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# Proposed Future Collaboration

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NNSA National Nuclear Security Administration

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# Introduction

- Collaboration within Initiatives and Partnerships
- Potential Collaboration Areas
- Simulation Examples
- Summary

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# Collaboration within Initiatives and Partnerships

- We are seeking partners for the Global Nuclear Energy Partnership (GNEP), the New Hydrogen Initiative (NHI), the Generation IV International Forum (GIF), and other new generation reactors.
- The GIF includes two reactors that are particularly suitable for MELCOR-H2 modeling: the gas cooled fast reactor (GFR) and the very high temperature reactor (VHTR).
  - Because of their high operating temperatures (850 and 1000 ºC, respectively), both are suitable for the production of hydrogen.
- The NHI (2003) lays out a foundation for an economy powered by hydrogen, as envisioned by the Department of Energy (DOE). It includes the usage of nuclear reactors for the production of hydrogen.
- GNEP is part of President Bush's and the DOE's Advanced Energy Initiative. It promotes nuclear power on a worldwide basis as economical and free of CO, while emphasizing non-proliferation.

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# Potential Collaboration Areas

- We are interested in partnerships, such as
  - Addition of other thermochemical cycles into MELCOR-H2 (e.g. UT-3, and so on)
  - Joint design and analysis of nuclear/thermochemical hydrogen plants
    - Generation IV reactors
  - Addition of new thermalhydraulic models into MELCOR-H2, including more advanced HTGR and secondary systems models
  - Simulation of experiments
    - direct closed Brayton cycle with series (or parallel) feed.
    - SI chemistry plants
    - Note that experiments and code simulations go hand in hand; one helps to further understand the other—with the ultimate goal of designing the best possible system.

# Potential Collaboration Areas, Cont.

- A fully-coupled nuclear/hydrogen plant can be modeled in steady-state and transient mode.
- MELCOR-H2 could also be used to design a nuclear/hydrogen plant.
  - Feedback from any of the system components to the rest of the system can be tracked. Adverse effects can be mitigated.
  - Which system configuration can generate the most economical hydrogen and electrical output?
    - For example, changes in IHX design will affect hydrogen production and electrical output.
  - Scalability issues
  - Evaluation of the potential for safe operation under normal and abnormal conditions
  - Parametric design calculations

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# Potential Collaboration Areas, Cont.

- For a given system configuration, we can track the total amount of hydrogen production, chemical species inventory, electrical output, plant efficiency, and component feedback. In the future, we will be able to compute hydrogen production cost in $/kg (or ¥/kg).
- As of May 2007, we will be able to model system start-up, and turbine and compressor transients.
- Ultimately, MELCOR-H2 serves to optimize hydrogen and electrical output, while assessing a given plant's safety.

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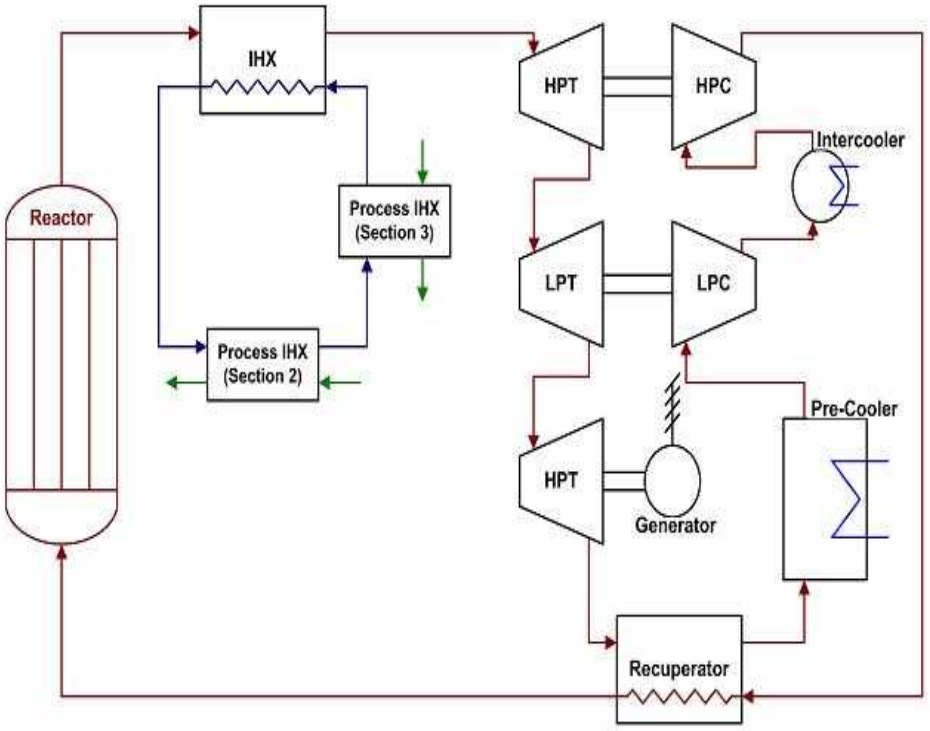
# Simulation Example: Modeling of Closed Brayton Cycle

- As an example, MELCOR-H2 can be used to model a direct closed Brayton cycle with series feed, as shown in the figure.

