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HYBREC

Reactor system for the production of solar fuels from H₂O, CO₂, and CH₄

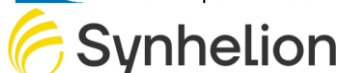


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The authors bear the entire responsibility for the content of this report and for the conclusions drawn therefrom.



Zusammenfassung

Das HYBREC Projekt untersucht die Ceroxid-basierte Redox-Trockenreformierung. Der Prozess wird durch konzentrierte Sonnenenergie angetrieben, welche die für die endothermen Reaktionen erforderliche Hochtemperaturprozesswärme liefert. Das Endprodukt ist Synthesegas – ein Zwischenprodukt für die Herstellung von flüssigen Kohlenwasserstofftreibstoffen. Im vergangenen Jahr gab es vor allem Fortschritte im Bereich der Reaktormodellierung für die Strömungssimulation (CFD) des Prozesses. Das numerische Programm porousRedoxFoam wurde innerhalb der OpenFOAM-Umgebung entwickelt, um reversible heterogene Reaktionen zu modellieren. Die numerischen Simulationsergebnisse zeigen eine gute Übereinstimmung im Vergleich zu den experimentellen Resultaten. Das Modell wird nun in einem weiteren Schritt für das Design und die Optimierung des Reaktorrohrs verwendet und dient als Werkzeug für die Skalierung der Technologie.

Summary

The HYBREC Project considers the ceria-based redox dry reforming. The process is driven by concentrated solar energy, which provides the high-temperature process heat required for the endothermic reactions. The final product is syngas – a precursor to drop-in liquid hydrocarbon fuels. The past year saw progress mainly with respect to the computational fluid dynamic (CFD) reactor model to simulate the process. A solver, porousRedoxFoam, has been developed within the OpenFOAM environment to model reversible heterogeneous reaction. Numerical results show good matching when compared to experimental tests. The model is then used for design and optimization of a reactor tube and serves as a tool for the scale-up of the technology.



Main findings

The HYBREC Project centers on the ceria-based redox dry reforming process to produce syngas, driven by concentrated solar energy. Syngas can be further processed to drop-in fuels for the transportation sector. The project has evolved through multiple phases, namely: theoretical thermodynamic modeling, lab-scale experimental investigation, scaled-up and on-sun testing of a directly-irradiated solar reactor in a solar tower, techno-economic evaluation, and development of a computation fluid dynamic (CFD) solver for modeling the process in a fixed-bed tubular reactor. All project areas share a common overarching goal, which is the development of the science and technology for the solar production of high-quality syngas through the innovative solar-driven ceria-based redox dry reforming process.

Experiments carried out in a lab-scale tubular reactor aided in comparing various ceria morphologies and detailed the importance of the microstructure. Ultimately, a pellet morphology was chosen which showed CH₄ conversions of 85% at 1000°C, significantly higher than previous conversions (35%) obtained with the standard reticulated porous ceramic (RPC) when tested under the same operating conditions. Thermodynamic modeling justified observations made during experimentation; namely that cycling in a reduce state, at higher nonstoichiometries, improved syngas selectivity. The core of this thermodynamic model was later implemented in the CFD model. In a collaboration with IMDEA Energy Institute in Madrid, the process was tested on a scaled-up, directly-irradiated solar reactor. The reactor operated with an input solar radiative power of 10 kW (560 suns) and temperatures around 1000°C. Peak CH₄ conversions reached 70% and solar-to-fuel efficiencies reached 16%. When operating in a co-feeding manner, the solar-to-fuel efficiencies increased to 27%. A technoeconomic study made use of a process flow diagram (PFD) to evaluate a solar-to-methanol plant. Heat, power, and mass streams were calculated over one year in order to evaluate the plant economics in terms of capital expenditures (CAPEX), operating expenditures (OPEX), and levelized cost of methane (LCOM). Solar fuels offer favorable environmental benefits compared to other fuel production methods, and the long-term viability of solar fuels is sensitive to location, CO₂ source, and OPEX. A CFD model, porousRedoxFoam, was developed for simulating an indirectly-irradiated tubular fixed-bed reactor. The numerical program runs in the OpenFOAM environment and is tailored for solving heat and mass transfer processes involving heterogeneous reactions with nonstoichiometric oxides. The CFD model has been validated versus experimental results obtained with a lab-scale prototype and will ultimately be used in the design, optimization, and scale-up of the reactor technology.



