Integrated Energy Systems

Case Study: Nuclear-Driven Chemical Conversion Processes

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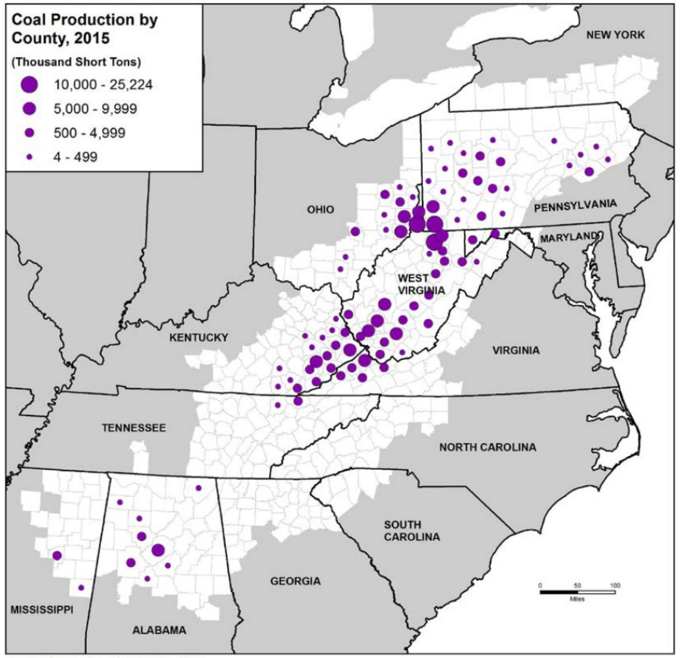
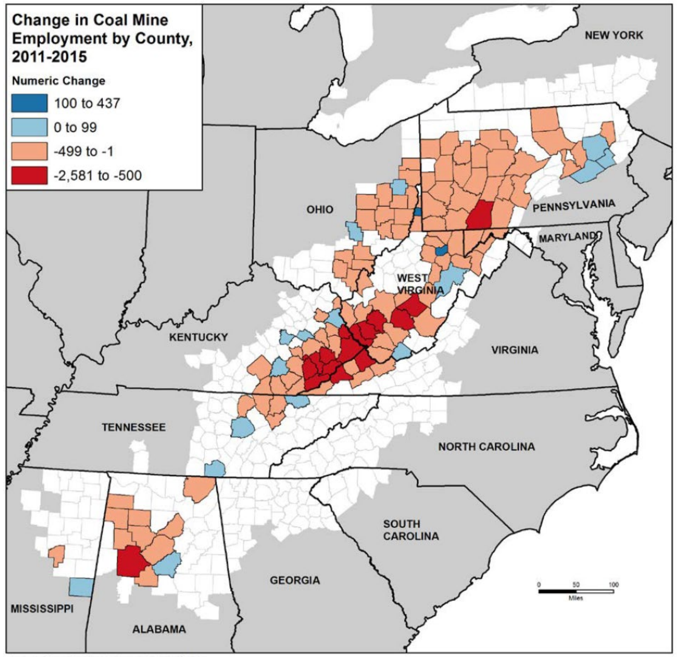
Project Motivation

- Limit the negative impact of decarbonization goals on local economies
- Focus on the coal industry in the Appalachian region of the United States
- From 2004 to 2014, coal production in Appalachia decreased by 45%, compared to 21% nationally



Appalachian Regional Commission, 2016
Data source: U.S. Mine Safety and Health Administration



