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Modeling of a Z-IFE Hydrogen Plant Using MELCOR-H2

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A Z-Inertial Fusion Energy (IFE) plant was coupled to a sulfur iodine (SI) thermochemical cycle using a new version of MELCOR called MELCOR-H2. MELCOR-H2 was designed to model nuclear reactors that are coupled to thermochemical plants for the production of electricity and hydrogen [Rodriguez, 2006a].

The Z-IFE input model consisted of three major system components—a fusion heat source, an SI loop, and a Brayton secondary system. The components were coupled in order to investigate system feedback and hydrogen production. The input model was modified so that various parametric studies could be conducted. Particular emphasis was placed on plant operating temperature and hydrogen maximization.

I. Introduction

Many researchers are currently investigating fusion devices, including Idaho National Laboratory (INL) [ANS newsletter, 2003], General Atomics (GA) [Shultz, 2004; GA website], Sandia National Laboratories (SNL) [Olson, 2006; Rodriguez, 2006b]. GA has shown interest in fusion reactors that are coupled with the SI thermochemical cycle for the production of hydrogen [Shultz, 2004]. Shultz cited the potential for massive production of hydrogen from fusion reactors because they generate heat at very high temperature.

II. A. Problem Description

The SI cycle is divided into three distinct sections: the decomposition of sulfuric acid (H_2SO_4), the decomposition of hydriodic acid (aqueous HI), and the Bunsen reaction, where the acids are reconstituted. Sulfuric acid is decomposed into H_2O and SO_3, and then the SO_3 is decomposed into O_2 and SO_2. The decomposition of the acid can occur at relatively low temperature. However, at 700 ºC, the hydrogen generation efficiency is only about 10%. The efficiency increases asymptotically as the temperature is increased. For example, the hydrogen generation efficiency is about 60% at an operating temperature of 1000 ºC.

For this research, a fusion heat source will be coupled to an SI loop and a Brayton secondary cycle (Fig. 1). The impetus for this research is to assess the potential of hydrogen production via fusion reactors.

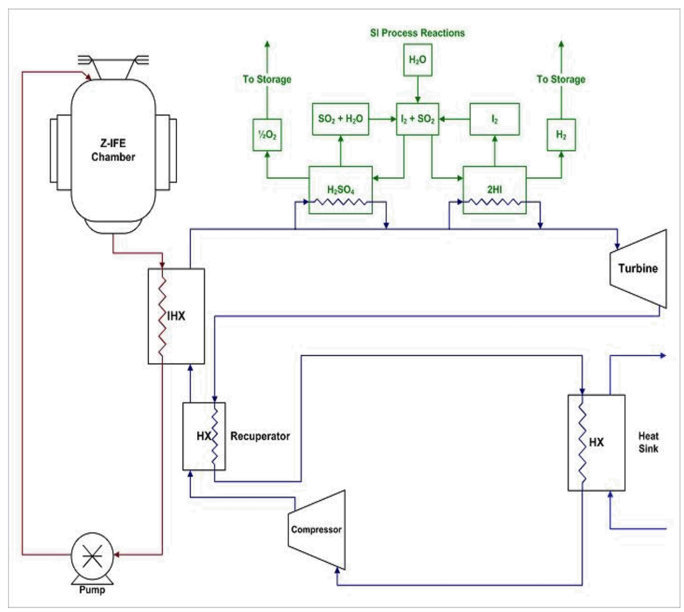

Fig. 1. Z-IFE Chamber Coupled with a Thermochemical Cycle and a Brayton Loop.

II.B. MELCOR-H2 SI Transient Chemistry

The SI chemistry considers the decomposition of sulfuric acid by heating the liquid into gas form, and then dissociating the gaseous sulfuric acid directly into SO_2. Thus, the computation assumes that all SO_3 is immediately converted into SO_2. This assumption is reasonable, given that Huang showed that at temperatures higher than 700 ºC, the decomposition of sulfuric acid

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into SO_3 approaches 100% completion [Huang, 2005]. From the standpoint of increased hydrogen production efficiency, this endothermic reaction should be allowed to proceed at 850 ºC or higher.

The decomposition of HI is computed by considering both the forward and backward rate kinetics. The endothermic reaction occurs at a lower temperature, about 450 ºC.

Finally, the exothermic Bunsen reaction allows the low-temperature (about 120 ºC) reconstitution of the two acids.

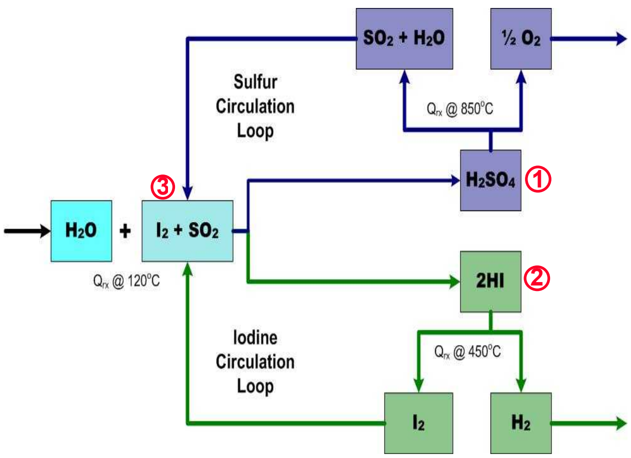

Fig. 2. MELCOR-H2 SI Chemistry.