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Abbreviations

CAPEX	capital expenditures
CFD	computational fluid dynamics
DNI	direct normal irradiation
ETH	Swiss Federal Institute of Technology
HTF	heat transfer fluid
LCOM	levelized cost of methanol
ODE	ordinary differential equation
OPEX	operating expenditures
P&ID	pipng and instrumentation diagram
PFD	process flow diagram
PREC	Professorship of Renewable Energy Carriers
RPC	reticulated porous ceramic
TES	thermal energy storage

E_a	activation energy
H_f	enthalpy of reaction
K_{eq}	equilibrium constant
k	rate constant
k_0	pre-exponential factor
k_f	forward rate constant
k_r	reverse rate constant
n	reaction order
R_u	universal gas constant
T	temperature
t	time

ΔG^0	standard Gibbs free energy of reaction
ΔH^0	standard enthalpy of reaction
ΔS^0	standard entropy of reaction
δ	ceria non-stoichiometry
ρ_s	density of solid

[i]	concentration of species i
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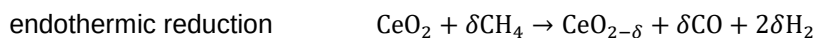
1 Introduction

1.1 Background information and current situation



Figure 1: Dry redox reforming process to produce drop-in liquid fuels

High-temperature solar thermochemical processes offer an efficient pathway to the production of sustainable fuels. This report focuses on the thermochemical pathway for producing syngas (H_2 and CO) from concentrated sunlight and CO_2 via a ceria-based redox reforming process which uses CH_4 as a reducing agent. Using CH_4 lowers the temperature of the endothermic reduction step by $500^\circ C$, when compared to the pure process which reduces ceria thermally in a low oxygen pressure environment. The process can be operated isothermally ($800-1200^\circ C$) and can achieve higher non-stoichiometries (δ), resulting in a higher proportion of O_2 exchange. Dry redox reforming is represented by two steps:



Recent experiments and analysis have shown the benefits of combining the two redox steps (i.e. co-feeding reactants), yielding the net dry reforming reaction [1]:



The main challenges associated with the technology are achieving high reactant conversions and syngas selectivities at low temperatures while avoiding unwanted side-products (e.g. carbon depositions) and side-reactions.

This report mainly describes the progress made in 2023.

1.2 Purpose of the project

The HYBREC Project focusses on developing the science and technology behind the process including the fundamental dynamics: thermodynamics, kinetics, fluid dynamics, and heat and mass transfer. Through this theoretical basis, experimental testing and modelling, the reactor technology can be developed, optimized, and scaled up for industrial production of solar fuels.

1.3 Objectives

The main objectives of the HYBREC Project are:

- 1) To study the fundamentals of the process and test the reactor technology at lab-scale
- 2) To develop modelling tools for the thermochemical reactor of which will be utilized for the optimization/scale-up and subsequent commercialization of the technology



2 Description of facility

The research facilities used during the HYBREC Project are:

- 1) **ETH Zurich, Switzerland:** The laboratory offers the facilities to manufacture various materials and structures, and to test them using scanning electron microscope, gas adsorption analyzer, thermogravimetric analyzer, and lab-scale tubular reactor (see Figure 2). The tubular reactor is used for testing of different morphologies and as a means of validating the CFD reactor model. The unit was also used to run experiments outlining the benefits of countercurrent chemical looping, the study being published this past year [2].
- 2) **IMDEA Energy Institute, Spain:** This location was used during the second half of 2020. The institute offers a solar tower concentrating facility, with the potential of delivering 50 kW of solar radiative power into a 16-cm diameter of the reactor's aperture. This facility was used when testing the redox reforming process on a scaled-up and directly-irradiated solar reactor which has been published in the past year [3].

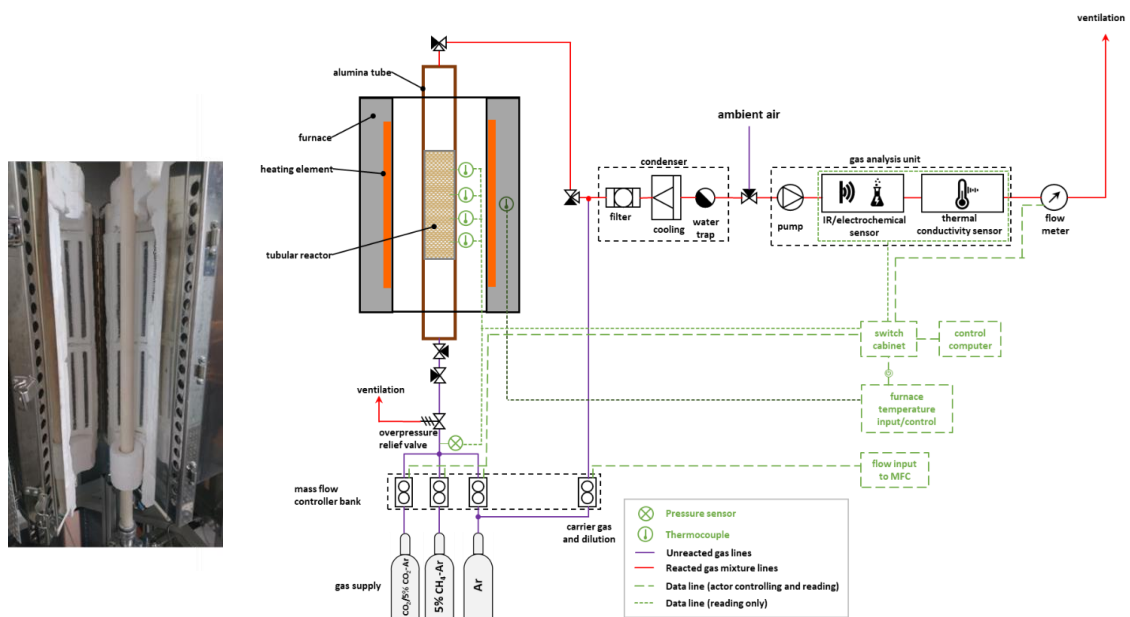


Figure 2: Lab-scale tubular reactor located at ETH Zurich (left).
The P&ID of the tubular reactor system filled with a packed bed of ceria redox material (right)



