Modelling Study of a Photo-Thermal Catalytic Reactor for rWGS Reaction Under Concentrated Irradiation

David Brust[a], Michael Wullenkord[a], Andrii Cheilytko[b], Hermenegildo García Gómez[c], Josep Albero[c]

a German Aerospace Center (DLR), Institute of Future Fuels, Schneiderstrasse 2, 52428 Juelich, Germany
b German Aerospace Center (DLR), Institute of Solar Research, Linder Hoehe, 51147 Cologne, Germany
c Departamento de Química/Instituto Universitario de Tecnología Química (CSIC-UPV), Universitat Politècnica de València, Avda. De los Naranjos s/n, 46022 Valencia, Spain

Photo-Thermal Catalytic (PC) Reactor

- Flow reactor for gas phase reaction
  - rWGS: $\mathbf{CO_2 + H_2 \leftrightarrow CO + H_2O}$ $\Delta H_R^{298} = 41\ \mathrm{kJ/mol}$
- Heterogeneous photo-thermal catalysis
  - RuO_2-$SrTiO_3$ catalyst [1] immobilized on porous support
  - Chemical conversion facilitated by heat / light
- Concentrated light irradiation in DLR's *High Flux Solar Simulator (HFSS) [2]*
  - 40-100 Suns concentration factor
  - Photon-management: homogeneous flux profile on catalyst

- Pre-mixed feed: H_2/CO_2 = 1/1 max. 5.6 L_s/min*
- Max. irradiaton power: 1.4 kW
- Atmospheric pressure operation

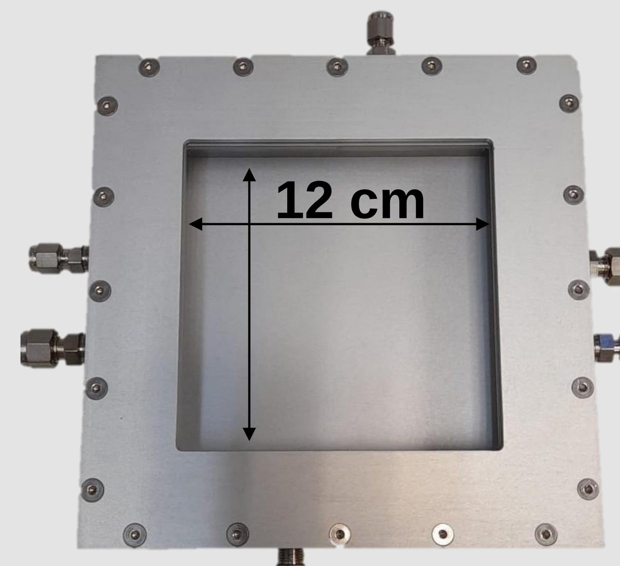
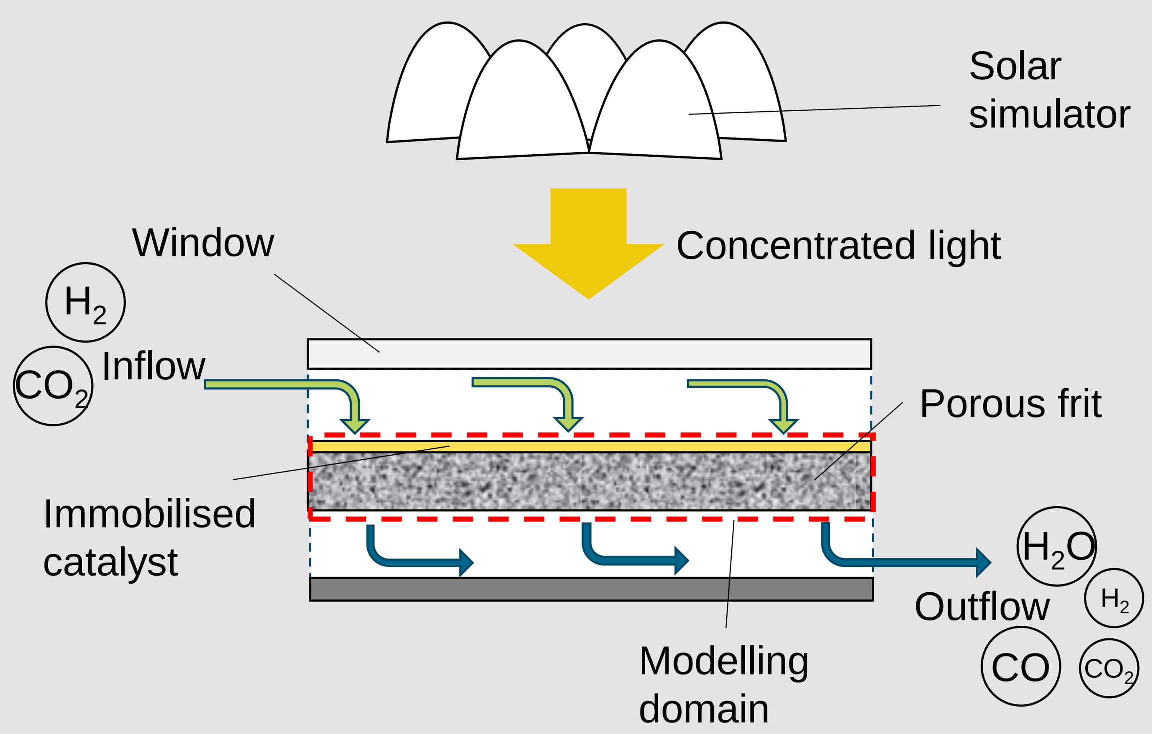


