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Quarterly report: High Efficiency Generation of Hydrogen Fuels using Solar Thermochemical Splitting of Water – Cadmium Quenching Modeling

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Introduction

Metals are attractive candidates for storage and transport of energy, and they can be used to produce hydrogen through water-splitting reactions (Steinfeld et al., 1998). In the Cd/CdO thermochemical cycle, the cadmium vapor at high temperature needs to be quenched (Steinfeld et al., 1999). In order to effectively guide the design of solar decomposer and vapor quencher receiver, it is of critical importance to understand the mechanisms of transport phenomena inside them. However, very little work has been reported about vapor condensation of metal. The objective of the present work is to develop a computational fluid dynamics (CFD) model for the purpose of investigating vapor condensation of cadmium inside the decomposer and quencher.

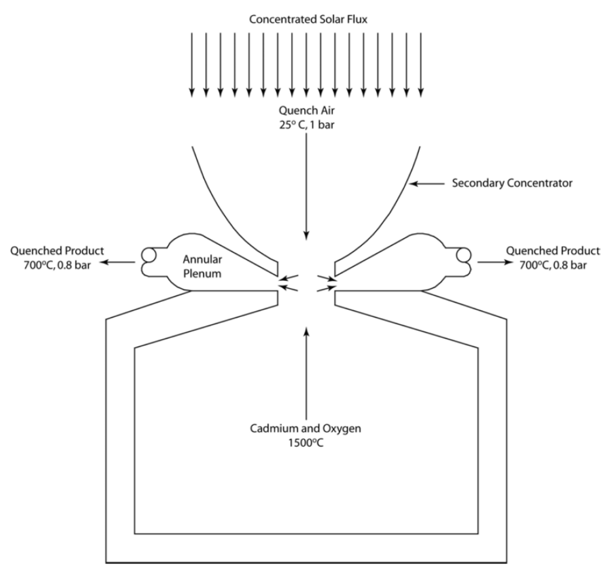
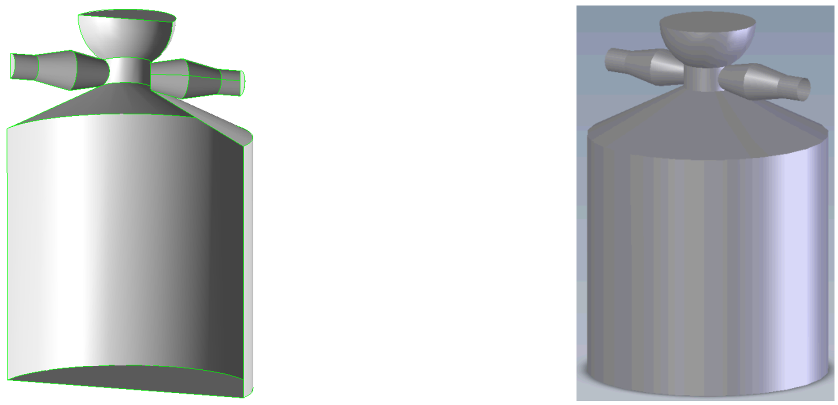


Fig. 1 Windowless beam-down concept (Brown et al., 2007)

Problem Statement and Numerical Methods

Based on the concept as shown in Fig. 1, a simplified conceptual design was devised for numerical modeling. A schematic of the investigated cadmium quencher is shown in Fig. 2. In this simplified model, some assumptions were made during the numerical simulation. This quencher has two inlets: one is at the top with a diameter of 0.4m and the other is at the bottom with a diameter of 1m. At the bottom inlet, it is assumed that a mixture of cadmium vapor and oxygen flows into the decomposer with a uniform temperature of 1450 K. The mole fractions of cadmium vapor and oxygen are assumed to be 0.6667 and 0.3333, respectively. Quench air at

298.13 K and 1 atm is introduced from the top inlet, with a uniform velocity of 1 m/s. The cold quench air will be expected to meet the hot cadmium and oxygen mixture in the "bottleneck" section. Then, the mixture of cadmium, oxygen and air will flow through two annular expansion-contraction nozzles. The exit nozzle has a diameter of 0.1 m.