3 Procedures and methodology

The following sections outline the methodology and problem-solving approach behind the main components of the HYBREC Project.

3.1 Thermodynamic Analysis

The thermodynamic analysis is largely based off a thermodynamic description of non-stoichiometric ceria developed by Bulfin et al. [4]:

$$\Delta G^\circ = \Delta H^\circ - T\Delta S^\circ$$

$$\Delta H^\circ = 1000(395 - 31.4 \log \delta)$$

$$\Delta S^\circ = 160 + 2.9R_u(\ln(0.345 - \delta) - \ln \delta)$$

The above equations allow one to model the heterogeneous reactions between the solid ceria and gas. The standard Gibbs free energy (ΔG°) at various temperatures and nonstoichiometries (δ) can be calculated and the spontaneity of various reactions can be determined. Ellingham diagrams (Figure 3 and Figure 4) are used to display reaction trends. At low δ the complete CH_4 oxidation reaction is highly favourable while the oxidation reaction is not (see Figure 3). As δ increases the complete CH_4 oxidation reaction becomes less favourable (implying less unwanted side products), the main syngas forming reduction reaction remains favourable, and the oxidation reaction becomes favourable (see Figure 4). These trends continue as δ increases, implying syngas selectivity, and CO_2 conversion during oxidation both increase at higher δ . The diagrams also depict how the reduction of ceria in the pure process is highly unfavourable at temperatures below 1500°C .

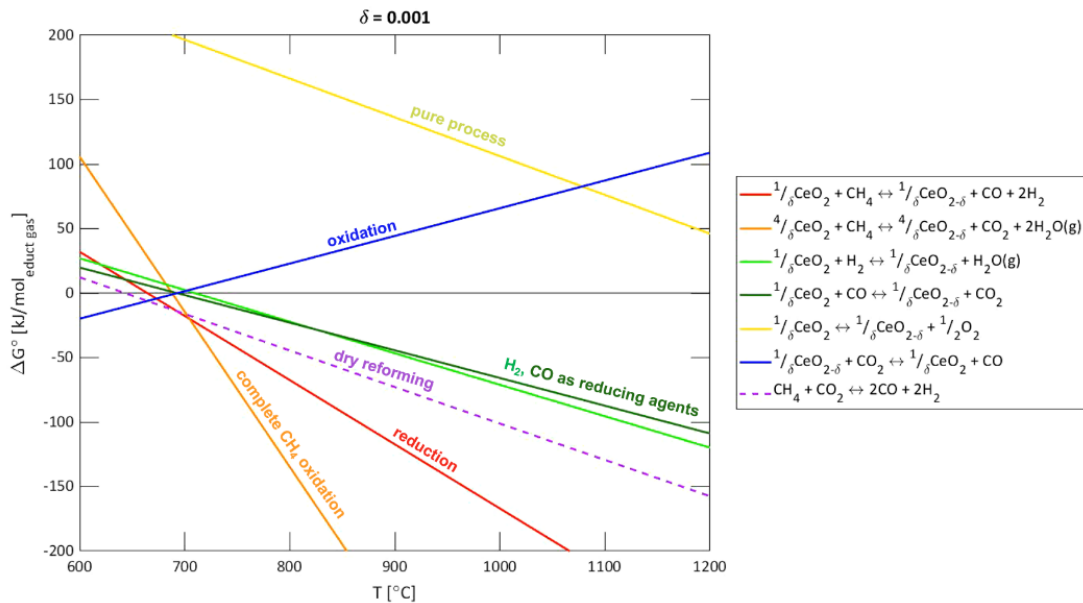


Figure 3: Ellingham diagram of the main reactions applicable to dry redox reforming at $\delta=0.001$.

Negative Gibbs free energy implies a spontaneous reaction.