Fig. 1 Investigated PC reactor for the rWGS reaction. Provided by Universitat Politècnica de València.

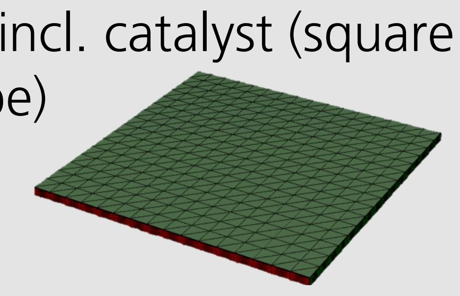
- Catalyst directly irradiated
  → locally high catalyst temperature
  → high activity



*p_s = 1.01325 bar, T_s = 293.15 K

Modelling Approach

- Scope / domain of interest
  - Porous foam, incl. catalyst (square prismatic shape)
  - Steady-state



- Mass / species transport
  - Convection-diffusion in porous medium: Dusty-Gas-Model [3]
  - Chemical reaction in catalyst layer incl. kinetics

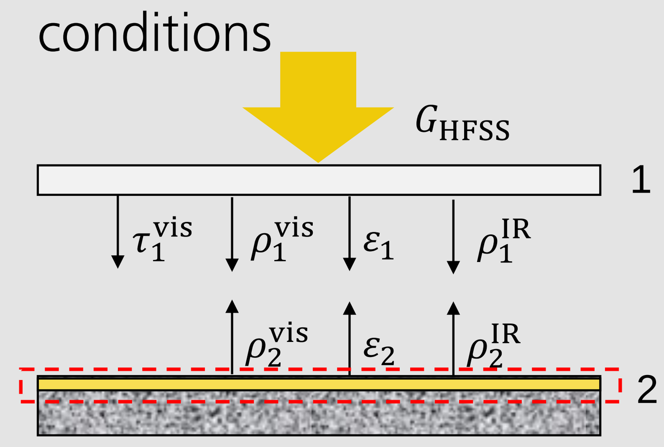
$$-\nabla \cdot \vec{N}_i + R_i = 0, i = 1 \dots \nu$$

$$\sum_{\substack{j=1 \\ j \neq i}}^{\nu} \frac{x_j \vec{N}_i - x_i \vec{N}_j}{D_{ij}^{\mathrm{eff}}} + \frac{\vec{N}_i}{D_{i,K}^{\mathrm{eff}}} = -\frac{\nabla p_i}{RT} - \frac{1}{D_{i,K}^{\mathrm{eff}}} \frac{p_i}{RT} \left(\frac{\kappa}{\mu} \nabla p \right)$$

