MELCOR Extensions for Simulation of Modular Power Cycles and Thermochemical Cycles for the Generation of Hydrogen via Nuclear Reactors

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ABSTRACT
Sandia National Laboratories (SNL) is currently extending MELCOR so that it can be used to simulate high-temperature nuclear reactors with modular secondary-side power components that are coupled to thermochemical cycles such as sulfur iodine (SI), the Westinghouse hybrid sulfur (HyS), and a generalized thermochemical cycle. To this extent, we will begin by extending MELCOR models for high-temperature gas cooled reactors, Brayton power cycles, an SI thermochemical cycle, and a graphical user interface (GUI). In addition, future versions of MELCOR will include a Monte Carlo module for uncertainty and optimization studies, modular components for major power cycles, a financial module, and a generalized thermochemical cycle.

KEYWORDS: MELCOR, SI Cycle, Thermochemical, Hydrogen Production, HTGR

I. INTRODUCTION
SNL continues to develop MELCOR for the U.S. Nuclear Regulatory Commission (USNRC). Over the years, MELCOR has evolved into a flexible, mechanistic modeling tool, with progressively more best-estimate capabilities. MELCOR thermal-hydraulics modeling employs a six-equation set with equations of state for water and noncondensible gases. In addition, MELCOR models core response and degradation, ex-vessel debris/concrete interactions, radionuclide release, aerosol and vapor transport, heat transfer to structures, and engineered safety features. MELCOR has been selected by the USNRC as its tool of choice for conducting integrated severe-accident analyses.

An SI cycle can be combined efficiently with a Brayton cycle, and this will be our starting point. The Brayton cycle will have modular components so that they can be used for modeling other power cycles. The GUI will allow the user to pause a calculation, modify a parameter, and observe its impact on the overall system behavior. The GUI will access a Monte Carlo module for use in optimization and uncertainty studies. Once these extensions have been tested, we will include additional modular power cycle components. This will allow the assembly of a power cycle that is appropriate for a given thermochemical cycle.

For enhanced modularity the new tool will allow analysts to simulate generic thermochemical cycles as specified by user input. There are at least 100 H₂-producing chemical reactions whose input is heat and water, and whose temperature range for the various reactions spans between 25 and 1000
°C [1]. Each thermochemical cycle is most efficient at a given temperature, and therefore is most productive in unison with a particular power cycle. The new tool will allow the analyst to match easily thermochemical cycles with power cycles, and to conduct design/optimization studies for the maximization of hydrogen production at a cost-efficient production rate while demonstrating safety to the public and environment.

II. MODEL DESCRIPTION
The key idea is to develop a modular version of MELCOR that can be used for generalized modeling of fully-integrated systems consisting of a high-temperature nuclear reactor, secondary system, and chemical plant for the production of hydrogen [2, 3]. Other attempts have been made to couple secondary systems with thermochemical cycles, but these have excluded the nuclear reactor and/or were designed solely for certain power cycles and thermochemistry [4, 5].

Figure 1 shows a nuclear reactor that has been coupled to the secondary system and a simplified SI cycle. In essence, the nuclear reactor heat is transferred to the secondary system through an intermediate heat exchanger (IHX). The heat is then transferred from the secondary system to the chemical cycle through a series of heat exchangers, thus allowing the SI chemical reactions to proceed. As shown schematically, the net input is heat and water, with the net products being oxygen and hydrogen. The integral model, as it would be implemented into MELCOR via modules, is shown in Figure 2.
II.A. Nuclear Reactor

MELCOR is uniquely qualified for analysis of the entire production plant system because it is capable of modeling current nuclear reactor designs. In addition, it has added flexibility afforded by its control volume (CV), flow path (FL), and control function (CF) capabilities that allow simulation of complex nuclear systems [6]. Other reactor systems codes were considered for the reference code for the production of hydrogen. SCDAP/RELAP5 may not be as suitable because it is not able to model events outside of the reactor pressure vessel [7]. The MAAP4 code has fixed components, and a new code version is required when geometry changes are made to standard reactor designs [7].

