INL/MIS-24-78576-Revision-0

Highlights: Model documentation and validation for chemical conversion processes added to the HYBRID library

December 2023

Changing the World's Energy Future

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Idaho National Laboratory

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Model documentation and validation for chemical conversion processes added to the HYBRID library:

Nuclear-driven chemical conversion pathways

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Report highlights

14 December 2023

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Purpose of the study

Context

- Coal-based electricity generation is declining, leaving behind communities whose economies rely on coal mines, refineries, and power plants.
- To strengthen such economies, projects study the feasibility of converting coal into non-fuel products using nuclear heat and electricity.

Objectives and impact

- Create a comprehensive model of a simulated coal refinery to investigate:
  - Alternative uses for coal other than electricity or fuel production.
  - Technical feasibility of using nuclear-sourced heat and electricity to convert coal to non-fuel products.
  - Most appropriate markets for coal-based products.
  - Capture and conversion of all of the refinery's released CO_2 to products.

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Methodology

- Explore markets and technologies for converting coal to products (completed in FY-22).
- Model the simulated coal refinery.
  - Develop models for coal pyrolysis, syngas cleaning, activated carbon production and methanol production (see next slide).
  - Add models to the HYBRID Library, an open-source repository for process models.
- Assess feasibility of a nuclear-integrated coal-to-methanol process by determining heat, electricity and hydrogen requirements.
- Assess feasibility of converting the refinery's captured CO_2 to formic acid by evaluating nuclear heat and electricity capacity requirements.

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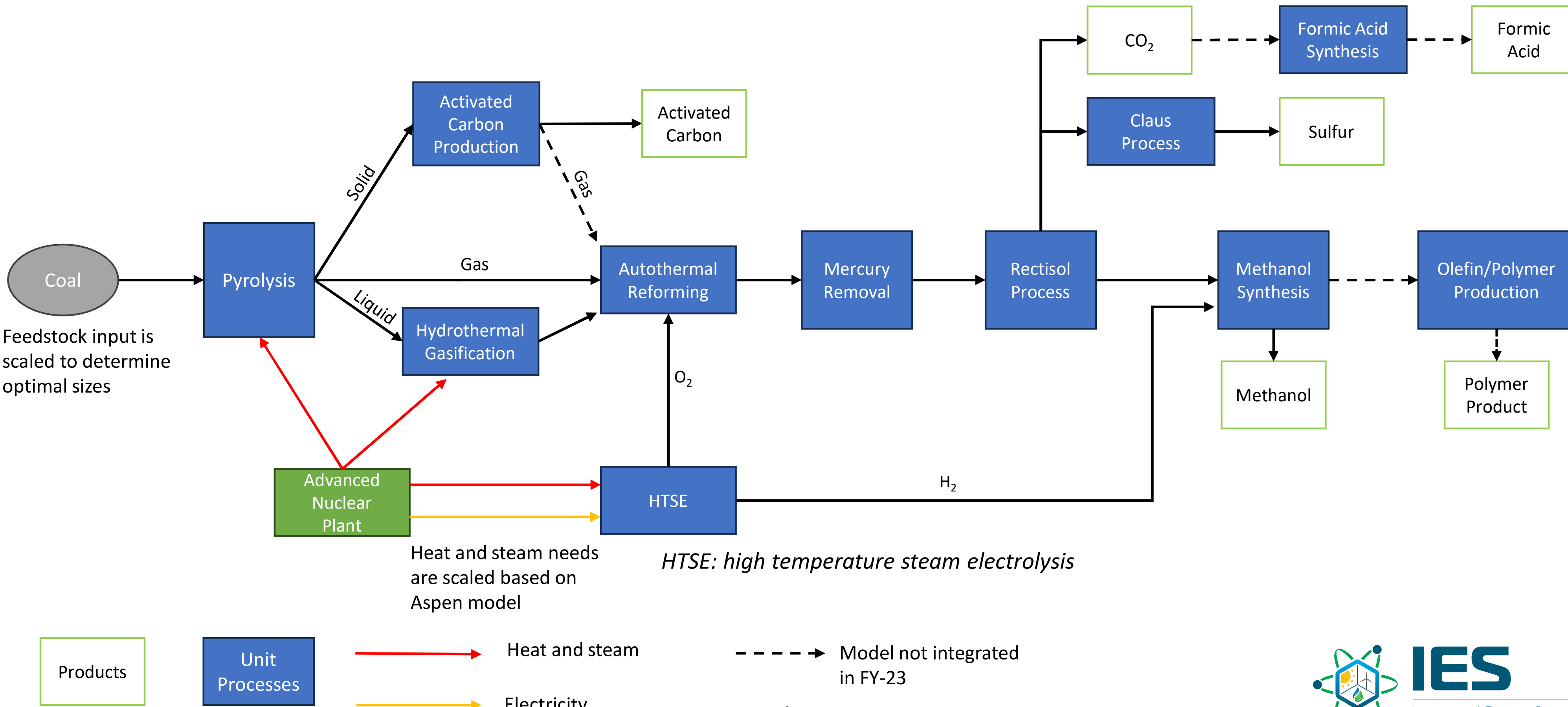
Methodology—“Carbon Refinery” model