Appalachian Regional Commission, 2016
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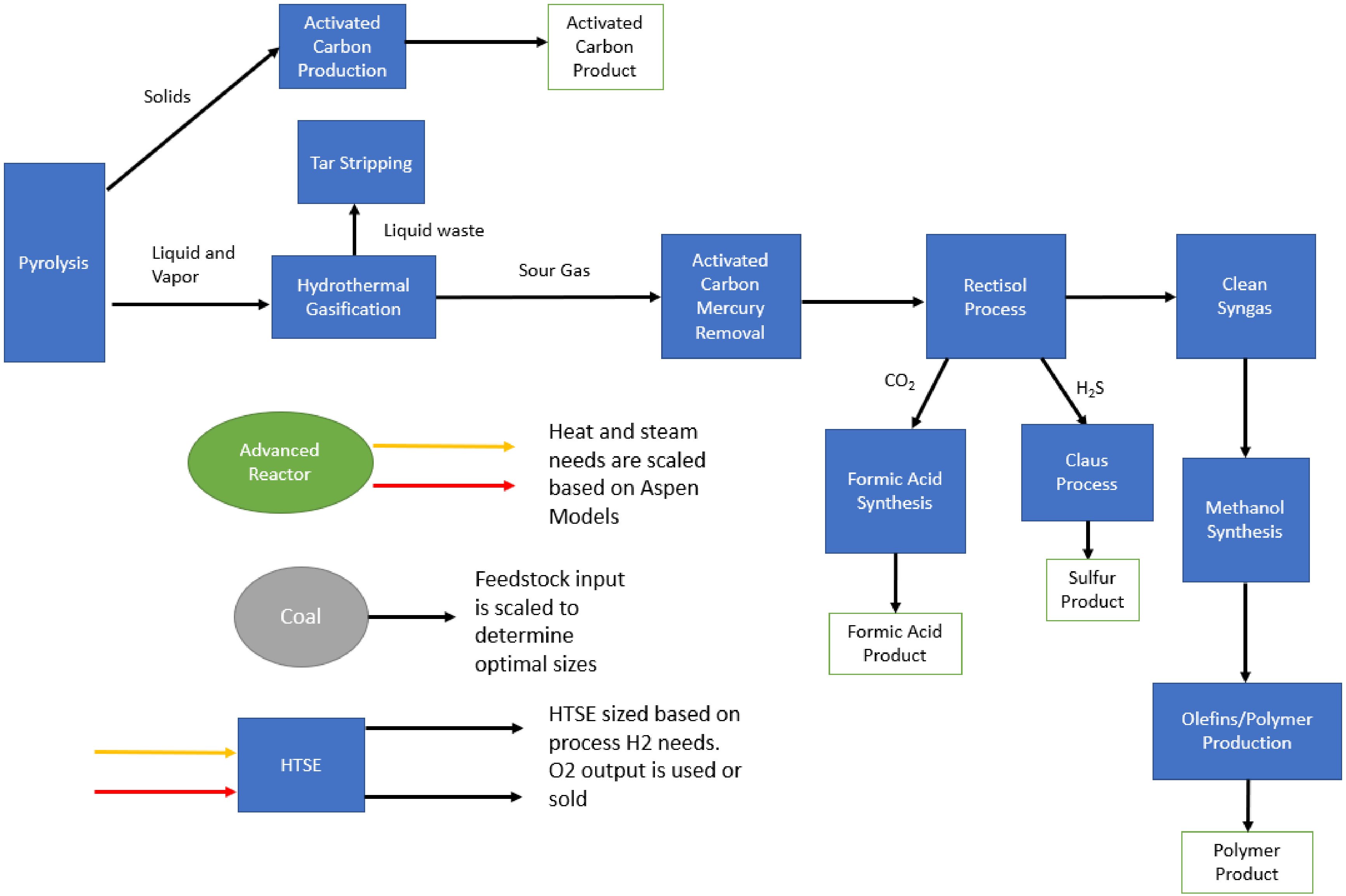
Carbon Conversion Refinery