- If so desired, the analyst can modify the input deck to reflect component changes, such as using a parallel feed instead of a series feed.

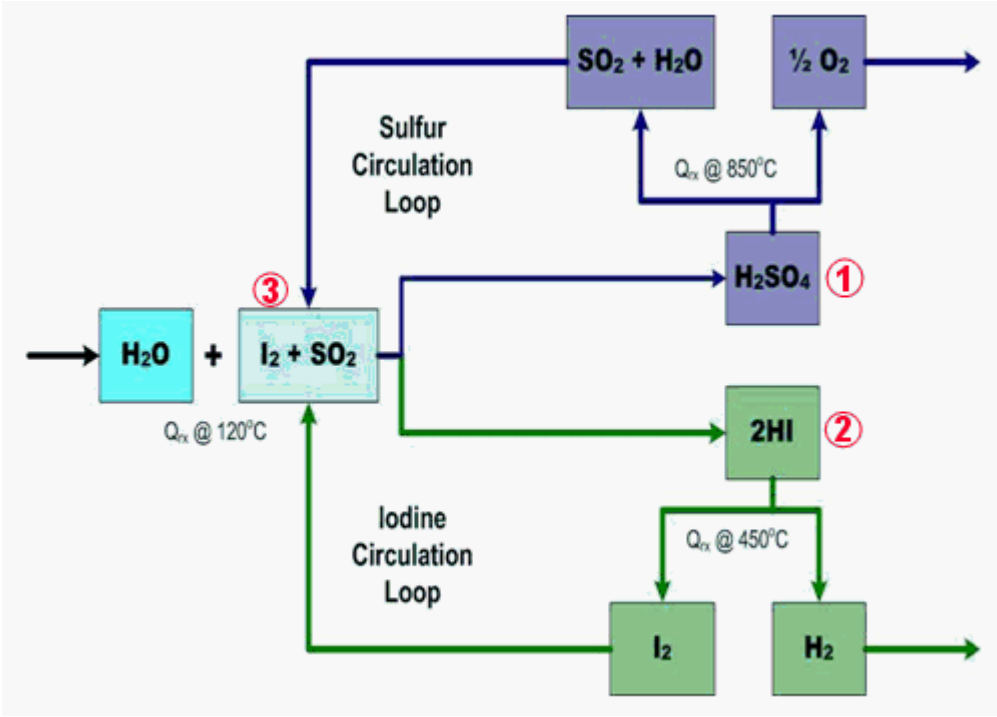



Direct Closed Brayton Cycle with Series Feed.

# Simulation Example: Chemical Imbalance

- Chemical species imbalance can be sought and eliminated. This will control the chemical processes before chemical imbalances can shut or otherwise interfere with the production of hydrogen.

- For example, if sulfuric acid decomposition occurs faster than the Bunsen reaction, H2 production will eventually stop.

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# Summary

- We are seeking partners for GNEP, NHI, GIF, and other new generation reactors.
- There are at least two reactors that are quite suitable for GIF (GFR and VHTR), which due to their high operating temperatures, are great candidates for the production of hydrogen. MELCOR-H2 can be used to design and model these reactors for the production of hydrogen.
- Additionally, collaboration can occur as follows
  - Development of additional MELCOR-H2 models
    - Thermochemical cycles
    - More advanced thermalhydraulic and secondary system models
    - More advanced GIF models
  - Simulation and design of experimental facilities
  - Design and analysis of thermochemical cycles

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# Summary, Cont.

- Analysis of
  - system feedback
  - chemical imbalances
  - integral effects
  - steady state and transient behavior
- Investigation of SI cycle chemistry improvements--Experiments.
- Other thermochemistry cycle experiments.

- **Because MELCOR-H2 is a generalized, modular, fully-coupled, and transient code, it is ideally suitable for the simulation of nuclear/hydrogen systems.**

- **We are open for suggestions, collaboration.**

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