Originally a fast-running, simplified code for plant risk assessment, MELCOR is the successor to the Source Term Code Package [8]. MELCOR retains some features of the earlier code versions that render it especially appropriate for the proposed work. In particular, sensitivity coefficients (SCs), which are user-controlled input parameters, allow the user to vary physics model parameters for sensitivity studies. The ability to implement these changes without necessitating reprogramming of the code itself makes MELCOR an ideal testing code.

For demonstration purposes, we developed a pebble bed modular reactor (PBMR) input deck consisting of 21 vertical COR cells and five radial cell rings (Figure 3) [9]. To model the area underneath the active fuel region, axial levels one through four were not loaded with spheres. The center ring was represented with pure graphite spheres in the pebble-loaded levels. The second ring was defined with equal parts consisting of graphite and fuel-loaded spheres. This ring accounted for the diffusion of the spheres between the fueled and non-fueled regions as they are dropped into the core region and move downward through the core region. The three outer rings corresponded to the active core region. The spheres in these rings were fuel spheres. A token 1 milligram of UO$_2$ was specified in each ring in the lowest active fuel level (Level 5) provided the code with a reference location for distributing axial power.

The CV-FL concept and the CF features render MELCOR suitable for modeling Generation IV reactors because it allows for simulation of reactor volumes of any geometry. Therefore, the helium flow channels and unique core geometries of high-temperature reactors may be represented by CV and FL connections without code modifications. For PBMRs, the spherical fuel pebbles may be
modeled as the particulate debris fuel component, with newly assigned thermal properties in the input. The fuel sphere diameter is conveniently specified as the hydraulic diameter of the particulate debris. In using the particulate debris component to model spheres, an objective is to force MELCOR to use the Ergun Equation for estimating core-pressure drop. Analysis output showing calls to the flow blockage models confirmed that this equation was indeed employed in the calculations and resulted in reasonable pressure drops.

For our test input model, the COR package defined the masses of only the uranium and graphite present in the active fuel region, which produced the desired effect of packed bed flow blockage in the CV Hydrodynamics (CVH) package, but was not a true reflection of the thermodynamic properties of the TRISO fuel in the core. A new material model is being developed to create a more accurate simulation of the core flow area and heat transfer mechanics. It will be implemented in future modifications of the input deck. This enhancement will represent more accurately realistic flow areas and increase heat transfer modeling in the core region.

The COR package required that heat structures be implemented on the boundaries of the reactor core. These heat structures were built similarly to those implemented recently [10]. Each heat structure was a composite built with layers representing the actual composition of the PBMR pressure vessel. The properties used for the materials in the heat structure will be improved in subsequent model revisions.

Figure 4 shows the particulate debris temperatures in Ring 4, Levels 5 through 9. These represent the hottest helium temperatures in the core and illustrate that helium temperatures were rising relevant to the distance traveled through the active core region, as expected.

![Figure 3. MELCOR Model of a PBMR Core.](image)
II.B. Secondary System

In order to model secondary systems, we added new component models into MELCOR such as turbo machine (e.g., turbine or compressor), heat exchanger (flexible design), and process connection point for external models. These components are associated with the FL package. Component flow can occur through a series of FLs, and the model can account for flow reversal under off-normal conditions. Inlet conditions were obtained from upstream volumes in the coding. As of this publication, preliminary versions for turbo machine and heat exchanger models have been coded and tested. The coding included infrastructure and interfaces for input, text, and plot output.

The IHX was coded as part of a new package within the FL package. It couples two FLs and uses the difference in process temperatures to calculate heat transfer. Thus, the inlet conditions are from actual donor volumes, and the heat is transferred between acceptor volumes. The new MCH package was also coded within the FL package. The machine can impose a pressure boost (implying work). In future versions of the model, there can be entropic terms added to flow, such as irreversible work and additional heat transfer.