The transient numerical solution of the chemical reactions is based on solving

1) the rate kinetics ordinary differential equations for the decomposition of the acids (see 1 and 2 in Fig. 2) and the Bunsen reaction (3 in Fig. 2),

2) conservation of energy (including the vaporization of the acids and their eventual dissociation into various gaseous species), and

3) conservation of mass (moles).

As an example, consider the decomposition of sulfuric acid [Revankar, 2006], where

(1.1) $H_2SO_4(g) \rightarrow H_2O(g) + SO_3(g)$

and

(1.2) $SO_3(g) \underset{k_1}{\rightarrow} SO_2(g) + \frac{1}{2}O_2(g)$

As noted previously, it can be assumed that 100% of the SO_3 decomposes to SO_2. Therefore, it follows that the concentrations of sulfuric acid and SO_3 are the same.

The SO_3 reacts as

(1.3) $\dfrac{d[SO_3]}{dt} = -k_1 \cdot [SO_3]$,

where

(1.4) $k_1 = A_1 \cdot e^{-\frac{E_1}{RT_1}}$,

with constants k_1, A_1, E_1, and T_1. T_1 is the reaction temperature, while A_1, E_1 are the Arrhenius constants. We can now solve for the dynamic concentration of sulfuric acid, as follows,

(1.5) $[H_2SO_4]_t = [H_2SO_4]_0 - \Delta[SO_3]$

which is simplified to

(1.6) $[H_2SO_4]_t = [H_2SO_4]_0 - [SO_3]_0 \cdot (1 - e^{-k_1 t})$,

and which finally simplifies to

(1.7) $[H_2SO_4]_t = [H_2SO_4]_0 e^{-k_1 t}$.

The MELCOR-H2 chemistry coding was designed to provide flexibility to the user by allowing certain design parameters (e.g. reaction temperature and reactant inflow rate) to be input by the user. These are like initial and boundary conditions. Thus, the code takes the user input as the starting point, and then it recalculates the appropriate values based on rate kinetics, molar conservation, and energy balances. The calculated value cannot exceed the design value.

II.C. MELCOR-H2 Input Model

The MELCOR-H2 input model of the Z-IFE hydrogen system had three major system components—a fusion heat source, an SI loop, and a Brayton secondary system.

Because the Z-IFE fusion reactor design is ongoing, it was modeled simply as a heat source with a constant mass flow rate. This simplification permits the coupling of the Z-IFE heat source to the secondary side and SI chemistry. Future models will incorporate more sophisticated fusion reactor models. MELCOR has been used previously to analyze fusion reactors [Marshall, 2002].

The SI chemistry consisted of the reduced set of ordinary differential equations representing the three major chemical reactions discussed previously (see Fig. 2).

Finally, the Brayton secondary system was modeled using the new MELCOR-H2 intermediate heat exchanger (IHX), heat exchanger, turbine, and compressor models. The models employ simple thermodynamic equations, but in FY07, we will incorporate more mechanistic thermalhydraulic models that include turbine blade angle, number of stages, chord length, maximum camber, component pressure losses, and so on [El-Genk, 2006].

II.D. Modeling Results and Discussion

Before testing the base Z-IFE model, it was decided to test the MELCOR-H2 SI chemistry models by oscillating the source temperature on the primary side from 500 to 950 K (see Fig. 3). Consequently, the temperature oscillation was expected to result in a similar oscillation in hydrogen production because the rate kinetic equations are in the form Arrhenius expressions, as discussed previously.

Fig. 4 shows the decomposition of sulfuric acid. Note that the quantity of sulfuric acid decomposition peaked when the temperature peaked. The calculation showed that the production of hydrogen followed the temperature excursion, as expected—the production of hydrogen was zero at low temperature and peaked as the primary system temperature peaked. Certainly, during normal plant operation, it would be advantageous to have a steady primary side temperature.

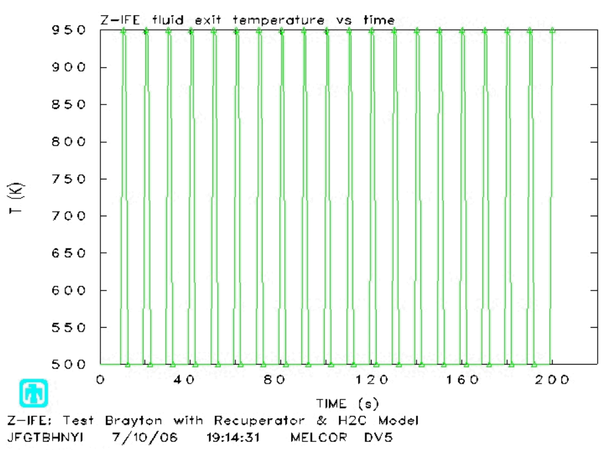

Fig. 3. Test Case with Oscillating Primary System Temperature: Temperature History.

