THESIS PROPOSAL

Title: Multiphysics modeling of a ceria-based receiver reactor for solar thermochemical fuel production.

Type of thesis: modeling thesis

Tutor/s: Domenico Ferrero, Francesco Orsini, Massimo Santarelli

Duration: 6 months, starting September 2024 or earlier

Topic: Simulation of an indirectly irradiated ceria-based receiver reactor for solar thermochemical fuel production. Investigation of configuration, and impact of shape, morphology, and design parameters on the reactor performance

Keywords: Chemical looping, solar fuels, reactor simulation, Multiphysics modeling

Description:

In the framework of chemical looping (CL) processes aimed at synthetic fuels production from H_2O and CO_2, the thesis activity is aimed at investigating the solar thermochemical hydrogen production (STCH) cycle by simulating the multiphysical process in COMSOL Multiphysics. The oxygen carrier (OC) is assumed to be state-of-the-art ceria, but also novel perovskites can be considered in principle given the availability of experimental data. After a detailed literature review on the topic, the thesis foresees to explore the following reactor-relevant aspects:

1. Selection of one or two relevant OC shapes/reactor geometries. The selected geometry(ies) will be assessed in terms of suitable performance metrics. Novel designs can be considered here, while having a thorough look to the literature.
2. Selection of suitable reactor materials capable to withstand the extreme operating temperatures (~1500 C). This can be accomplished looking at the state-of-the-art literature.
3. An indirectly irradiated receiver reactor (IIRR) configuration will be considered.
4. Once the OC shape and the reactor geometry will be defined, as well as all the materials to be used, the morphology will be addressed more in detail. The state-of-the-art literature suggests using reticulated porous ceramics (RPC) structures. This kind of structures will be implemented in the model based on well-established empirical correlations. The thesis aims then to tune some of the morphological parameters, e.g., porosity and mean pore diameter, to explore the related impact on the reactor performance (more specifically: morphology-induced T and non-stoichiometry fields, and following fuel production).
5. Parametric sweep can be also performed with respect to some design (e.g., geometrical) and operational (e.g., flow rates, inlet temperatures) parameters.
6. The model should address the entire redox cycle – reduction and oxidation. From one to few cycles will be simulated at steady-state operation. Convergence studies will be performed.

The model should couple the fluid flow (inert during reduction, and steam during oxidation), the chemistry (redox reactions), and the heat transfer. Particular attentions will be given to radiative heat transfer, that typically drives the process. Suitable radiation approximations will be used in line with the literature. Also, energy balance will be performed to assess the nature of thermal losses in the system, in order to drive the next design steps. A preliminary reference modeling will be accomplished with close relation to reference literature, with the aim of validating the physics implementation (i.e., modeling of a geometry from the literature, and results comparison, prior to moving to the new models).

The outputs of the thesis should encompass:

i. A complete overview of the current trends in numerical modeling of STCH reactors.

ii. The detailed physics implementation and following benchmark/validation with reference modeling works.
iii. The definition of the impact of shape, morphology and selected design or operational parameters on the IIRR performance.
iv. Hints for the following modeling steps in order to improve the performance, where needed or where possible, based on the obtained results.

The thesis activity will be monitored with weekly/biweekly meetings.