Development of Design and Simulation Model and Safety Study of Large-Scale Hydrogen Production Using Nuclear Power

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Abstract

We are conducting research for the design of a large-scale hydrogen production plant, and to demonstrate its economic viability and safe operation. The work includes design of the nuclear and chemical component, and development of computational models for the nuclear reactor and the chemical plant plus the coupling of these models. The simulation model will analyze the three most promising high temperature cycles, namely the sulfur-iodine (SI) cycle, the calcium bromide-iron oxide cycle, and the Westinghouse cycle. The effects of various reaction temperatures on overall efficiency and hydrogen production will be investigated. Additionally, various ranges of flow rates for both the reaction gases and the heat transfer fluid will be combined with heat exchanger parameters to calculate heat transfer coefficients and assist in designing heat exchangers for the processes in the reactions.

The SI-cycle, in particular, has shown high potential for large-scale hydrogen production. In order to provide a large power source for the SI-cycle, a nuclear plant capable of producing steam up to 850 C will be considered. The reactor design study will evaluate high temperature gas-cooled and molten salt reactor designs, and select the optimal design for producing high temperatures in order to maximize hydrogen production on a massive scale. The options in the design include the reactor core design, thermal hydraulics, and safety. Simulation models will be developed for the SI-cycle and for the coupled plant analysis. The latter will be based on the MELCOR code and will be coupled to the simulation model for SI plant performance. MELCOR has a strong, worldwide reputation as a premiere safety analysis tool for nuclear reactors.

This research will result in the first fully integrated, fully coupled code that can be used to simulate the entire nuclear and thermochemical plant, maximize hydrogen production, and evaluate the potential for safe operation under normal and abnormal conditions. It can also be used to address scalability, hydrogen production cost, and design optimization.

Research Objectives

The research and development phase of the project will last approximately two years, followed by one year of application studies and further refinement of the tool. The first step in the research will modify MELCOR so that it can simulate high-temperature gas-cooled reactors. The code will be tested on an input deck designed to model a prototypic high-temperature reactor. Then, the code will be further modified so that it can be fully coupled to thermochemical cycles that generate hydrogen (see Figure 1).

The SI cycle will be modeled first, as it appears to be the most promising thermochemical cycle. Basically, it is based on three chemical reactions, with the net input being water and high temperature heat, and the output being oxygen and hydrogen (see Figure 2); the sulfur and iodine are recirculated. The coupling of a high temperature reactor onto a thermochemical cycle will be achieved by explicitly modeling a Brayton cycle that includes an intermediate, high-temperature heat exchanger. In addition, the coding will include a Monte-Carlo module and a financial module. These will allow the analyst to perform design and parametric calculations, and to estimate the associated cost in dollars per kilogram for hydrogen. The coding will be accessed via a graphical user interface (GUI). The economic impact of the O₂ and supplementary processes (e.g. desalinator) will also be considered. A conceptual description of the modules is found in Figure 3.

Work on the new modules has begun, and the code is expected to be ready for testing on or before May 2006.

There exists a tremendous incentive for the economic production of hydrogen. As shown in Table 1, a small increase in reactor operating temperature will result in significantly more hydrogen production. For example, at 800 °C, 65.3 million kg of H₂ plus 90.4 MW of electricity can be generated per year. The net energetic output equals 88.2 million gallons of gasoline. However, by increasing the system temperature by just 100 °C, the energetic output of an extra 38 million gallons of gasoline can be generated. The new tool will help perform this type of analysis, and many others. A further benefit of hydrogen production via a nuclear reactor is the lack of CO₂ generation.



Figure 1. Coupled nuclear reactor and thermochemical cycle.



Figure 2. SI process reactions.



Figure 3. MELCOR analysis tool for nuclear reactors coupled to thermochemical cycles.

Table 1. Yearly Hydrogen Production and Electrical Output from a 1000 MW_{th} Plant.

Temperature	Mass of H ₂	Plus Additional	Equivalent
(°C)	Generated	Electrical	Energy
	(Millions of	Output	Output from
	Kg)	(MW)	Gasoline
			(gallons)
700	17.8	24.1	23,898,000
800	65.3	90.4	88,200,000
900	93.5	129.6	126,420,000
1,000	105.8	146.9	143,220,000

Figure 4 shows that hydrogen production via thermochemical cycles can be competitive with other technologies. Certainly, multiple technologies and approaches should be considered, and the production of hydrogen from nuclear energy is clearly an invaluable option.



Figure 4. Hydrogen production cost for various technologies.

In summary, the new tool will allow users to computationally analyze the coupling of hydrogen production to nuclear power generation. In addition, it will enable the investigation of hydrogen maximization, scalability, and safety issues. The tool will be designed such that different thermochemical cycles can be compared. It will also allow the analyst to perform parametric calculations of a given plant design, and to estimate the associated cost in dollars per kilogram of hydrogen generated. Finally, the research will allow for the design of a large-scale hydrogen production plant such that hydrogen production is optimized under a safe plant design.

Conclusion

The new version of MELCOR will be used to

- Assess hydrogen production cost in \$/kg for various thermochemical cycles as well as nuclear reactor designs.
- Determine the production of hydrogen as a function of design parameters (e.g. operating temperature, thermochemical cycle, etc).
- Allow the user to investigate the hydrogen-generating potential of a particular reactor by easily switching among various thermochemical cycles.

Investigate hydrogen maximization, cost, scalability, and safety issues.

The economic impact of the O_2 and supplementary processes (e.g. desalinator) will be considered, as preliminary studies indicate that they can contribute to the overall profitability of the system. The code will be ready for testing around May 2006.

*Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under Contract DE-AC04-94AL85000.