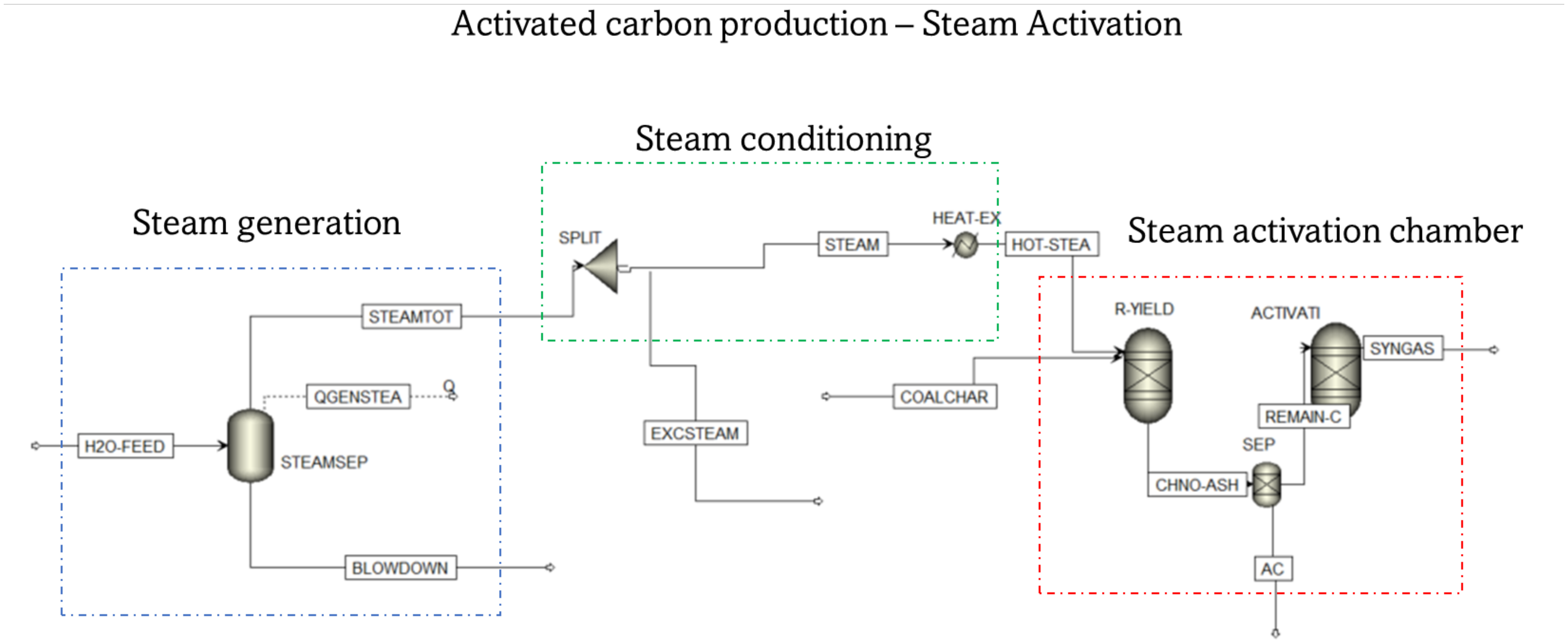
- Convert coal to valuable products via pyrolysis and gasification
- Reduce waste by utilizing products in other parts of the refinery
- Capture CO_2 and convert it to products as opposed to carbon sequestration
- Maximize revenue from various product streams
- Include High-Temperature Steam Electrolysis (HTSE) for hydrogen generation



Aspen Modeling for Hybrid

- Building models for basic chemical processes that can be put in the hybrid library for future use cases
- Models can be verified using data from previous Idaho National Laboratory (INL) Aspen use cases
- Feedstock is Pittsburgh #8 Coal
- Mid-fidelity models are intended to be accurate enough to project a material input/output ratio and cost estimate but generic enough to be used with different feedstocks/use cases.
- See following slides for Aspen process model examples:

