Sandia National Laboratories

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Standardizing Solar-to-Hydrogen Efficiency Calculations for the Evaluation of New Water Splitting Materials

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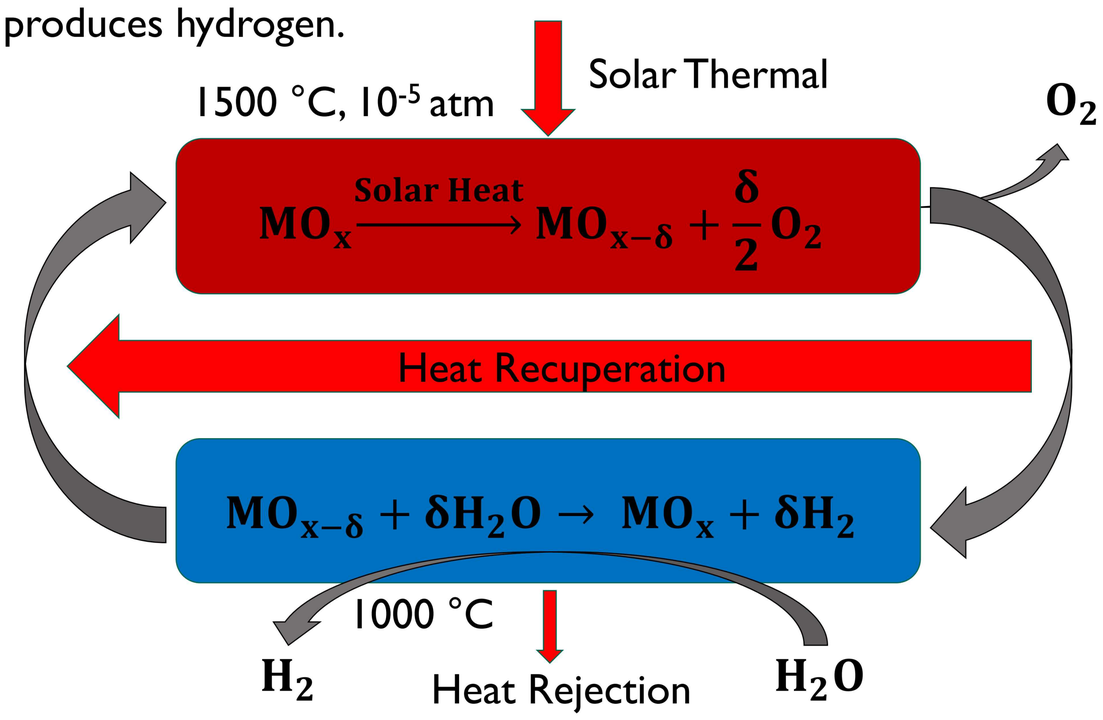
Introduction

Solar thermochemical hydrogen (STCH) production is a two-step redox process that utilizes solar thermal energy to produce chemical fuels. Concentrated sunlight can be used to thermally reduce a metal oxide leaving it in an oxygen deficient form. Subsequent exposure of the reduced metal oxide to steam at lower temperatures reoxidizes the material and produces hydrogen.



Numerous computational modeling studies have been conducted on the metal oxide ceria ($CeO_{2-\delta}$). However, the thermodynamics are insufficient for achieving hydrogen cost and efficiency targets set by DOE. Therefore, the development and selection of new non-stoichiometric oxide materials is required to improve the solar-to-hydrogen efficiency and lower hydrogen production cost.

Material Efficiency Model

Material research has led to the need for a standardized evaluation tool for computing system efficiencies with new material formulations. The goal of the tool is to compare solar-to-hydrogen efficiencies based on thermodynamic data of new materials.

Objective: *Create an open source system model for evaluating solar-to-hydrogen efficiencies of novel water splitting materials.*

Model Development

Desired Model Characteristics:

- Non-proprietary platform
- Graphical interface
- System component models can be reconfigured
- Easily modify/implement new material thermodynamics

The model is currently being developed in *OpenModelica*, which *is an* object-oriented modeling language that allows for component development with generality and a graphical interface.