- Thermal energy transport
  - Convection/conduction through porous medium: effective thermal conductivity [4]

$$-\nabla \cdot \left(\lambda_{\mathrm{eff}} \nabla T - \sum_i^{\nu} \vec{N}_i h_i \right) = 0$$

  - Radiative transport boundary conditions



- Discretization / numerical method
  - Finite Volume Method
  - *VoronoiFVM.jl* [5] package for the *julia* programming language

Energy Balance

- Energy flows over reactor bounds
- Determine importance of loss mechanisms → design optimisation

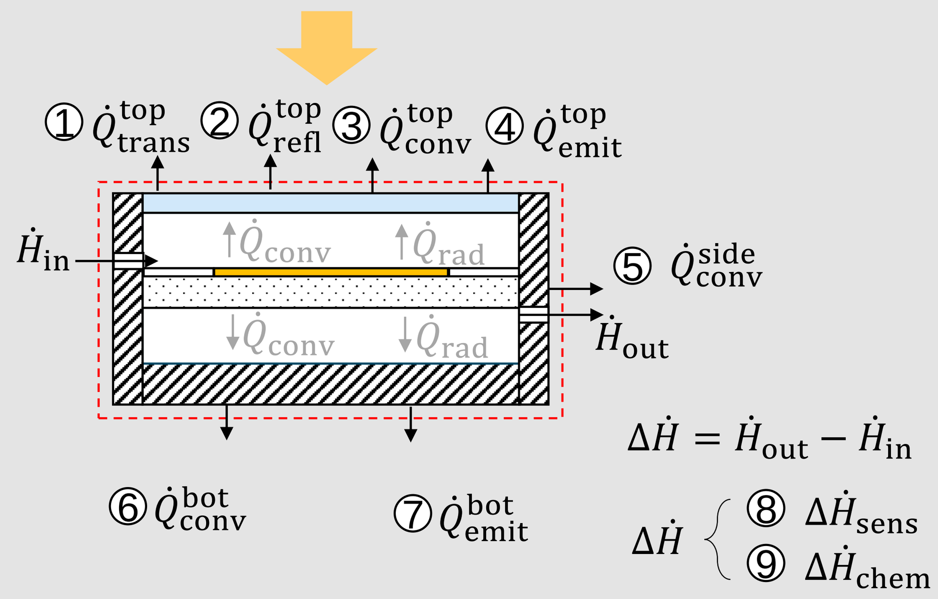


Fig. 4 Illustration of heat and enthalpy flows across the system boundary considered in the energy balance.

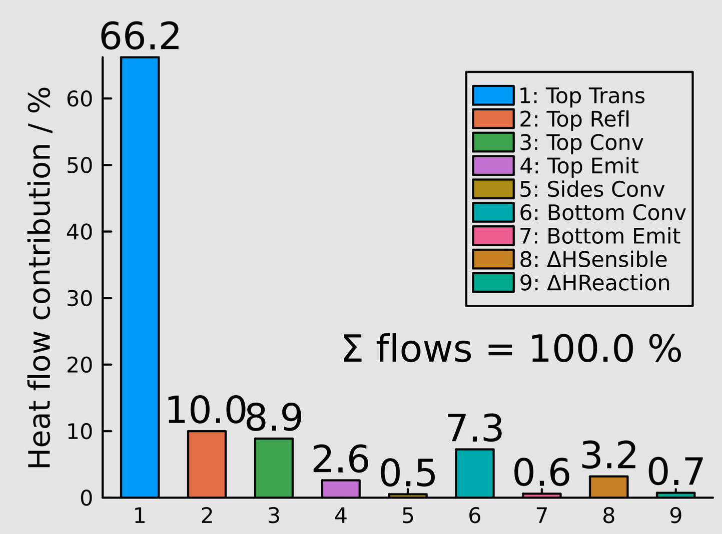


Fig. 5 Exemplary relative contributions of heat flows across the system boundary (Fig. 4) normalized to total irradiation power of 980 W on the aperture.