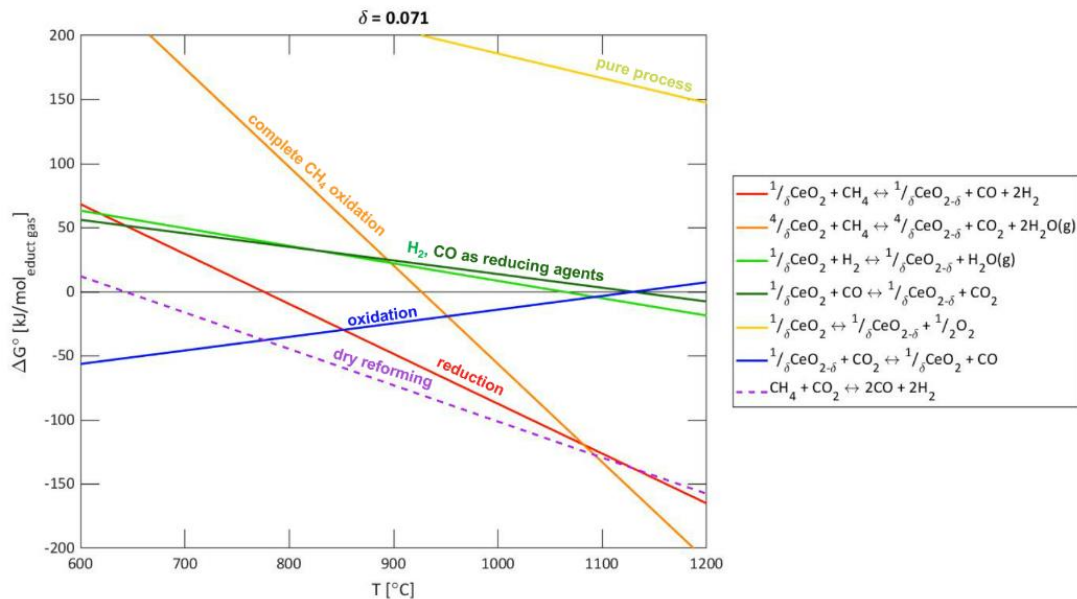


Figure 4: Ellingham diagram of the main reactions applicable to dry redox reforming at $\delta=0.071$.

Negative Gibbs free energy implies a spontaneous reaction.

3.2 Kinetic Analysis

A kinetic rate equation resembling that of the apparent reaction rate within the tubular reactor system is to be imposed. The general rate equation is given by:

$$\frac{d\delta}{dt} = k_0 e^{-\frac{E_a}{R_u T}} \cdot f(\delta) \cdot [\text{CH}_4]^n \cdot \rho_s$$

$$f(\delta) \propto K_{\text{eq}}(\delta)$$

Experiments in the tubular reactor are used to determine an apparent reaction rate that represents the reactor conditions.

3.3 Experimental Assessment

Two main setups are used for the experimental assessment:

- 1) **Tubular reactor, ETH Zurich:** The tubular reactor is electrically heated and allows for roughly 100g of material. Typical operating conditions are: 900-1050°C, 0.25-2.0 L_n/min, 5% reactant flow diluted in argon, ambient pressure, redox cycling and co-feeding. Tests were conducted involving a ceria pellet morphology and used to validate the numerical model against gas analysis readings. Parameters to vary include flowrate, temperature, operating mode (redox reforming cycling vs. co-feeding), and reactor tube diameter.
- 2) **Solar reactor, IMDEA Energy Institute:** On average the solar reactor operated with 10 kW of input, and can be filled with 25 kg of redox material. Typical operating conditions were: DNI>750 W/m², 800-1200°C, 100 L_n/min, 3-40% reactant flow diluted in argon, ambient pressure, redox reforming cycling and co-feeding. This setup was used to analyse the challenges when operating under the directly irradiated conditions as well as assessing the process in scaled-up conditions. Future tests are not planned nor expected at this site.



3.4 Numerical CFD Reactor Model

The computation fluid dynamics (CFD) model of the reactor considers chemical thermodynamics, kinetics, heat transfer (convection, conduction, and radiation), mass transfer, and fluid dynamics. Each feature of the model is configured and validated against analytical solutions whenever possible. Following the implementation of all features the model is validated against experimental results. The CFD model is created with the open source package OpenFOAM, and named porousRedoxFoam. It is developed on two base solvers, reactingFoam and porousGasificationFoam. reactingFoam is a “transient solver for turbulent flow of compressible reacting fluids” [OpenFOAMWiki] and is often used in combustion applications. porousGasificationFoam was developed by Žuk and considers limited heterogeneous irreversible reactions through a fixed porous media [5]. porousRedoxFoam is developed to allow for additional solver capabilities such as reaction thermodynamics, reversible reactions, δ dependency, and improved flexibility when defining chemical reactions.



4 Activities and results

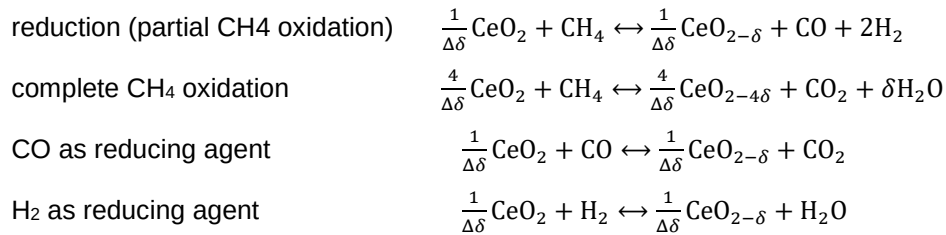
The following section outlines the main advancements during the past year only, with a focus on the numerical CFD reactor model.