Current Status

System component models for a simple two-step thermochemical cycle have been developed.

Components:

- Solid and gas thermodynamic and transport properties
- Reactors (Solar Reduction Receiver, Water Splitting Reactor)
- Heat Exchangers (Solid and Gas Phases)

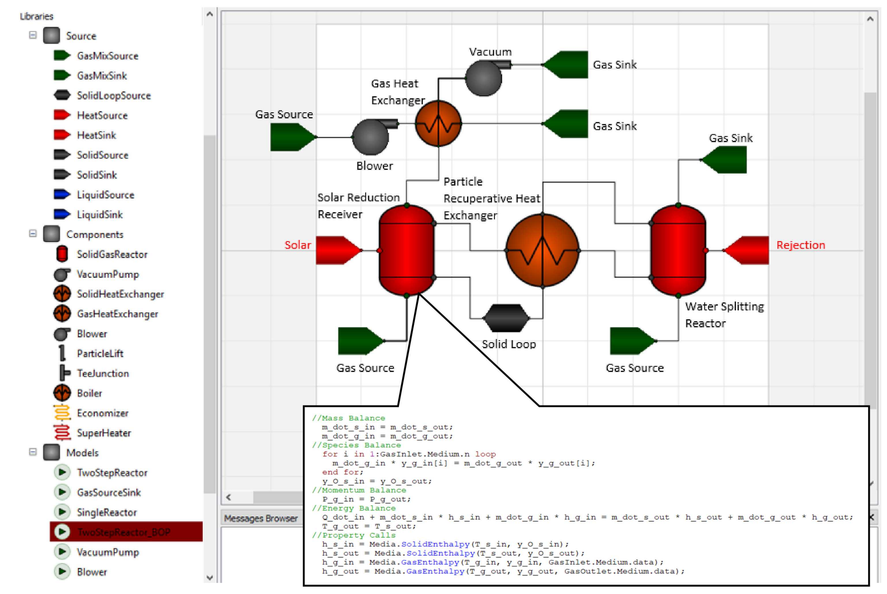


Figure 1: Libraries and partial two-step solar thermochemical system model in *OpenModelica*.

Future Work

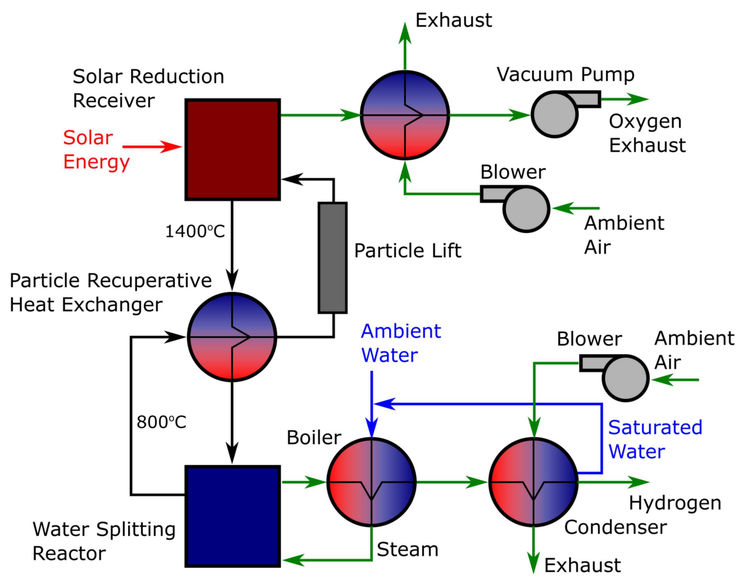


Figure 2: Complete two-step STCH system with balance-of-plant components.

- Finish modeling the balance-of-plant components (boiler, condenser, particle lift, radiation heat transfer)
- Develop a standard system model with ceria material thermodynamics
- Standardize the material thermodynamic property functions to accept new materials
- Document the code and make publicly available

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