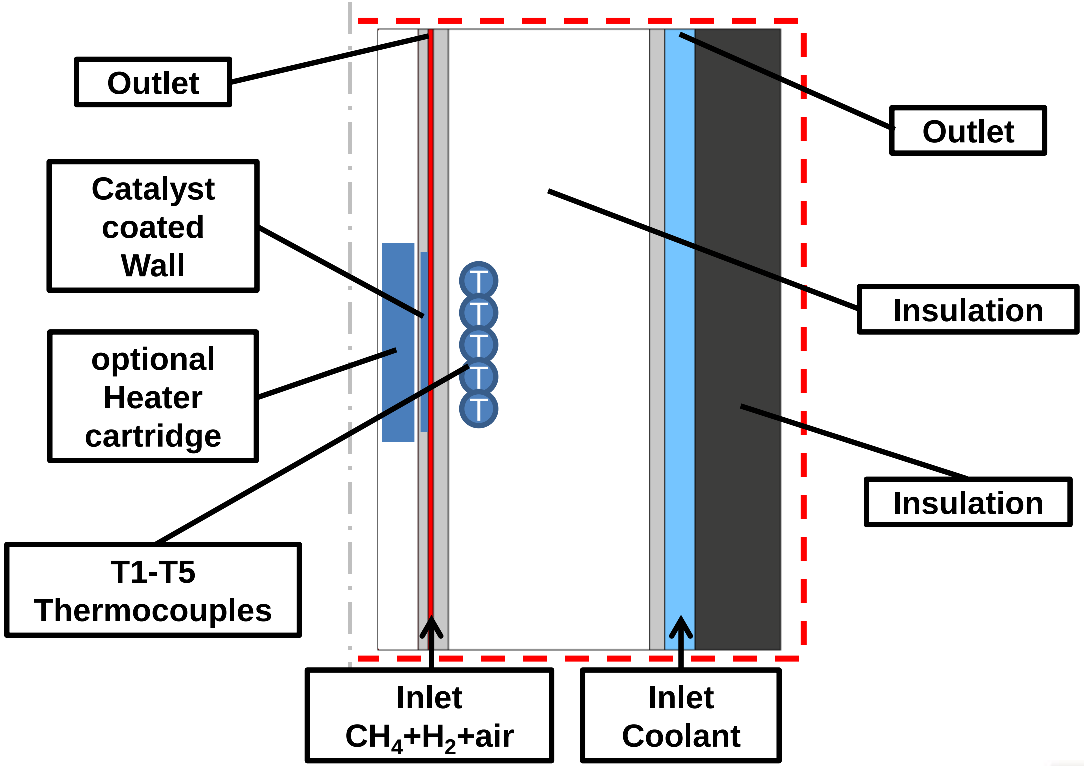
In: *Combustion and Flame* 45, S. 171–190. DOI: 10.1016/0010-2180(82)90043-8.