(*a*) (*b*)

Fig. 2 Simplified Windowless quenching decomposer

Due to flow symmetry, only one quarter of the fluid domain was selected as the computational domain in order to save computational time cost. The computational domain together with some of the operating parameters is shown in Fig. 3. Numerical simulations of cadmium quenching process in generation of hydrogen fuels using solar thermochemical splitting of water were performed. In this quarter, results in two aspects were obtained: effects of cadmium vapor flowrate, and development of the condensation model.

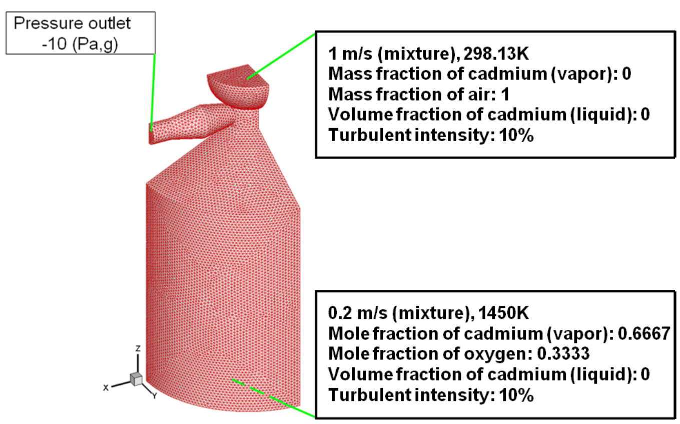


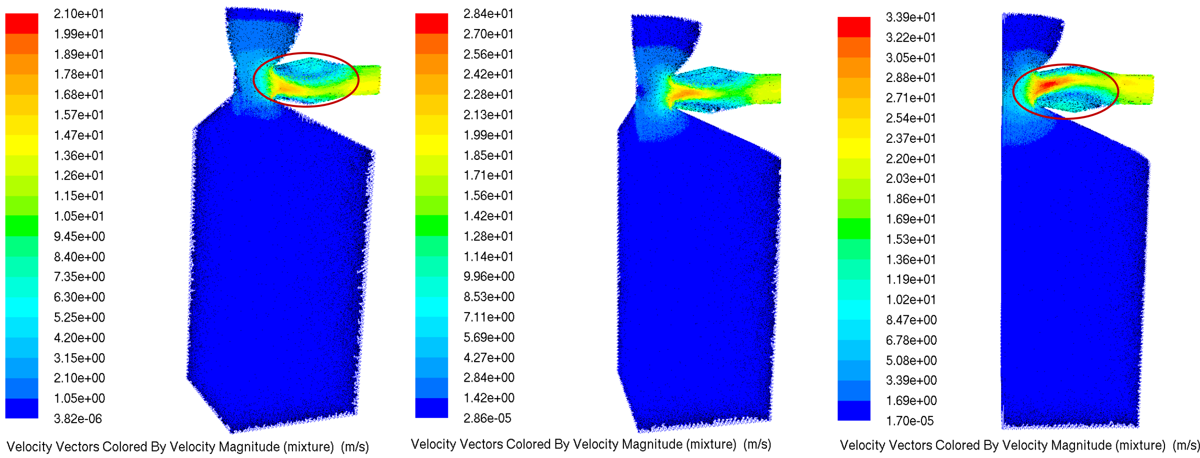
Fig. 3 Computational domain

Results and Discussions

Investigations of cadmium vapor effects

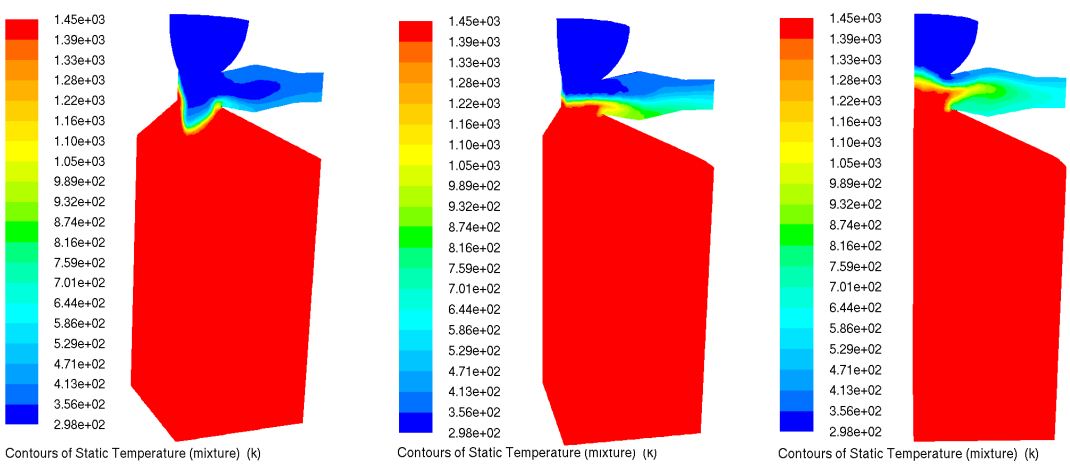
It was assumed that flow velocity of quench air at the upper inlet is fixed at 1 m/s. Three different flow velocities for cadmium/oxygen mixture at the bottom inlet (u_{vapor} = 0.1, 0.2 and 0.3 m/s, respectively) were studied. Numerical results including the velocity and temperature distributions of cadmium are shown in Figs. 4 and 5.

