SOLZINC REACTOR MODELING AND EXPERIMENTAL VALIDATION

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A numerical model is formulated for the SOLZINC solar chemical reactor for the production of Zn by carbothermal reduction of ZnO. The model involves solving, by the finite-volume technique, a 1D unsteady-state energy equation that couples heat transfer to the chemical kinetics for a shrinking packed bed exposed to thermal radiation. Validation is accomplished by comparison with experimentally measured temperature profiles and Zn production rates as a function of time, obtained for a 5-kW solar reactor tested at PSI's solar furnace.

1 INTRODUCTION

Solar-made zinc offers the possibility of storing and transporting solar energy. It is a compact solid fuel that finds applications in Zn/air fuel cells and batteries. Zinc can also be reacted with water and form high-purity hydrogen. In either case, the chemical product from these power generation processes is ZnO, which in turn is solar-reduced to Zn. The cyclic process from solar energy to electricity via solar-processed Zn/air fuel cells is being investigated within the European Union's project SOLZINC.

The thermal dissociation of ZnO into its elements requires temperatures above 2200 K, and the product gases need to be either quenched or separated at high temperatures to prevent their recombination. The reduction temperature can be significantly lowered and the recombination avoided by using carbonaceous materials as reducing agents. The carbothermic reduction of ZnO can be represented by

$$ZnO + \lambda C = Zn + (2\lambda - 1)CO + (1 - \lambda)CO_2$$

where λ denotes the stoichiometric molar ratio C/Zn. This reaction proceeds endothermically (ΔH°_{1400K} = 352.5 kJ/mol) at temperatures above 1200 K.

2 REACTOR MODELING

A scheme of the SOLZINC solar chemical reactor is shown in Figure 1. It features two cavities in series, with the first (top) one functioning as the solar absorber and the second (bottom) one as the reaction chamber. A common SiC plate separates them. The first cavity is made of SiC and contains a windowed aperture to let in concentrated solar radiation. The second cavity is a well-insulated cylinder and contains a packed bed of a ZnO/C mixture that is subjected to irradiation emitted by the SiC plate. Reactants are placed in the reaction chamber before the run for batch operation; gaseous products exit continuously via an outlet port located on the lateral wall.

A transient reactor model is formulated that couples radiation and conduction heat transfer with the chemical kinetics. The model domain consists of the packed-bed of ZnO and C, undergoing shrinking due to the chemical reaction. The reaction rate is determined experimentally by thermogravimetry.

The 1D unsteady-state energy conservation equation is given by

$$\rho_{bed} C_p \frac{dT}{dt} = \frac{d}{dx} k_{eff} \frac{dT}{dx} + q'''$$

where q''' is the volumetric heat sink due to the endothermic reaction. The effective thermal conductivity k_{eff} of the packed bed is found by matching numerical calculated and experimentally measured temperatures, using the radial heat flow method. The packed bed is discretized into disk-shaped layers (control volumes), each with a decreasing thickness as the reaction progresses. The fully implicit finite-volume scheme is applied and the resulting system of equations is solved iteratively. Further details are found in [1].

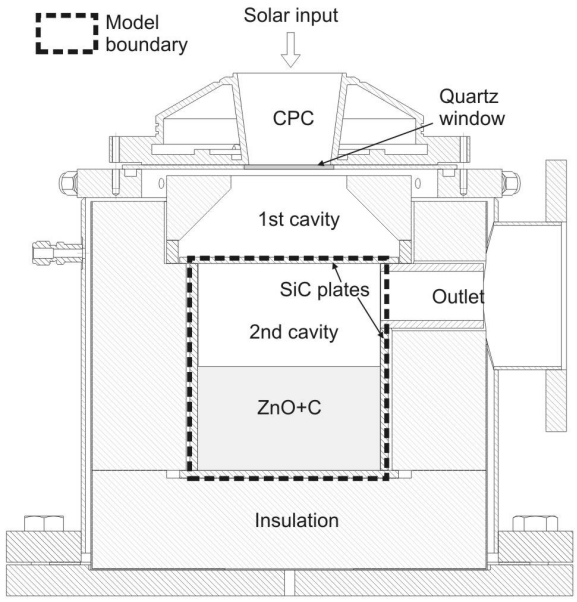

Fig. 1: SOLZINC solar chemical reactor configuration for the carbothermic reduction of ZnO.