4.1 Numerical CFD Reactor Model - porousRedoxFoam

The past year saw a major focus on advancing the numerical CFD model of the reactor. The transient solver is derived from based solvers reactingFoam and porousGasificationFoam and solves a total of seven conservation equations in the gas (i.e. species mass, continuity, energy, momentum) and solid phase (i.e. species mass, continuity, energy) [5]. The most notable additions and changes to the base solvers are:

- compatibility with openfoam9
- corrections to conservation equations
- adaptation of molar units (OpenFOAM primarily works in mass units)
- reversible reactions such that thermodynamics and the Gibbs relations can be imposed (see **3.1 Thermodynamic Analysis**)
- multi-reaction/multi-product reactions with reaction orders
- a normalized δ variable
- δ dependency on K_{eq} , H_f , and $k_{f\&r}$

The addition of reversible reactions allows one to impose the thermodynamics of the system. This becomes important due to the many competing reactions within the ceria redox reforming process. The four main heterogeneous reactions considered are:



The thermodynamic favourability of each reaction is governed by the Gibbs free energy (see **3.1 Thermodynamic Analysis**) and is related to the equilibrium constant by:

$$\Delta G^\circ = -R_u T \ln(K_{eq})$$

In the case with ceria, the Gibbs free energy and hence the equilibrium constant varies with non-stoichiometry (i.e. state of the reactor),

$$K_{eq} = f(\delta, T)$$

and generally,

$$K_{eq} = \frac{k_f}{k_r}$$

where k_f and k_r resemble the forward and reverse reaction rate constant, respectively. The solver uses the rate constants to drive the reactions, hence to model thermodynamics the reverse reaction rate must also be considered. The result is a Jacobian ODE matrix where concentration of each species is to be solved after each numerical iteration, eventually converging to the equilibrium solution.



Following the implementation of the above components into the porousRedoxFoam solver, initial simulations were conducted on a two-dimensional axisymmetric model mimicking that of the tubular reactor, as shown in Figure 5.

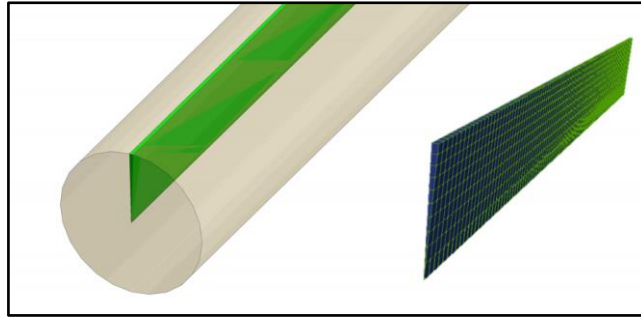


Figure 5: Wedge of tubular reactor (left), used as computational mesh domain (right)

4.1.1 Theoretical Verification

Theoretical verification is performed to substantiate that the newly imposed chemical thermodynamics is behaving accurately in porousRedoxFoam. The theoretical result is derived based on the thermodynamic definition by Bulfin et al. [4] and using Cantera, an open source suite of tools for chemistry, which allows one to predict product concentrations. Cantera's 'equilibrate' uses a Sundials CVODES solver which is not equivalent to solving the Jacobian ODE as done in OpenFOAM.

The OpenFOAM simulation behaves as a 0-D simulation without any flow. Methane is initialized at 100% and the product composition at equilibrium is compared at varying δ for a fixed temperature (1000°C). Figure 6 shows the comparison of results between the theoretical values and OpenFOAM simulation. The results indicate that the implementation of the reversible reactions within OpenFOAM was done correctly and the solver is able to accurately solve the Jacobian ODE matrix.

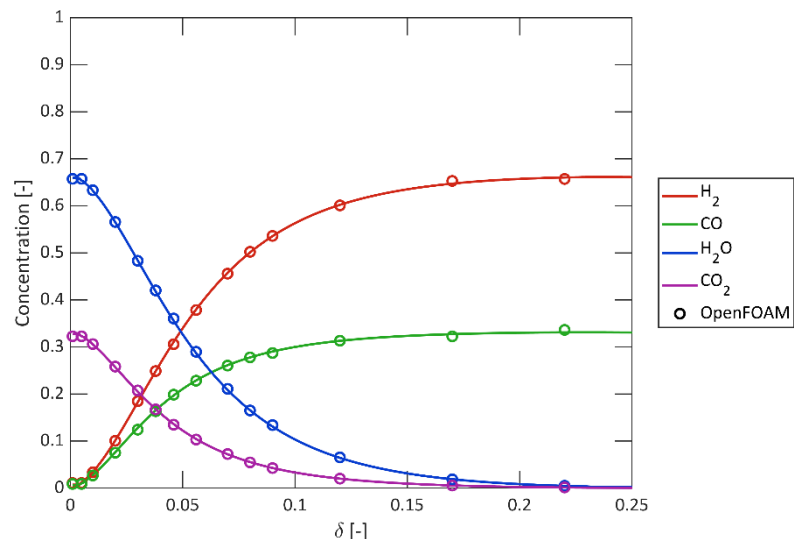


Figure 6: Equilibrium product composition as a function of the ceria non-stoichiometry δ at 1000°C.
Theoretical values (lines) compared to OpenFOAM results (circles).