Catalytic combustion of H_2 and CH_4
The reaction engineering module 1D

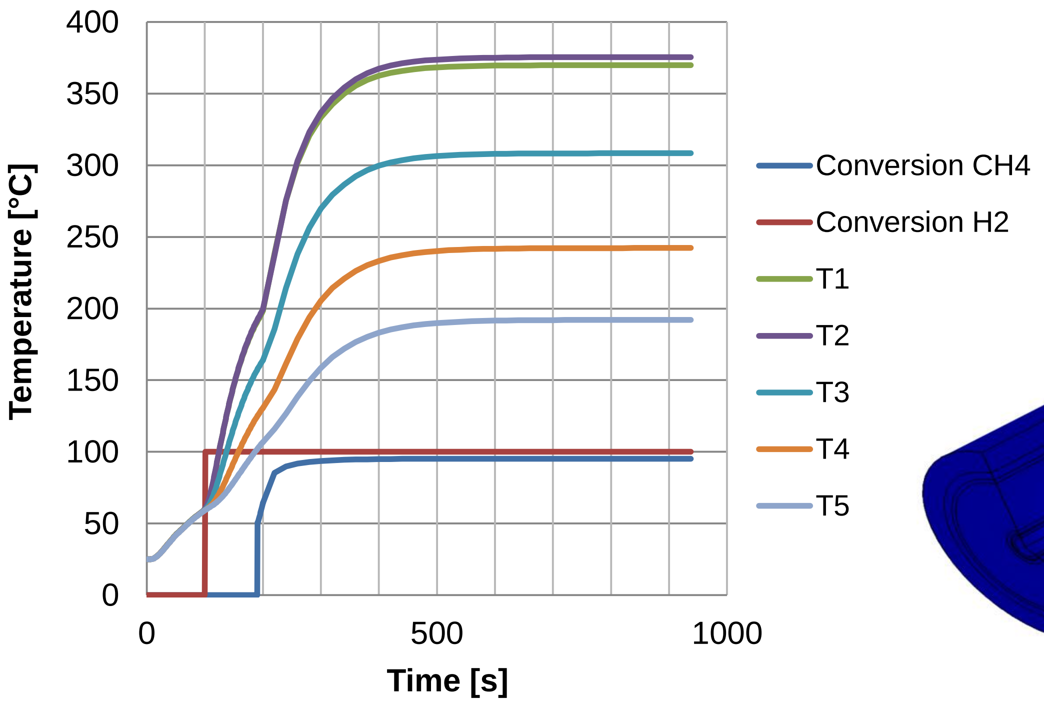


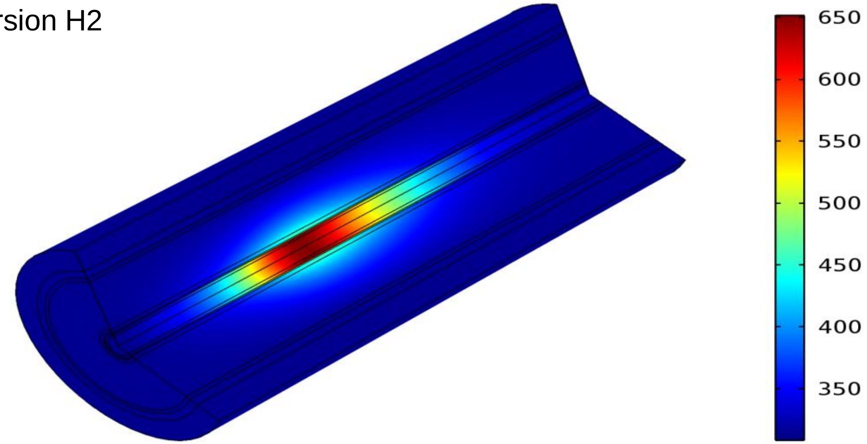
Calculation domains
2D axisymmetric time dependant model