Feedstock input is scaled to determine optimal sizes

Heat and steam needs are scaled based on Aspen model

HTSE: high temperature steam electrolysis

Main results and conclusions

- The nuclear capacity requirements (36 MWt and 111.2 MWe) could be supplied by a small modular reactor (SMR).
- 24 tons of hydrogen that is generated through high temperature steam electrolysis (HTSE) replace the water-gas-shift unit traditionally used to adjust the ratio of H_2 to CO in syngas for methanol production.
- The activated carbon production unit is highly exothermic and produces ~63 MW of heat that could be recovered for the pyrolysis process.

Summary of Model Results (mass balance)

Coal-to-Methanol Process

Unit [metric ton/day]	*IN*	*OUT*
Coal	1,000	—
Activated Carbon	—	339
Ash	—	102
CO_2	—	428
Water	7,632	7,546
Oxygen	478	—
Hydrogen	24	—

Unit [metric ton/day]	*IN*	*OUT*
Light Gas	—	532
Methanol	—	398
Sulfur	—	~2
$HgCl_2$	—	Small

CO_2 Utilization Process

Unit [metric ton/day]	*IN*	*OUT*
CO_2	428	85
Hydrogen	31	--
Formic Acid	—	513

Summary of Model Results (energy balance)

	Heat Input From Nuclear (MWt)	Electricity Input From Nuclear (MWe)	Heat Output From Processes (MWth)
Coal Refinery	23	24	83
Hydrogen Production (For Coal Refinery)	6.1	35.3	--
CO_2 Utilization	--	6.3	--
Hydrogen Production (For CO_2 Utilization)	6.9	45.6	--
Total	36	111.2	83

Main results and conclusions

- A nuclear power plant (NPP) could supply heat to this coal refining process.
  - This heat requirement could also potentially be met by recovering heat from activated carbon and methanol production.
- If all CO_2 from the simulated coal refinery (using 1,000 tons per day coal, or 0.09% of the U.S. daily coal consumption) is processed into formic acid, it would generate 25% of the annual global formic acid production.
  - More CO_2 utilization options should be explored, or the coal refinery capacity would be limited by market capacity.
- With the small heat and electricity capacity required from an NPP, the coal refinery option could be sited with a large reactor or SMR built on a retired coal site.
  - This would help coal communities to retain jobs in both utilities and mining.

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Next steps

- Explore heat recovery to lessen the thermal requirements from the NPP.
- Explore more options for CO_2 use or sequestration.
- Increase the methanol production output by including syngas generated from activated carbon production.