4.1.2 Experimental Validation

Following verification of the reversible reactions, the tubular reactor is used for validation of the model. The temperature of the furnace is set to 1016°C, and 5% CH₄ diluted in argon is fed into the reactor at a flow rate of 1 L_n/min for 900 seconds. The boundary conditions from the experiment (e.g. wall



temperature profile, inlet flowrate and concentration, outlet pressure) and thermophysical properties (e.g. specific heat capacity and thermal conductivity of ceria, porosity) are imposed in the OpenFOAM simulation to accurately represent real-world conditions. The outlet product composition between the experiment and simulation are compared and shown in Figure 7.

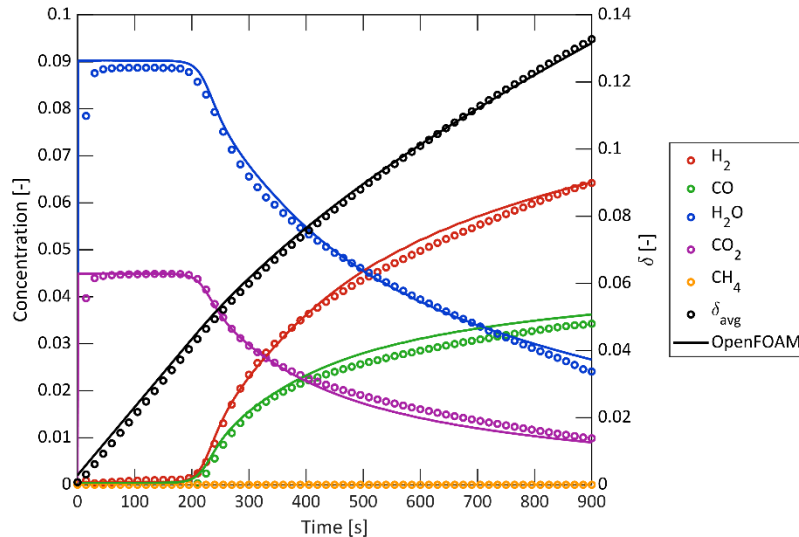


Figure 7: Temporal variation of the product composition and δ during 900 seconds of reduction (5% CH₄ diluted in Ar at 1 L/min). Experimental data (circles) compared to OpenFOAM results (lines).

The OpenFOAM simulation results show good agreement to that of the experimental results, which suggests the model is validated for the reduction step and can subsequently be used for a trusted optimization and scale-up analysis.

5 Evaluation of results to date

The experimental campaign helped validate the porousRedoxFoam solver for the reduction reaction. The outlet product composition shows good agreement between the numerical simulation and the experimental run. The aforementioned comparison case focusses solely on a reduction case in which the methane is fully converted. The simulation results indicate a fully working model coupling chemical reactions, reaction enthalpies, heat and mass transfer, as well as fluid dynamics.

6 Outlook

The next steps are to use the porousRedoxFoam solver on the oxidation step as well as on cases in which methane does not fully convert (i.e. at lower temperatures). Following validation of the oxidation reaction and reductions at lower temperatures, a design optimization of a single tube will be conducted. The syngas yield per reactor volume will be optimized for a given temperature profile along the tube. The main parameters being varied include the tube diameter and flow rate of the reactant gas stream. The intended use of the model is for dry redox reforming cycling; however, a short study will be conducted to determine the viability of the model when cofeeding CO₂ and CH₄. Further studies with the model include a deeper investigation into the benefits of counter current feeding [2, 6].



A journal paper on the CFD reactor model is in preparation. Correspondingly, the porousRedoxFoam solver will be made available as an open-source contribution.

All of the simulations and recent work have been on a tubular reactor, not a directly irradiated reactor (e.g. cavity-receiver). The concept is based on employing a solar receiver to heat up a heat transfer fluid (e.g. steam) which could be fed downstream into a tubular reactor (i.e. heat exchanger) to drive the reactions (see Figure 8). A future project (outside the scope of HYBREC) could see the scale up of this configuration to an on-sun system similar to the one outlined by Zuber et al. [3].