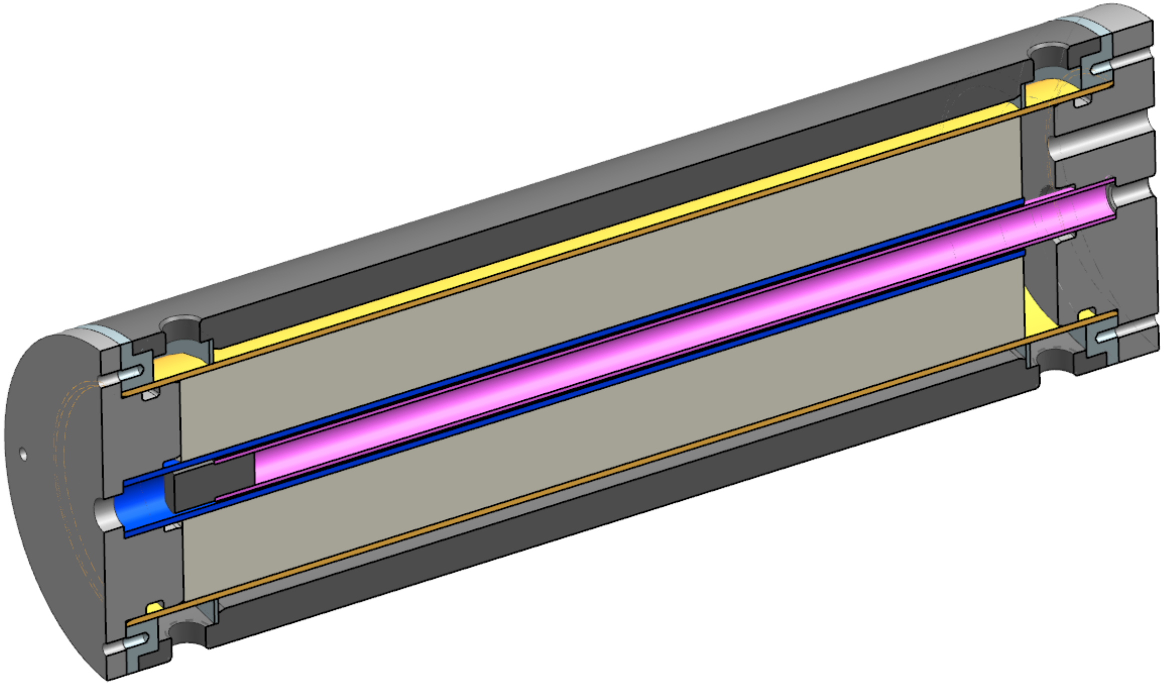


Interim results

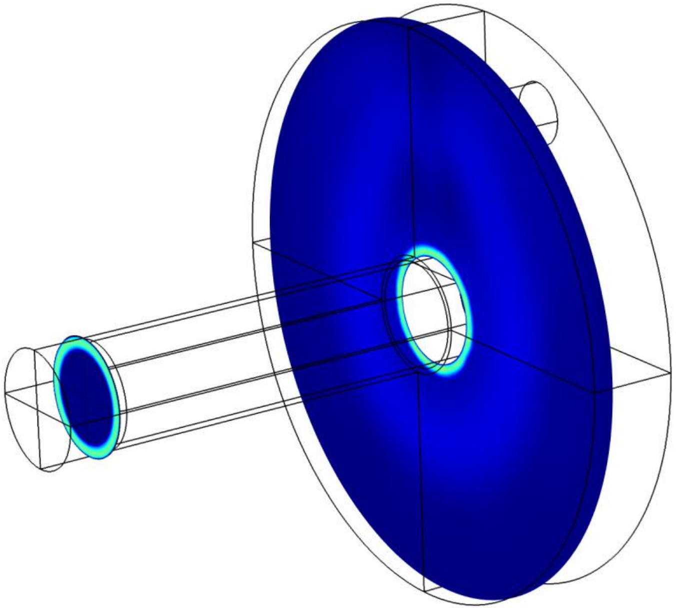


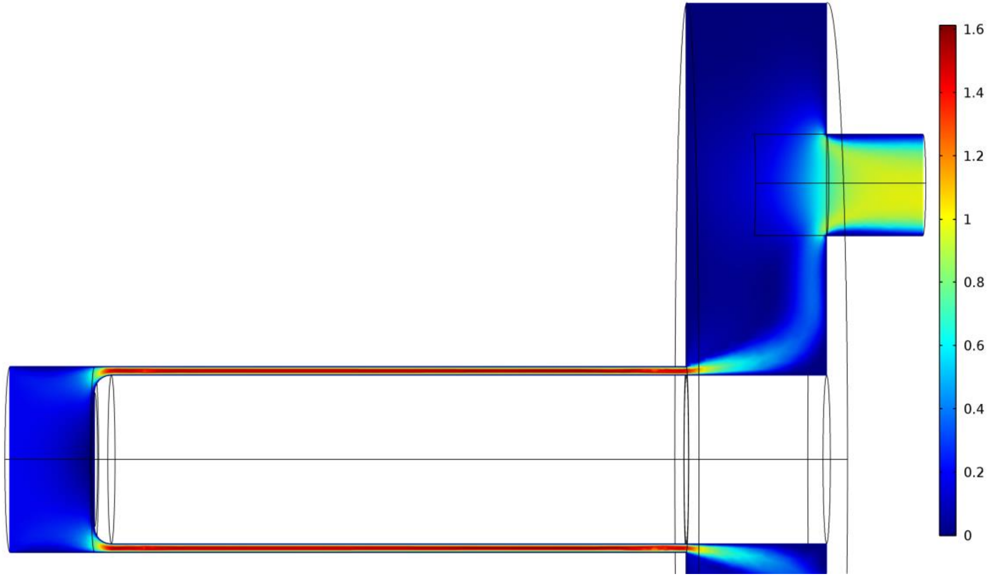