It was shown from numerical results that flow is relatively low in the decomposer and close to the bottom and the top inlets. The maximum velocity develops in the region near the entrance of the quenching nozzle. Temperature of the mixture varies a lot in the "bottleneck" region, where the cold quench air from the top and the hot cadmium/oxygen mixture from the bottom meet and mix. Temperature distribution in this region is directly affected by the ratio between the cadmium vapor from the bottom and the quench air from the top. Pressure drop primarily occurs inside the nozzle.



(*a*) u_{vapor} = 0.1 m/s; (b) u_{vapor} = 0.2 m/s; (c) u_{vapor} = 0.3 m/s

Fig. 4 Distributions of the velocity field

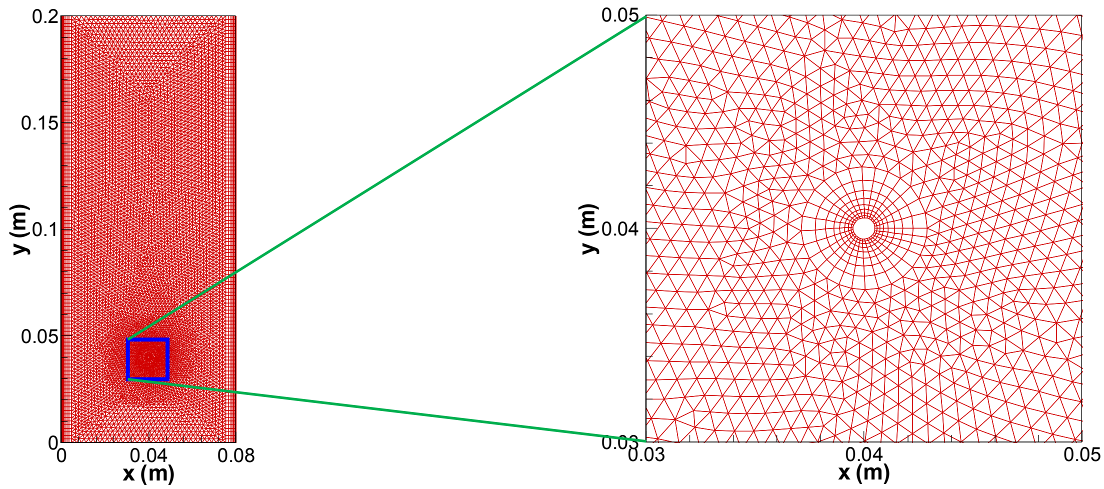


(*a*) u_{vapor} = 0.1 m/s; (b) u_{vapor} = 0.2 m/s; (c) u_{vapor} = 0.3 m/s

Fig. 5 Distributions of the temperature field

Development of condensation model

2-D modeling of cadmium condensation around a cold cadmium droplet was performed. The used computational domain is shown in Fig. 6. It consists of a channel with a width of 0.08 m and a length of 0.2 m. The used coordinate system is included in Fig. 6. The circular cylinder is placed in the center of channel in the spanwise *x*-direction. The center of cylinder is 0.04 m downstream from the inlet and 0.16 m upstream of the exit section. It is assumed that the cadmium droplet has a diameter of 1 mm.