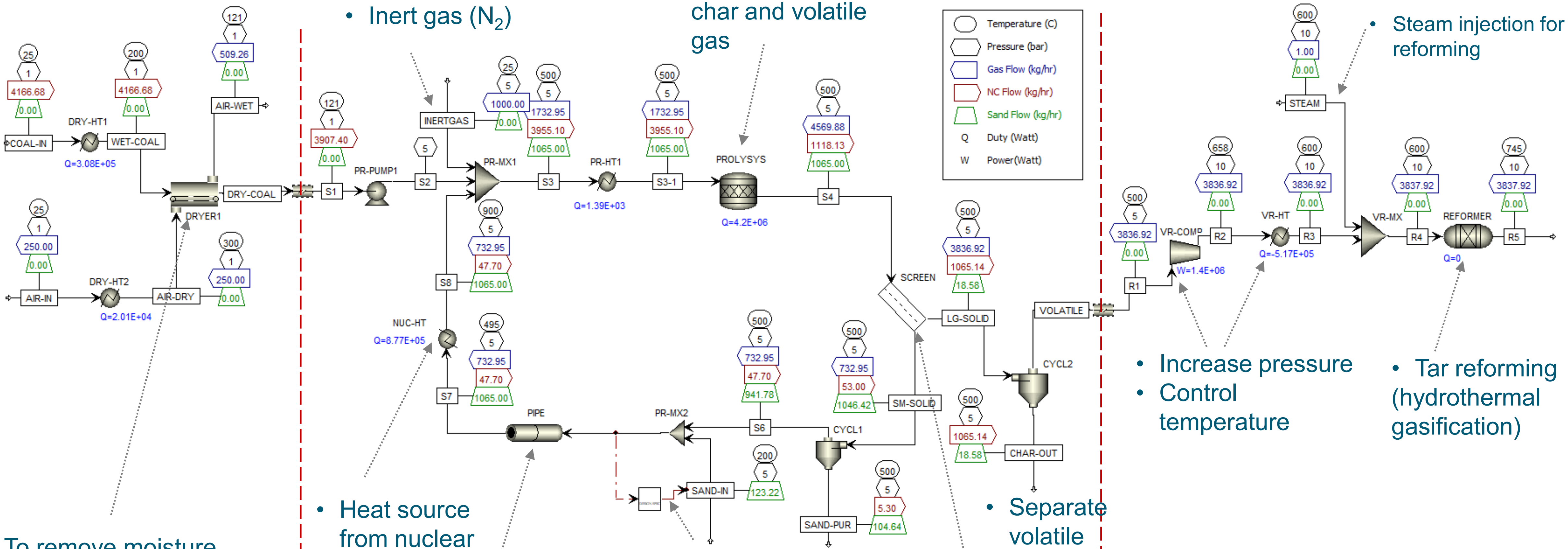
Example: Activated Carbon Production



Coal dryer

Pyrolysis and coal/sand circulation

Gas reforming



- Inert gas (N_2)
- Pyrolysis reactor converting coal to char and volatile gas
- Steam injection for reforming
- To remove moisture inside coal using hot air
- Heat source from nuclear reactor
- Calculate gas velocity required for particles (sand) to flow over
- Sand makeup
- Sand purge
- Separate large solid particle (char) from small particles (sand)
- Separate volatile material from char
- Increase pressure
- Control temperature
- Tar reforming (hydrothermal gasification)

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Aspen HYSYS and APEA

- Models will be converted from Aspen Plus to Aspen HYSYS
- HYSYS models will focus on balance of plant (BOP) and equipment needed to move heat and materials through the system
- Aspen Process Economic Analyzer (APEA) will provide a cost estimate for this equipment and will help determine scaling factors

Process Optimization in HERON

- Detailed process models from Aspen will be simplified into smaller input/output blocks
- Aspen Plus model provides the material input/outputs
- Aspen HYSYS model provides the heat and electricity duties (to size the reactor)
- APEA results will determine capital costs based on each process size
- Reactor costs will be based on estimates from recent literature
- Holistic Energy Resource Optimization Network (HERON) will optimize the system net present value (NPV) by comparing cost benefits of scaling versus product revenue