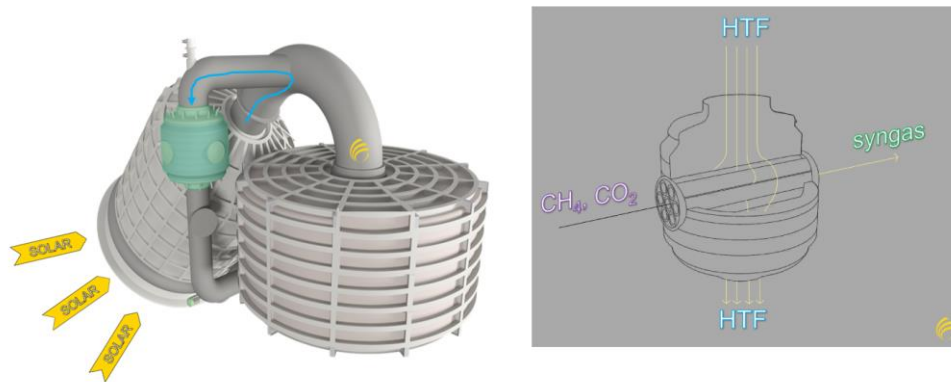


Figure 8: Example of a solar receiver feeding an HTF downstream to a reactor, with a thermal energy storage (TES) attached (left)
Example of a tubular reactor heat exchanger with HTF and reactant flow (right). Images adapted from Synhelion SA
(<https://synhelion.com/>)



7 Synhelion: Advisory Role and Technoeconomic Assessment

7.1 Advisory Role

Synhelion consistently provides essential consulting assistance in project definition and management, as well as in ongoing scientific dialogues. Throughout the on-sun campaign at IMDEA, Synhelion supplied the necessary support for the entire project, including equipment provision, design, manpower, and scientific/strategic planning. Currently, Synhelion is aiding in the development of the numerical CFD reactor model by engaging in frequent discussions on the status of the simulations and what steps to take. Information and knowledge on the latest advancements and state-of-the-art in their range of projects is also shared. Synhelion also provides expertise into real-world implementation via their experience in scaling up the process chain. Additionally, via other collaborations (e.g. with Prof. Scheffe's group at the University of Florida [7]) new insights into the dry redox reforming process are shared and considered within the scope of this project.

7.2 Review of Technoeconomic Assessment

A process flow diagram (PFD), Figure 9, illustrates the major components from sun to liquid fuels. The PFD includes a solar unit and methanol synthesis unit. The solar unit includes the solar field, receiver, TES, reactor, and steam reformer. The PFD model calculates heat, power, and mass streams on a minute basis over one year, and can ultimately be used to justify plant configuration and estimate CAPEX, OPEX, and levelized cost of methanol (LCOM).

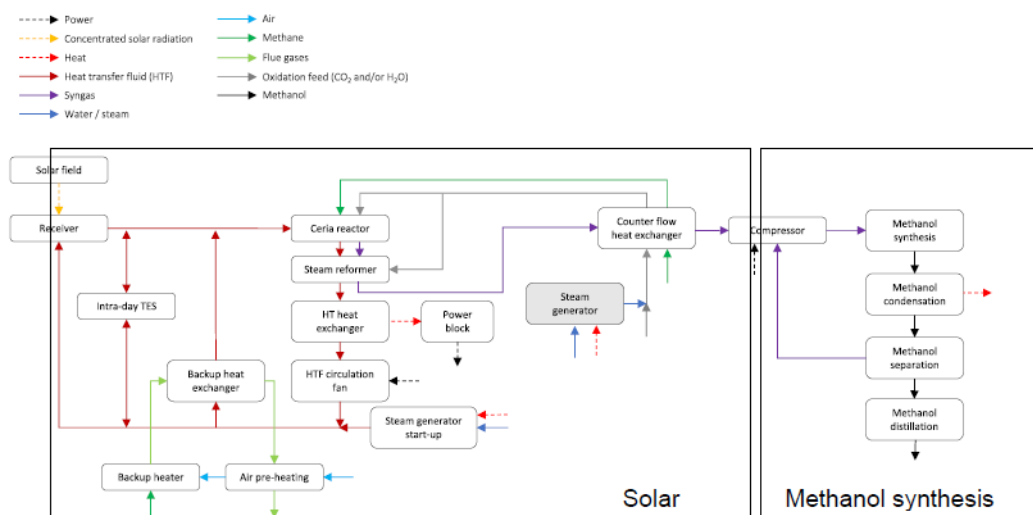


Figure 9: Process flow diagram of the solar plant and the methanol synthesis plant

The steam reformer is used to convert unreacted methane and additional steam into syngas. As it operates at lower temperatures the steam reformer can be placed in series with the redox reactor, and can further cool the HTF. A lower conversion of CH_4 in the redox reactor means the more the steam reformer is being utilized, and thus can allow for a lower overall HTF temperature, thus aiding efficiency.