Experimental design

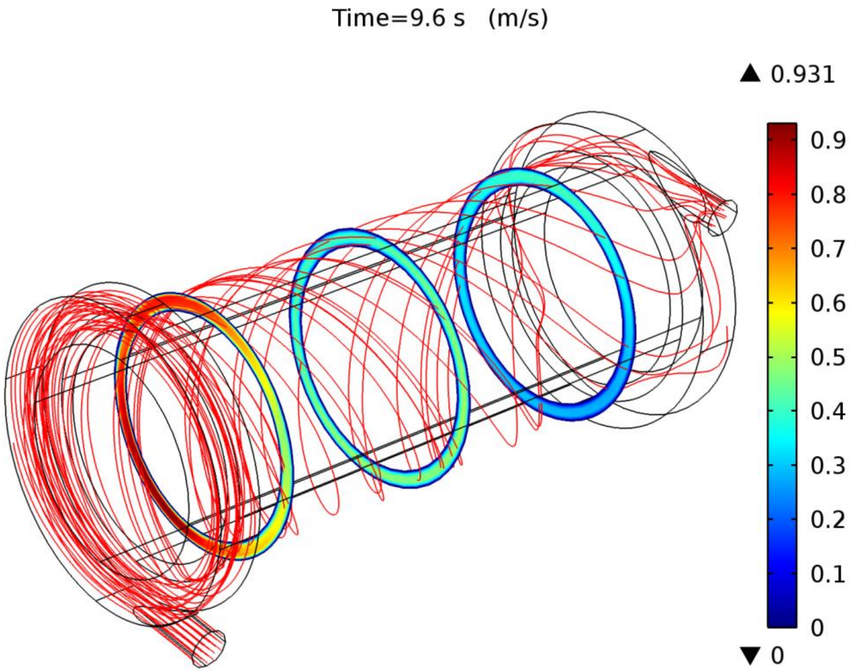


2D axisymmetric boundary conditions
influence of the inlet and outlet