Once the above test calculation was performed, the base case Z-IFE input model was run for 200 transient s in order to achieve a steady state where the power generated by the fusion source was explicitly used to produce hydrogen and to generate energy that is available for electrical conversion.

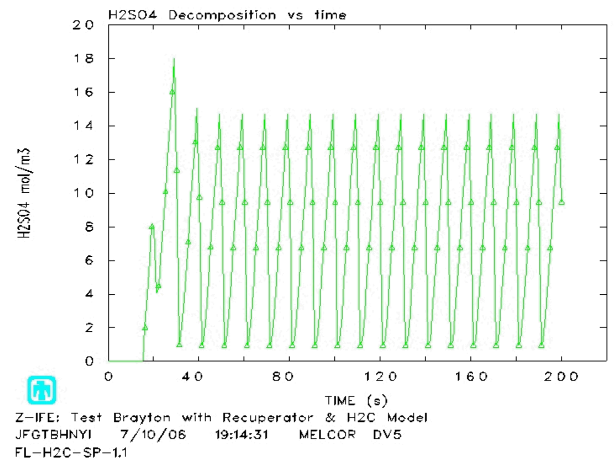

Fig. 4. Test Case with Oscillating Primary System Temperature: Decomposition of Sulfuric Acid.

The base case simulation started at time 0, when heat was being transferred to the secondary side. By user input, the SI chemistry was inactive during the first 30 s. This allowed the system to approach a steady state on the secondary side before activating the chemistry. Certainly, for an actual fusion plant, the SI chemistry will become active at a much later period.

Fig. 5 shows the cumulative production of hydrogen. Hydrogen production was initially zero, until the system was allowed to react the chemicals 30 s into the simulation. Thereafter, the rate of hydrogen production was constant at about 0.6 kg/s. This implies a net hydrogen generation of 18.9 million kilograms per year.

A clear advantage of fusion reactors over fission reactors is that fusion reactors can operate at higher temperatures. As shown by Fig. 6, the higher the operating temperature, the higher the hydrogen production efficiency.

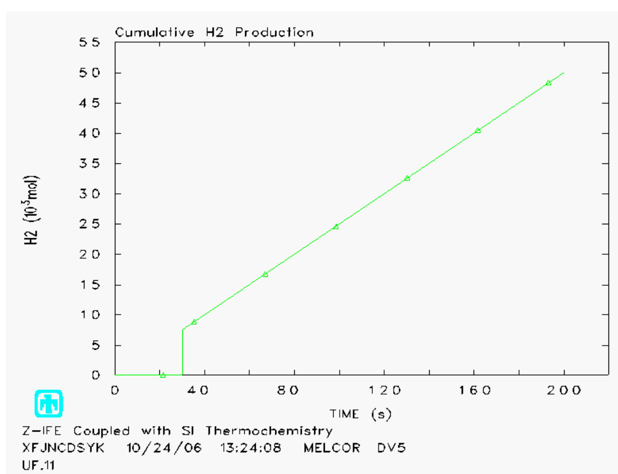

Fig. 5. Cumulative Hydrogen Generation Based on Base Case Calculation.

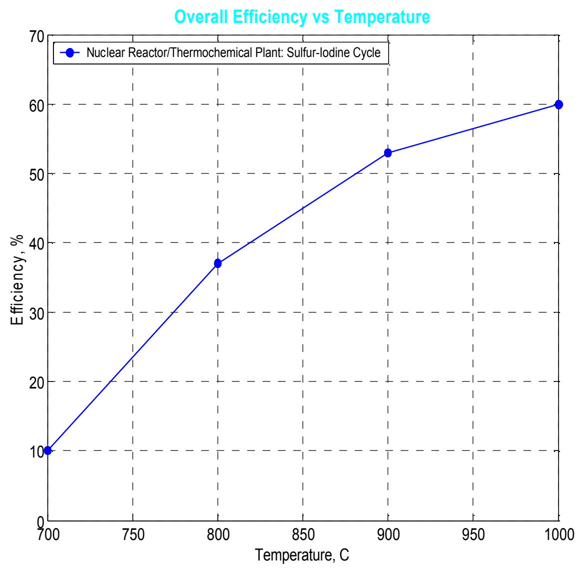

Fig. 6. Projected Hydrogen Production Efficiency as a Function of Temperature.

III. CONCLUSION

Research shows that fusion reactors have much potential for the production of massive amounts of hydrogen because they supply heat at very high temperatures. SNL has developed MELCOR-H2, a transient tool that can be used to simulate fission and fusion reactors that are coupled to thermochemical plants for the production of hydrogen and generation of electricity.

For this research, the authors coupled an SI cycle to a hypothetical Z-IFE fusion reactor. The results show that this hydrogen plant can produce significant amounts of hydrogen. In agreement with the GA studies, the higher the process temperature, the higher the hydrogen production efficiency.

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