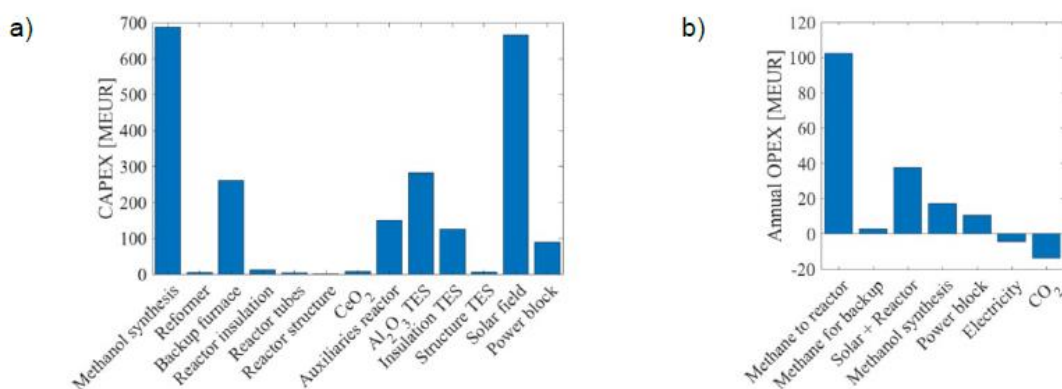


Figure 10: a.) Non-actualized CAPEX (Total: 2299 MEUR) and b) annual OPEX of components (Total: 153 MEUR/year)

Figure 10 details the CAPEX and OPEX of the units within the PFD. The methanol synthesis and solar are the major contributors to the capital costs, each totaling roughly 30% of the total CAPEX. With respect to operating costs, the methane to reactor step totals 65% of the total OPEX. This work is expanded upon in a paper by Moretti et al [8].

8 National and international cooperation

Synhelion SA, Switzerland

IMDEA Energy Institute, Spain

9 Communication

See 10. Publications.



10 Publications

The following is a list of published materials to date.

10.1 Journal Papers

- M. Zuber et al., "Methane dry reforming via a ceria-based redox cycle in a concentrating solar tower," *Sustainable Energy & Fuels*, 2023, doi: 10.1039/d2se01726a.
- B. Bulfin, M. Zuber, O. Gräub, and A. Steinfeld, "Intensification of the reverse water–gas shift process using a countercurrent chemical looping regenerative reactor," *Chemical Engineering Journal*, vol. 461, 2023, doi: 10.1016/j.cej.2023.141896.
- B. Bulfin, M. Zuber, and A. Steinfeld, "Countercurrent Chemical Looping for Enhanced Methane Reforming with Complete Conversion and Inherent CO₂ Separation", **in preparation**
- *C. Moretti, V. Patil, C. Falter, L. Geissbühler, A. Patt, and A. Steinfeld, "Technical, economic and environmental analysis of solar thermochemical production of drop-in fuels," *Sci Total Environ*, vol. 901, p. 166005, Aug 2 2023, doi: 10.1016/j.scitotenv.2023.166005.

10.2 Conference Contributions

- Zuber M., Ackermann S., Furler P., Steinfeld A., "Solar Fuel Production from CO₂ and H₂O Via the Hybrid CeO₂-CH₄ Redox Cyclic Process", *2020 AIChE Annual Meeting*, San Francisco, USA, Nov. 15-20, 2020.
- Zuber M., Patriarca M., Ackermann S., Furler P., Romero M., González J., Steinfeld A., "Experiment Investigation of a Solar Reactor for Thermochemical Syngas Production Via the CeO₂-CH₄-CO₂ Hybrid Redox Cycle in a Concentrating Solar Tower", *2021 AIChE Annual Meeting*, Boston, USA, Nov. 7-11, 2021.
- Zuber M., Ackermann S., Steinfeld A., "Thermodynamic and Computational Modeling of Thermochemical Syngas Production Via the CeO₂-CH₄-CO₂ Redox Reforming Cycle in a Tubular Reactor", *2023 AIChE Annual Meeting*, Orlando, USA, Nov. 5-10, 2023.

10.3 Patents

- P. Furler, S. Ackermann, P. Good, G. Mazzanti, L. Geissbühler, and M. Zuber, "Process for the Production of Syngas," WO 2021/110667 & US 2023/0002225.

10.4 Colloquiums

- Zuber M., Ackermann S., Furler P., Steinfeld A., "Performance Optimization of the CeO₂-CH₄-CO₂ Redox Cycle for Solar Fuel Production", 1st Doctoral Colloquium of SFERA-III, Odeillo, France, September 11-13, 2019.
- Zuber M., Patriarca M., Ackermann S., Furler P., Steinfeld A., "On-Sun Experimental Investigation of a Solar Reactor for Thermochemical Syngas Production via Methane Reforming Utilizing a Ceria Redox Cycle", 2nd Doctoral Colloquium of SFERA-III, Almeria, Spain, October 7-8, 2021.
- Zuber M., Ackermann S., Steinfeld A., "Dry Redox Reforming", 3rd Doctoral Colloquium of SFERA-III, Zurich, Switzerland, September 12-14, 2022.
- Zuber M., Ackermann S., Steinfeld A., "Modeling the CeO₂-CH₄-CO Redox Reforming Cycle in OpenFOAM", 4th Doctoral Colloquium of SFERA-III, Cologne, Germany, September 11-13, 2022.



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