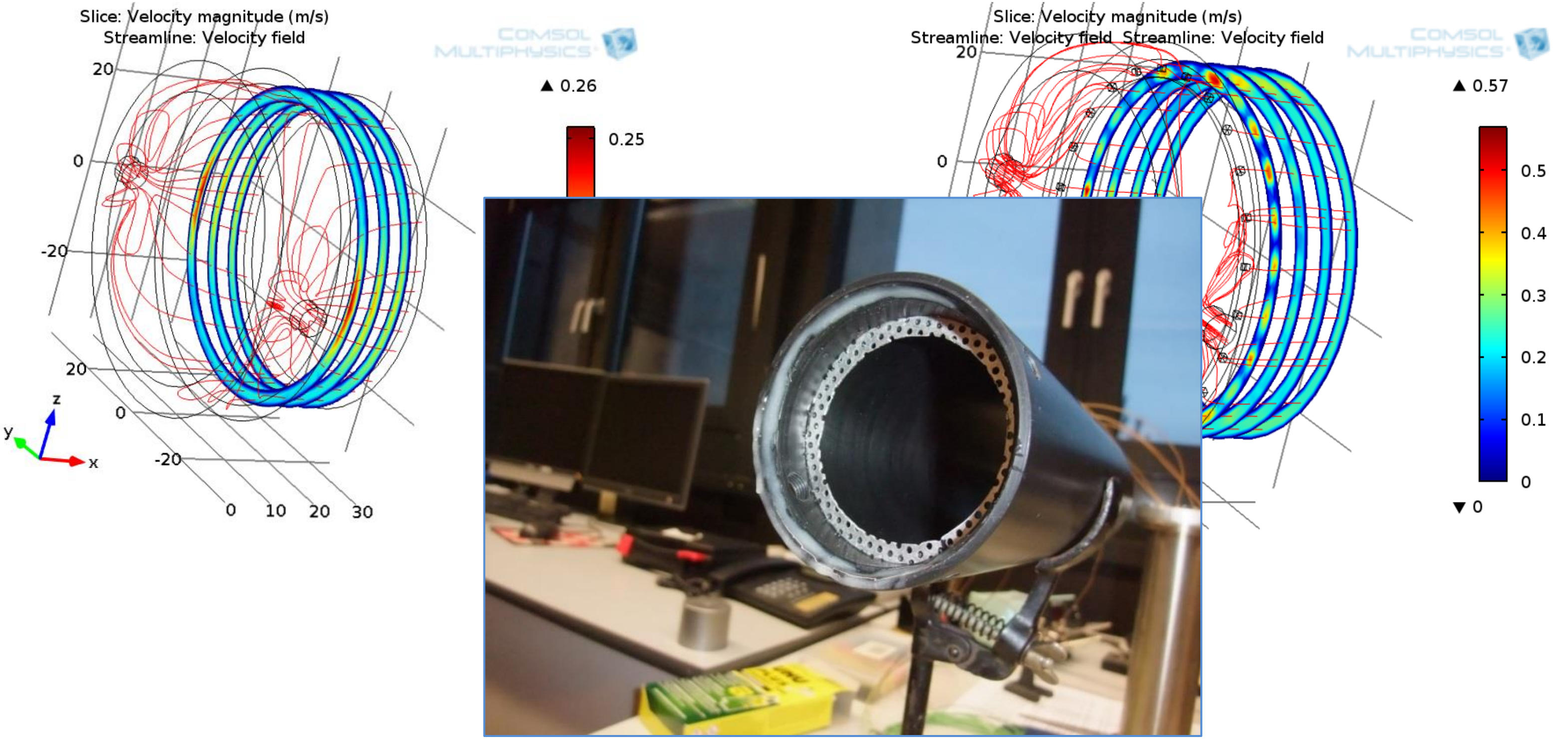




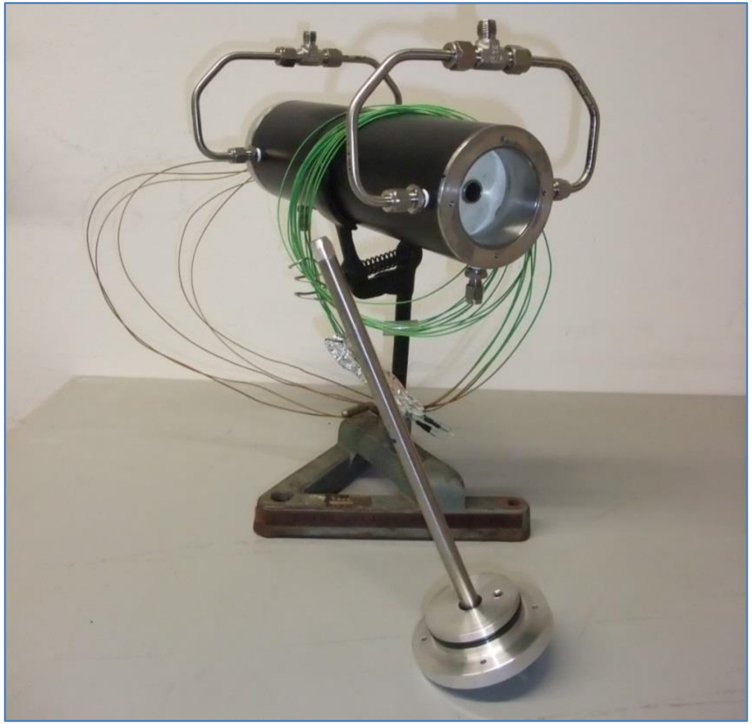
2D axisymmetric boundary conditions influence of the cooling jacket