(*a*) (*b*)

Fig. 6 Computational meshing system for the selected test case

At the inlet, flow of the cadmium vapor and oxygen mixture is assumed to have a uniform velocity of 7 m/s and a constant temperature of 1450°C. The mole fractions of cadmium vapor and oxygen are assumed to be 0.6667 and 0.3333, respectively. It is assumed that the cadmium droplet is maintained at a constant temperature of 350°C.

Temperature distribution is shown in Fig. 7. Noticeable temperature gradients appear only in the region very close to the cadmium droplet. This also can be seen from the mass fraction distribution of Cd vapor, as given in Fig. 8. It is determined that the average heat transfer coefficient at the droplet surface is 486.38 W/(m^2-K), and the specific heat flux through the droplet surface is 162.86 kW/m^2. Validations of the developed model are under the way.

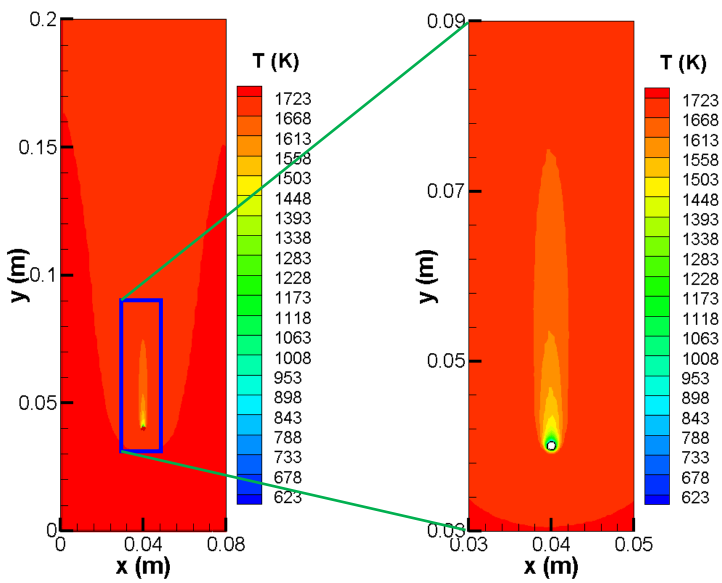


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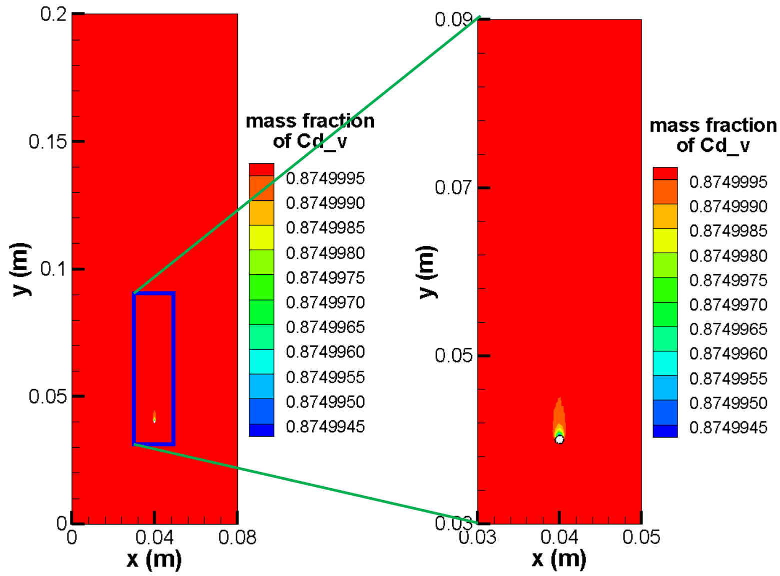
Fig. 7 Temperature distribution



(*a*) (*b*)

Fig. 8 Distribution of mass fraction of Cd vapor

References

L.C. Brown, B. Wong, and B. Buckingham, 2007, "Solar production of hydrogen using a cadmium based thermochemical cycle," In: 2007 AIChE Annual Meeting. Salt Lake City, UT.

A. Steinfeld, P. Kuhn, A. Reller, R. Palumbo, J. Murray, and Y. Tamaura, 1998, "Solar-processed metals as clean energy carriers and water-splitters," International Journal of Hydrogen Energy, 23(9), pp. 767-774.

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