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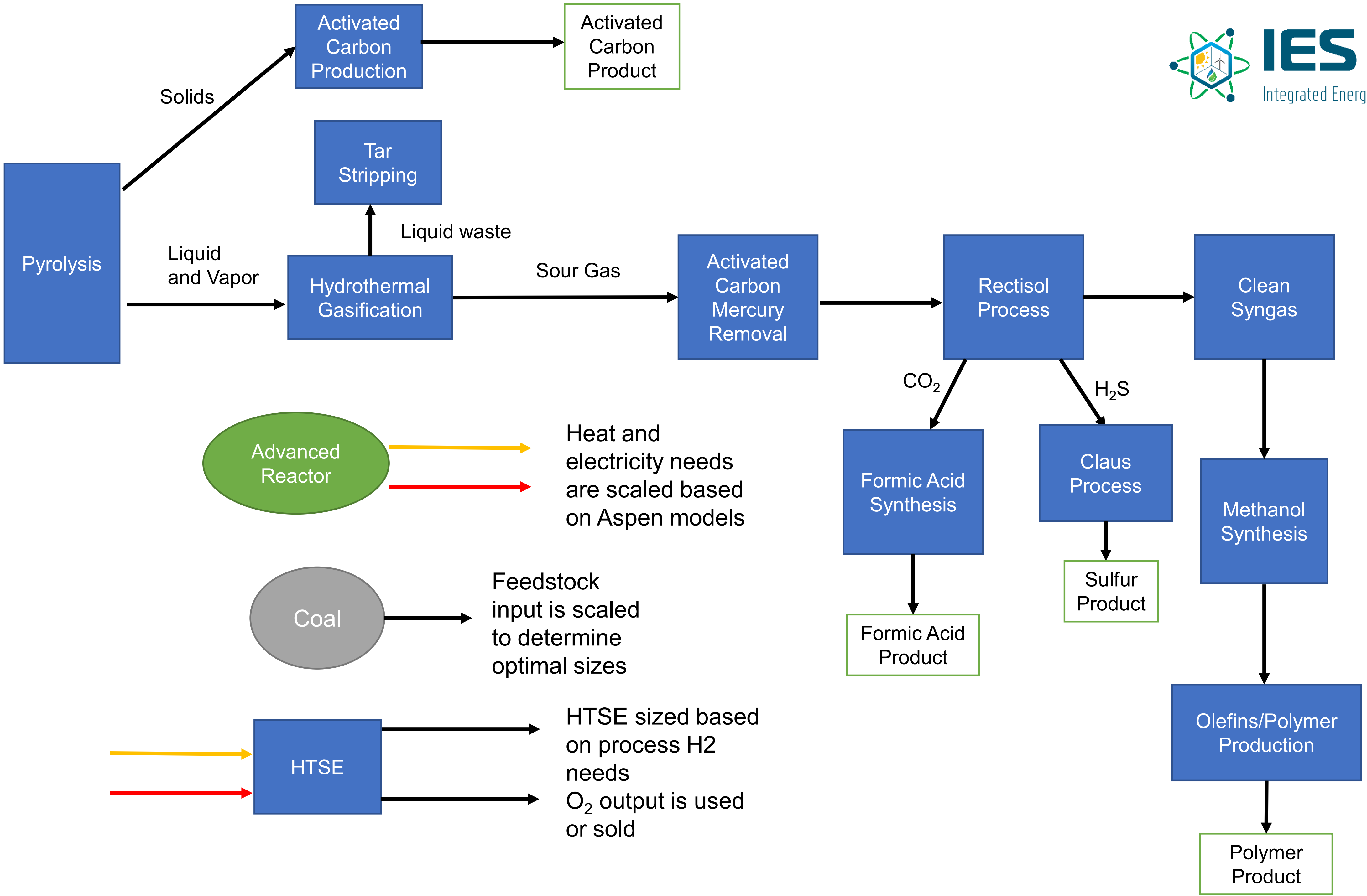
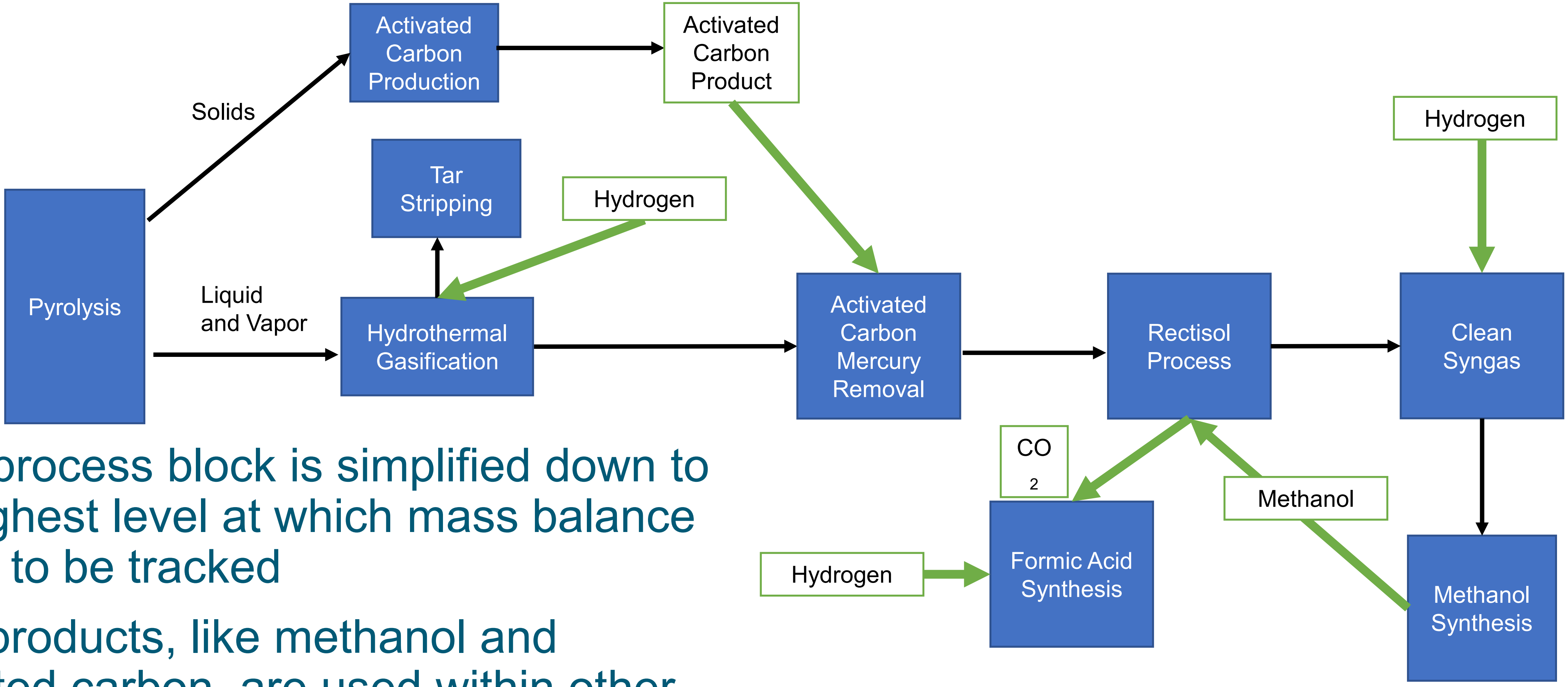

