Modeling of Concentrating Solar Reduction Reactor for Oxygen Separation from Air

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1. Introduction

Ammonia is an important ingredient in fertilizer and is a potential candidate for storage of thermochemical energy in a liquid fuel. Synthesis of ammonia via concentrating solar power reactors has the potential to generate a sustainable and renewable source of ammonia. The proposed route for ammonia production is a two-stage reduction-oxidation (redox) cycle. In the first stage, the N_2 necessary for the synthesis of ammonia is separated from O_2 in air via the oxidation of substituted strontium ferrite. The second stage involves cycling the N_2 with a novel metal nitride and H_2 to produce ammonia. Efficient metal oxide reduction and subsequent N_2 extraction from the air is important to the overall efficiency of the ammonia production cycle.

To this end, a benchtop, dense granular flow, oxide reduction reactor is being designed, with the aid of three-dimensional numerical modeling. The reduction reactor design employs a directly irradiated, inclined, dense granular flow configuration, in which the solid oxide particles are simultaneously the primary heat transfer media and the O_2 getter/carrier for thermochemical air separation. Substituted strontium ferrite is used in the air separation cycle due to its structural stability, high redox activity across attainable changes in temperature and O_2 pressure, and rapid uptake and release of O_2. Dense flowing [1] or falling [2] granular media have been proposed in solar thermochemical applications for potentially high absorption temperatures, efficiencies, and/or energy densities. The modeling results and subsequent reactor design will be presented.

2. Model Description

The physics of the inclined particle receiver are modeled as a three-region continuum: a reactor body comprised of the insulating and mechanical components of the reactor, a flowing particle bed, and a gaseous cavity region within the reactor. Simulation of the reactor involves modeling physical transfer within and between the three regions. Within the flowing particle region, a porous-mixture model is used to describe the relative transport of heat and mass. The advection velocity of the gaseous species through the flowing bed is given by an augmented version of Darcy's Law. Description of the velocity profile in the particle bed is modeled after the work done in [1] prescribing a depth dependent velocity. Thermodynamic models of the equilibrium redox extent for T = 400 – 1100 ºC and p_{O2} = 0.01 – 0.90 bar O_2 are used to couple the endothermicity of the thermal reduction and the accompanying O_2 release to the computational heat and mass transfer equations.

Within the cavity region, the Navier-Stokes equations are solved to provide the flow profile of gases. Heat and mass transfer are modeled within the cavity by their respective advection-diffusion equations. The reactor region solves for the diffusion of heat through its body, with reradiation and convection of heat along its boundaries. Mass and heat transfer between the particle bed and the cavity region are handled via robin-robin interfaces. Heat transfer from the particle bed and cavity to the wall is enforced though a contact resistance flux. Radiative heat transfer within the body of the reactor is modeled using enclosure radiation.

The High Flux Solar Simulator (HFSS) at Sandia National Laboratories provides input radiation to the reduction reactor. To characterize the HFSS lamps, flux maps are generated from digital images of beams reflected from a water-cooled Lambertian target. The target is mounted in the HFSS focal plane, and maps are determined using methodology based on [3]. The maps are used to tune a ray tracing of the HFSS lamps developed in the commercial software FRED via minimization of total power and spatial flux error. The ray tracing captures lamp characteristics and allows the generalized prediction of radiation delivered to 3D surfaces and volumes. Boundary conditions are thereby generated for the reactor geometry and input to the CFD model via an energy conservative, spatially-preservative ray mapping algorithm [4].

3. Results & Discussion

The reduction of the metal oxide at a given set of process parameters is of interest for the reactor simulation. As illustrated in Fig. 1, the reactor model took the mapped irradiation data from FRED simulations and generated flux distribution maps through the domain. The corresponding loss of oxygen from the bed is shown in Fig. 2. For this irradiation map, only a small region of the reactor was capable of sufficiently reducing the oxide. Efforts to modify the design to increase the active reduction area of the benchtop reactor are underway.

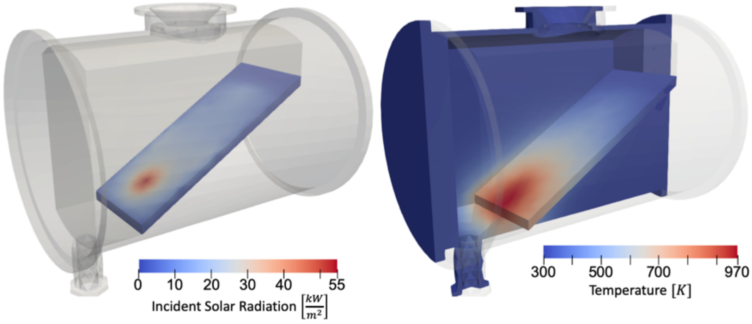

Fig. 1: (Left) Mapped irradiation data from FRED optical simulations to the surface of the flowing particle bed. (Right) Steady state temperatures reached inside the reactor for inert particles.

A survey of process parameters of the benchtop reactor design was conducted to observe the changes in exit temperature as irradiation intensity, particle feed temperature, and preheated reactor temperature were varied. Overwhelmingly, the intensity of incoming radiation was the leading driver in elevating particle temperature, with particle feed temperatures lending a smaller but significant contribution. Preheating of the reactor body did not provide any additional gains in the average exit temperature of the particles, nor did it significantly reduce the time required for the reactor to reach equilibrium operation.

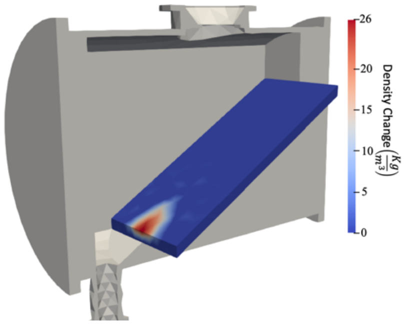

Fig. 2: Changes in particle bed density from the reduction of oxygen out of the strontium ferrite bed.

Acknowledgment

This material is based on work supported by the U.S. Department of Energy Solar Energy Technologies Office under Award No. DE-EE0034250. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525. SAND2020-4906 A.

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