Exemplary Thermal Results

- Total irradiation power: ~1 kW (avg. measured flux of 70 kW/m² in center of catalyst plane)
- Feed vol. flow rate: 3 L_s/min* (H_2/CO_2 = 1/1)

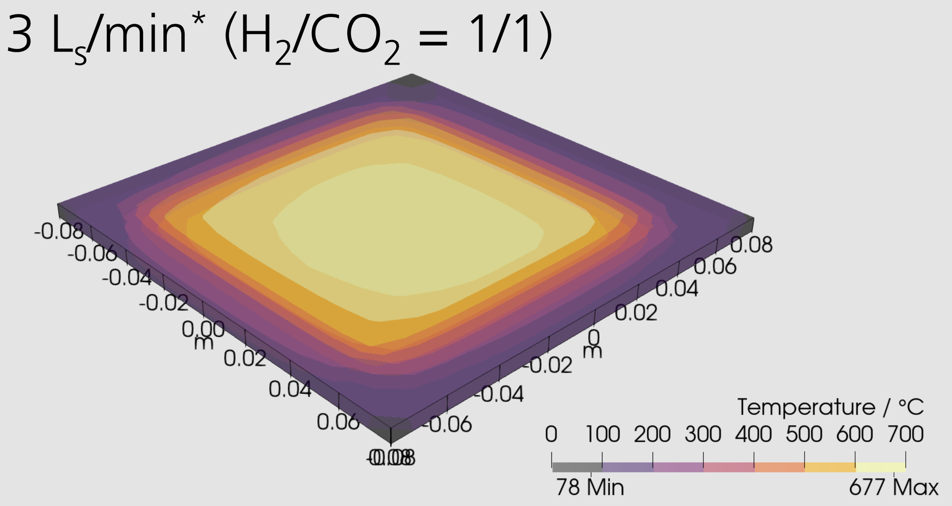


Fig. 2 Temperature distribution in reactor, with average temperatures of 636 °C (upper surface, center) and 477 °C (lower surface).

Exemplary Chemical Results

- Pressure ~ 1 atm
- Catalyst mass: 500 mg
- Chemical kinetics of Ni-Al_2O_3 for rWGS [6] (no kinetic model of Ru-$SrTiO_3$ available yet)

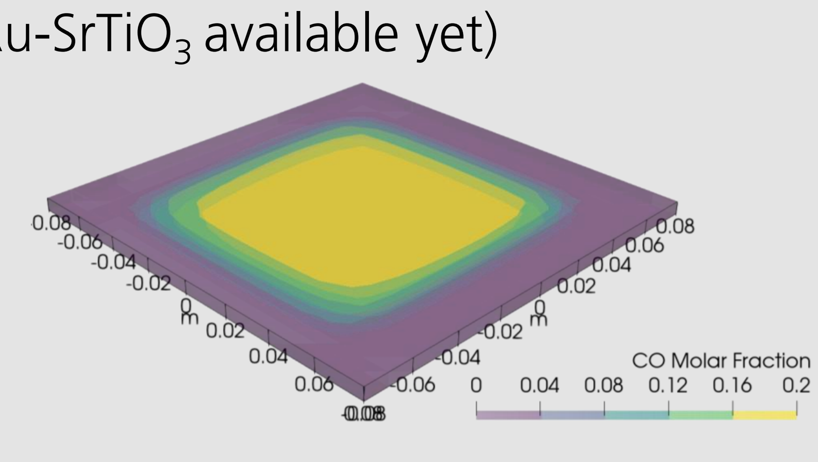


Fig. 3 Distribution of CO mole fraction in reactor, corresponding to a total production of 0.7 $\mathrm{mol_{CO}/h}$ with an average reaction rate of 1.4 $\mathrm{mol_{CO}/(h\ g_{cat})}$ and yield of 18% (CO_2 basis).

References

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Contact: **Institute of Future Fuels** | Chemical and physical fundamentals | Jülich, Germany | David Brust
Telephone: +49 2461 93730 321 | E-mail: david.brust@dlr.de

DLR Deutsches Zentrum für Luft- und Raumfahrt

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