3 EXPERIMENTAL VALIDATION

Solar tests over the temperature range 1350-1600 K were performed with a 5-kW reactor prototype at PSI's solar furnace [2]. Details of the fabrication of the reactor prototype, the experimental setup, and experimental results have been described by Osinga et al. [3].

The results produced by the model are compared to a solar experimental run carried out under the experimental conditions of Table 1.

C:ZnO molar ratio	0.8
Initial ZnO+C batch [kg]	0.5
ZnO+C residual [kg]	0.315
Initial bed temperature [K]	300
Solar input power [kW]	6.2
Mean solar flux at aperture [W/m^2]	1868
Reactor's aperture diameter [m]	0.065
Bed height at time=0	0.063

Table 1: Solar experimental conditions.

Figure 2 shows the calculated temperature profiles along the bed as a function of time (every 10 min). Three stages are observed. During the first 40 min, the upper portion of the bed is heated from ambient temperature to above 1000 K, but temperatures are not high enough for the reaction to occur. Afterward, the temperature at the top exceeds 1200 K, and the reaction proceeds at reasonable rates. The right ends of the temperature curves are shifted to the left with time because of the shrinking of the bed. Finally, after 87 min, the shutter is closed, the bed undergoes cooling, and the reaction stops. Also shown in Figure 2 is the temperature measured by a thermocouple submerged in the bed at a height of 30 mm. The agreement between calculated and measured values is within 1.6 ± 1%.

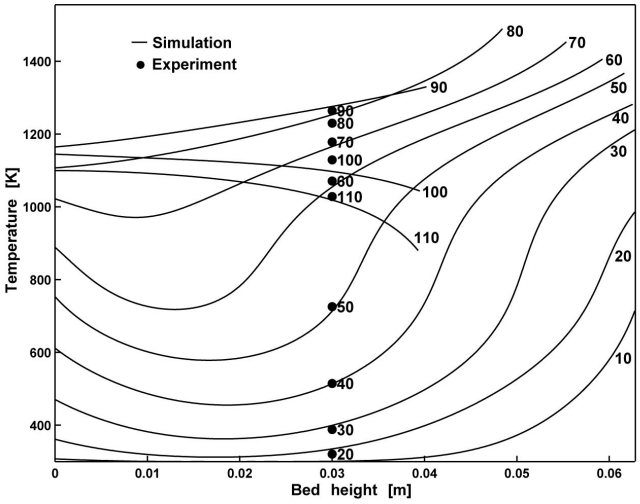

Fig. 2: Calculated temperature profiles along the packed bed determined every 10 min. The points correspond to the measured values.

The calculated (solid curve) and measured (dotted curve) rates of ZnO decomposition are shown in Figure 3. The calculated values are the result of the integration over the bed of the reaction rate for each control volume at each time step. The experimental values are recorded by on-line gas chromatography. The agreement between model and experiment is remarkably good. The validated model is now being used to predict the performance of an up-scaled reactor. Preliminary runs have shown that a large temperature gradient is obtained at the top layer, which is typical of ablation processes where heat transfer through the bed becomes the rate controlling mechanism.

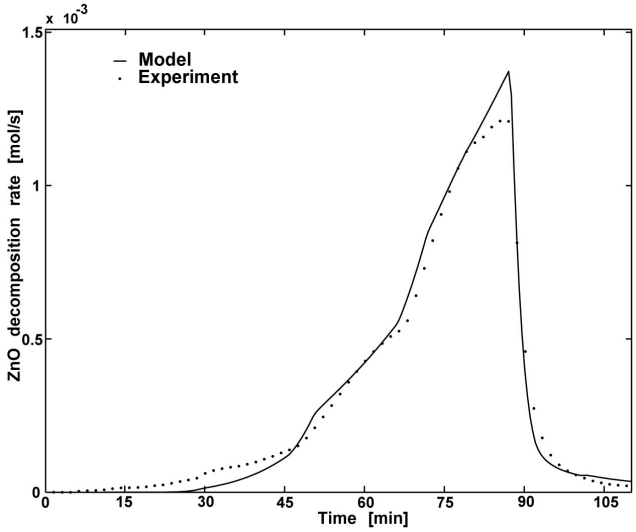

Fig. 3: Calculated and measured reaction rate vs. time.

4 ACKNOWLEDGEMENT

This study was performed within the framework of the EU research project SOLZINC. We gratefully acknowledge the financial support from the BBW - Swiss Federal Office of Education and Science.

5 REFERENCES

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