We tested the new coding by simulating a Brayton Cycle with a hot gas stream at 800 K, while the cold side was at 300 K (see Figure 5). Flow was allowed to ramp from zero to very large flow rates. There was no initial flow in the secondary loop. All secondary fluid was initially at 100.0 kPa and 550 K. Note that this startup transient was intended for test purposes only. The flow was forced by constant pressure drop machine characteristics. As the simulation proceeded, the flows reached steady state values, since they were limited by frictional losses (Figure 6). The flows stabilized eventually about 1 minute later. System pressure is shown in Figure 7. As a result of the flow stabilization, the system temperatures reached steady state, thus defining densities and velocities in frictional terms. During the transient, the initial temperature spiked because there was inadequate heat removal during the first eight seconds. However, the temperatures stabilized soon thereafter (see Figure 8).
Figure 5. MELCOR Brayton Cycle Test Model.

Figure 6. MELCOR Brayton Cycle Test: Volumetric Flow Rate.
Figure 7. MELCOR Brayton Cycle Test: Pressure.

Figure 8. MELCOR Brayton Cycle Test: Temperature.
II.C. Thermochemistry

An SI chemistry model is being implemented into MELCOR for the Sandia Hydrogen Generation Project, and the first version should be completed by April 30, 2006. The model includes the general and basic structures of the hydrogen chemistry package based on a simplified chemistry model [11, 12]. In particular, the model minimizes the chemistry significantly by modeling only the major chemical reactions: generation of sulfuric acid, decomposition of sulfuric acid, and decomposition of hydrogen iodide (see Figure 9). Figure 9 shows that each reaction is assumed to be in a reaction chamber with a uniform reaction temperature on which the reaction rate is based. In each chamber, the inventory of the inflow and outflow of the reactants and products are accounted during the simulation. The cumulative inventory of fresh water coming into the chamber and the output hydrogen and oxygen are also calculated. The reaction and sensible heat required to bring the reactants to the reaction temperature are acquired from the IHX that links the nuclear power plant to the secondary system.

A demonstration calculation will be provided as part of the code development testing. This demonstration will simulate the SI chemistry with three chamber volumes, and will be carried out with a fully integrated system that will include the primary and secondary loops of a nuclear power plant. Figure 10 shows the preliminary MELCOR nodalization for the SI cycle.

![Figure 9. Simplified SI Chemistry.](image-url)
II.D. Graphical User Interface

The graphical user interface (GUI) creates MELCOR input files based on user input, and directly interfaces with MELCOR. It allows the user to start a new simulation, or to resume a previous simulation on a single PC. In addition, the user may change the values of a set of selected variables while MELCOR is paused, then allow the calculation to start again with the new values. Additionally, it can be used to plot variables in real time, even if input is changed by the user during the simulation. The GUI can be used to terminate the simulation, and can provide error diagnostics, if necessary. Figure 10 shows a small subset of the MELCOR GUI capabilities [13].
III. CONCLUSION AND FUTURE PLANS

The first version of the MELCOR tool will be available by May 15, 2006. It will allow the analyst to determine the production of hydrogen as a function of design parameters (e.g. operating temperature, etc). In addition, the user will be able to investigate the hydrogen-generating potential of a particular reactor by switching easily among various thermochemical cycles as they are added into the model. Thus, the tool can be used to investigate hydrogen maximization, scalability, and safety issues.

The first phase of this research has produced the first fully integrated system analysis and design tool whose primary aim is to economically, safely, and reliably replace gasoline with hydrogen generated by nuclear reactors. Since no CO\(_2\) is emitted, the technology is also environmentally benign.

The MELCOR H\(_2\) tool is unique due to its modularity and fully-coupled system integration that can be used to
- simulate the entire nuclear and thermochemical plant,
- maximize hydrogen production,
- estimate hydrogen generation costs,
- design and optimize system configuration,
- address scalability, and
- evaluate the potential for safe operation under normal and abnormal conditions.

In future versions of the tool, we will incorporate a model to assess hydrogen production cost in $/kg for various thermochemical cycles as well as nuclear reactor designs. We will also consider the economic impact of the O\(_2\) and supplementary processes (e.g. desalinator). Finally, future versions of the tool will include additional thermochemical cycles and more advanced secondary-system thermalhydraulic models.
REFERENCES