COMSOL aided experimental design



Final design



12 Thermocouples

2 Mass flow controller

Coolant: 20 – 90°C

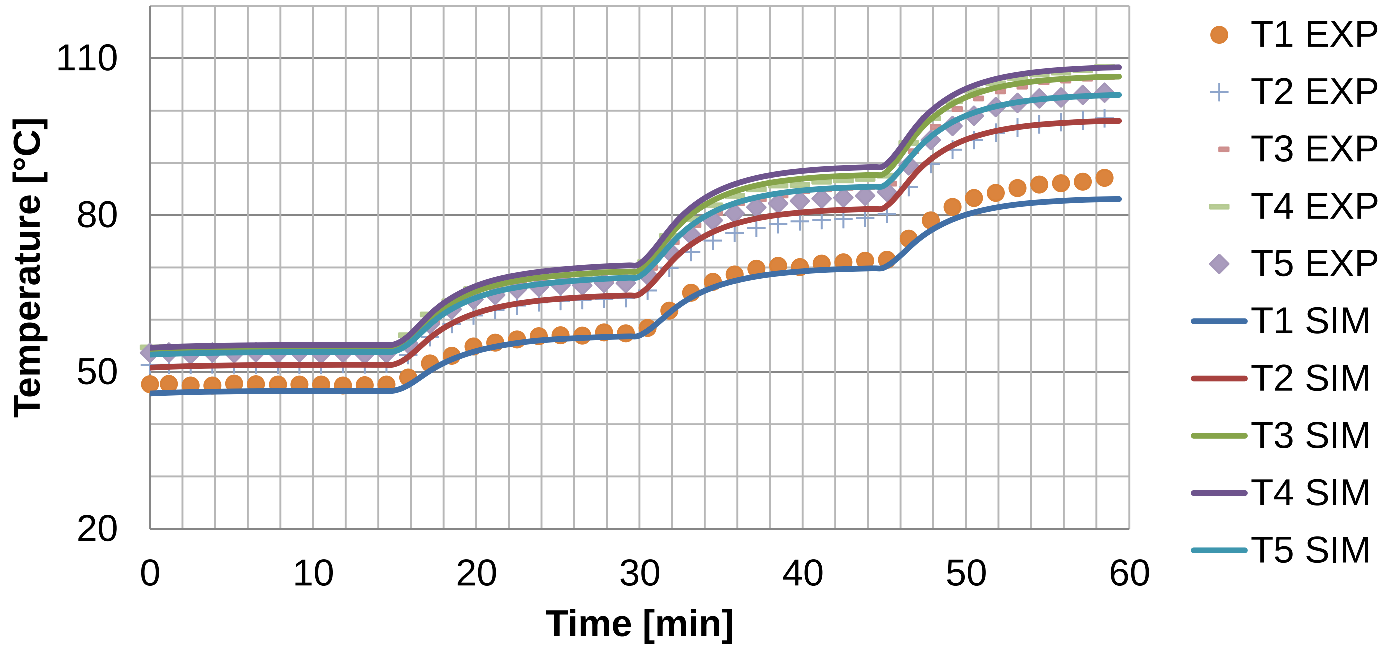
Heater: 0 – 350W

Temperature: 50 – 900°C

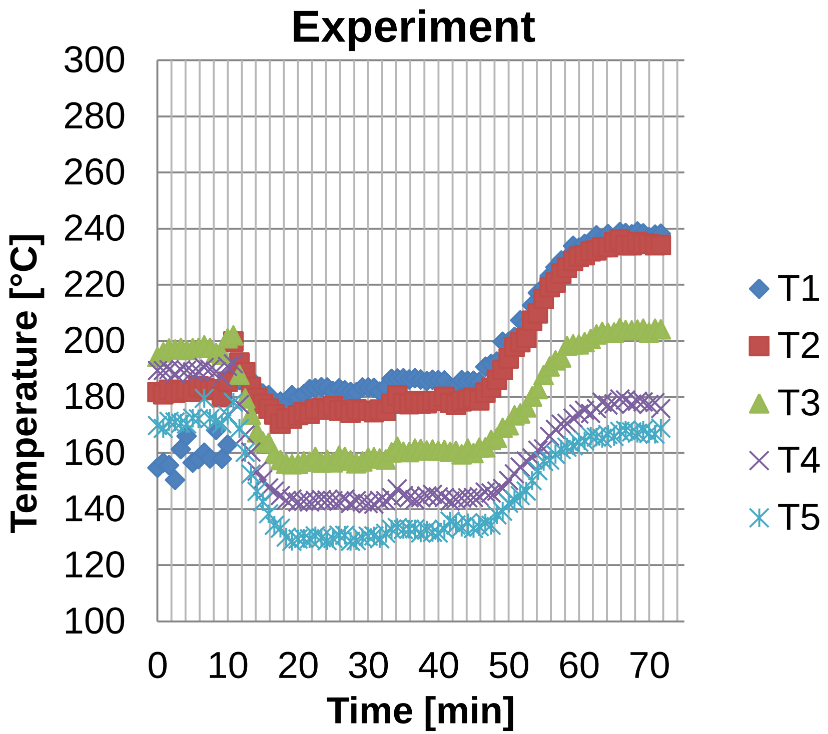
Variable gap size < 1000µm

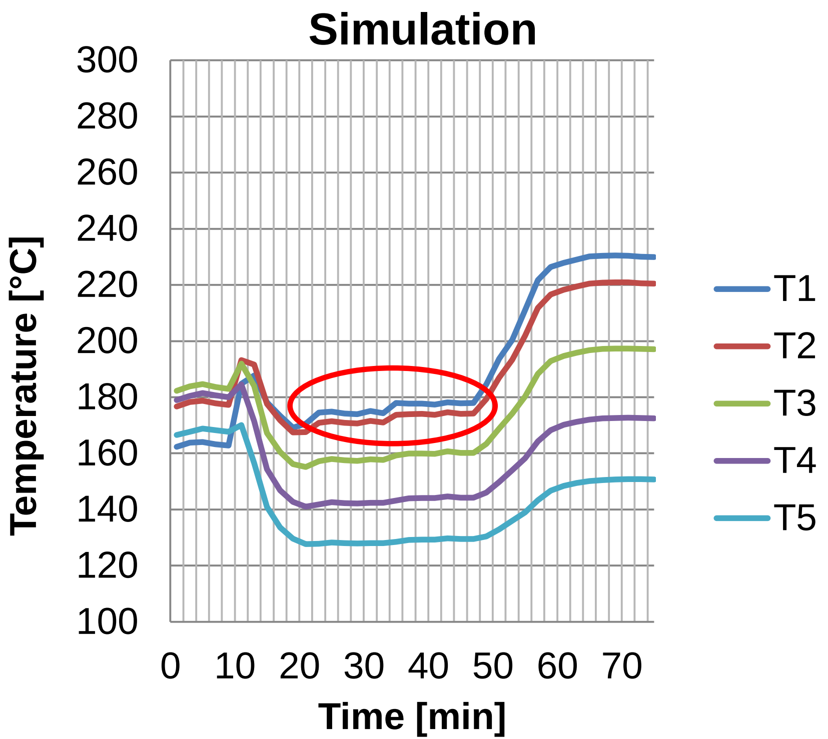
exhaust gas analysis by gas chromatography

Reactor validation with heat cartridge (15, 24, 33, 42W)



Transition from heater to H_2-Air reaction

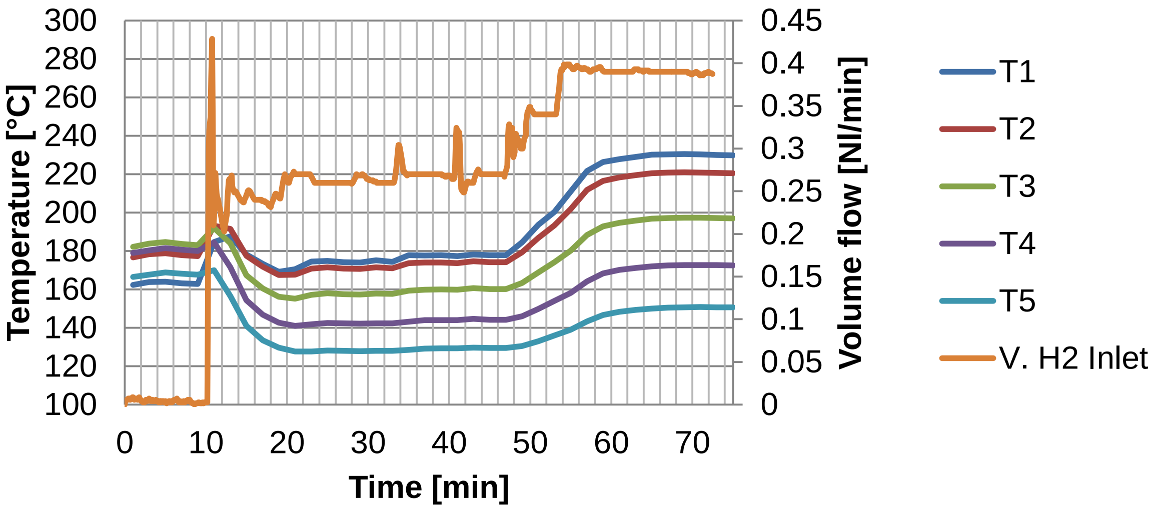




How to obtain an unsteady line as a simulation result?

Solution:

Import the actual volume flow from the experiment as a boundary condition in COMSOL:



Conclusion & outlook

Powerful development tool for chemical engineering.

- NASA polynomials | CHEMKIN → $c_p(T)$, $\Delta H_R(T)$, Transport properties

Virtual functional product development due to multiphysics

- Prediction of the dynamic behaviour of a chemical reactor

Superior pre and post processing

- Import time dependant boundary conditions
- Evaluation of ‘miscarried’ experiments

Catalyst deposition method needs revision: