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# Two-dimensional Modelling of a Non-isothermal PROX Reactor with Water Cooling for Fuel Cell Applications

**H. Beyer*[1], B. Schönbrod[1], C. Siegel[1], M. Steffen[1] and A. Heinzel[1,2]**

[1]Zentrum für BrennstoffzellenTechnik (ZBT) GmbH, Duisburg, Germany

[2]University of Duisburg-Essen, Institut für Energie- und Umweltverfahrenstechnik, Germany

*Corresponding author: Zentrum für BrennstoffzellenTechnik (ZBT) GmbH, Carl-Benz-Straße 201, D-47057 Duisburg, Germany

h.beyer@zbt-duisburg.de

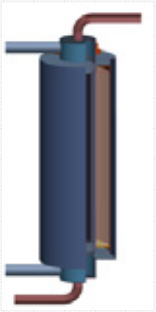
## 1. Introduction

- **Modelling of a PROX reactor using COMSOL Multiphysics on the basis of reaction kinetics from experimental investigations**

→ **Hydrocarbon reformate purification**
→ **Feed gas into PROX contains 0.5 mole-% CO**
→ **Product target CO mole fraction down to a few ppm**
→ **Exothermic reactions**
→ **Accurate cooling conception is mandatory**

- **Reactor design**

→ **Annular-gap-shaped PROX reactor**
→ **Inner and outer, coaxial cooling**
→ **Fuel cell cooling water used to cool PROX reactor and feed gas**
→ **Cooling water temperature and the educt gas temperature are assumed to be equal**



**3D coaxial reactor design**

## 2. Reaction kinetics

- **Two main reaction**

$$CO + 0.5 \cdot O_2 \rightarrow CO_2 \qquad \Delta H_R = -283.6\ kJmol^{-1}$$

$$H_2 + 0.5 \cdot O_2 \rightarrow H_2O \qquad \Delta H_R = -243.5\ kJ \cdot mol^{-1}$$

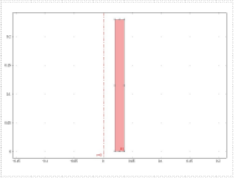
- **Methanation of CO and $CO_2$ and RWGS reaction are negligible**

- **Rate equations determined by experimental investigations**

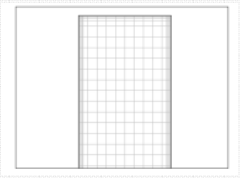
$$r_{CO} = 5 \cdot 10^{-5} \cdot \exp\left(\frac{-2.84 \cdot 10^4}{RT}\right) \cdot x_{CO}^{\ -0.5} \cdot x_{O_2} \qquad x_i = \frac{c_i}{c_{total}}$$

$$r_{H_2} = 2.6 \cdot 10^{-7} \cdot \exp\left(\frac{-1.8 \cdot 10^4}{RT}\right) \cdot x_{O_2}^{\ 1.16} \qquad L = \frac{c_{O_2}}{2 \cdot c_{CO}}$$

## 3. Use of COMSOL Multiphysics



**2D axial symmetric geometry**



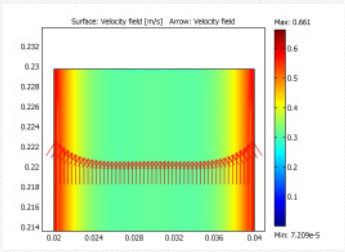
**Rectangular mesh (mapped mesh)**

**Chemical engineering application modes:**

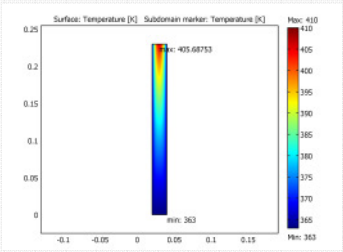
| | Governing equations | Boundary conditions |
|---|---|---|
| • **Mass transport (convection and diffusion)** | $\nabla \cdot (D_i \nabla c_i) = R_i - u \nabla c_i$ <br> $R_i = -r_i \cdot_{bulk} \quad i = H_2, CO \qquad R_{O2} = -0.5 \cdot (r_{CO} + r_{H2}) \cdot_{bulk}$ | Inlet → concentration <br> Outlet → convective flux |
| • **Energy balance (convection and conduction)** | $\nabla \cdot (-k \cdot \nabla T) = Q - \ _{gas} \cdot C_p \cdot u \cdot \nabla T$ <br> $Q = -\Delta H_{R,CO} \cdot R_{CO} - \Delta H_{R,H2} \cdot R_{H2}$ | Inlet → $T_0$ <br> Outlet → convective flux <br> Walls → heat flux <br> $q_0 = k_w \cdot (T_w - T)$ |
| • **Momentum transport (Brinkman, porous media)** | $-\cdot u = \nabla\left(p \cdot I + -\frac{1}{}\left( (\nabla u + (\nabla u)^T) - \frac{2}{3} (\nabla u) I \right)\right)$ | Inlet → laminar flow <br> Outlet → pressure |

A porosity profile for is implemented

## 4. Results

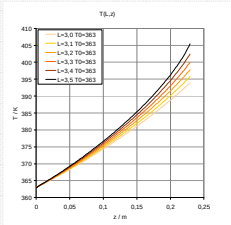
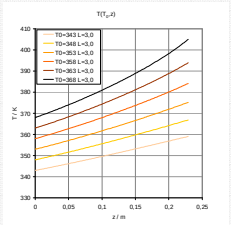
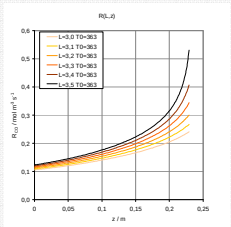
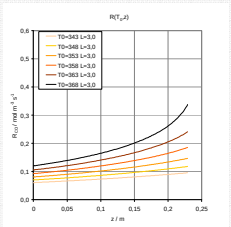
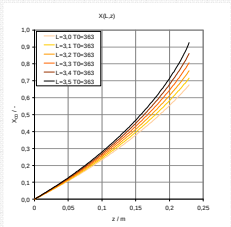
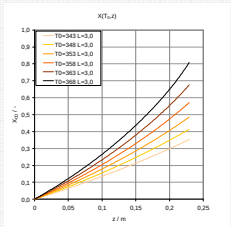
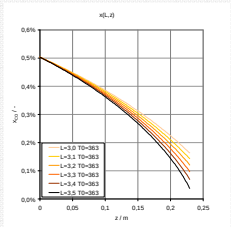
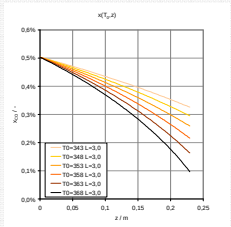


**Radial velocity distribution as result of - profile**



**Exemplary surface plot of temperature**

**Cross section plots**

| Lambda variation | | Inlet temperature variation |
|---|---|---|
|  | **Reaction temperature** $T$ |  |
|  | **CO reaction rate** $R_{CO}$ |  |
|  | **CO conversion rate** $X_{CO}$ |  |
|  | **CO mole fraction** $x_{CO}$ |  |

## 5. Conclusions

- **A compact PROX reactor was designed.**
- **Two rate equations were determined within kinetic experiments.**
- **2D geometry with axial symmetry was used in COMSOL Multiphysics v3.5a.**
- **Model combined mass, energy and momentum transport with chemical kinetics.**
- **Simulations confirmed model operability in principle and provided performance data.**
- **At higher reaction temperatures → no convergence or negative concentrations**
- **When the CO concentration approaches zero, numerical noise becomes significant in comparison to the concentration.**
- **Further CO conversion improvement is essential.**