Activated Carbon Production
Activated Carbon Product
Solids
Tar Stripping
Liquid waste
Pyrolysis
Liquid and Vapor
Hydrothermal Gasification
Sour Gas
Activated Carbon Mercury Removal
Rectisol Process
Clean Syngas
CO_2
H_2S
Advanced Reactor
Heat and electricity needs are scaled based on Aspen models
Formic Acid Synthesis
Claus Process
Methanol Synthesis
Coal
Feedstock input is scaled to determine optimal sizes
Sulfur Product
Formic Acid Product
HTSE
HTSE sized based on process H2 needs
O_2 output is used or sold
Olefins/Polymer Production
Polymer Product

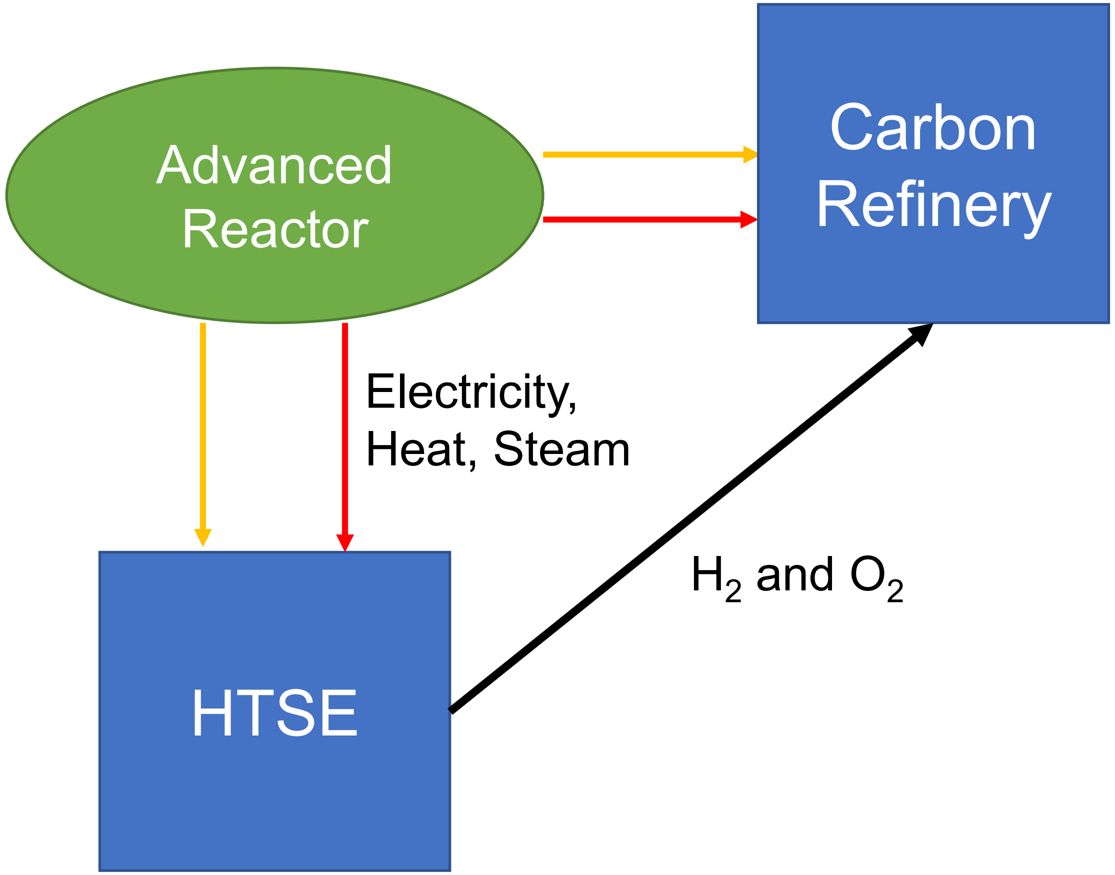
Material Balances



- Each process block is simplified down to the highest level at which mass balance needs to be tracked
- Final products, like methanol and activated carbon, are used within other components therefore scaling will affect the revenue

Heat and Hydrogen Balances

- Heat and electricity duty will be determined at system-level to size the reactor
  - Steam required for chemical reactions could be handled at a system level or as a "feedstock"
- Changes in sub-system duties due to scaling can be tracked in Aspen during the cost estimation process
- The HTSE process is considered its own component based on process models and cost estimates published by INL
  - HTSE is sized so that hydrogen is fully consumed by the carbon refinery
  - Some oxygen will be consumed by the refinery



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HERON Considerations

- HERON component-based models make system calculations more intuitive
- Unrestricted optimization could result in an unreasonable maximization of components
  - Product output will be limited by the estimated market potential (locally or nationally)
  - Add costs associated with tar disposal or unutilized carbon
- Parametric optimization studies to change material I/O based on operating conditions could be possible in the future
- Different reactor designs (light-water reactor vs. high-temperature gas-cooled reactor) could change optimization results

Figures of Merit

- Demonstrate the market viability of converting carbon sources to non-fuel products
  - $FOM = NPV_{refinery}$
- Validate integration of "self-sustaining" principles to utilize process byproducts in other areas of the plant
  - $FOM = (Revenue\ of\ AC\ Sold - Cost\ of\ AC\ Production) - Cost\ to\ purchase\ AC$ used
- Determine the economic benefits of scaling nuclear-driven hydrogen electrolysis between many processes
  - $FOM = NPV_{with\ CO2\ utilization} - NPV_{with\ CO2\ sequestration}$
- Perform a cost comparison of using LWRs and HTGRs for high-temperature processes
  - $FOM = NPV_{LWR} - NPV_{HTGR}$

Goals for Final Report

- Optimize the chemical process for coal conversion based on market needs
  - Validate integration of "closed loop" principles to utilize products within other areas of the process
  - Increase benefits of nuclear-driven hydrogen electrolysis by cost sharing between many processes
- Use NPV and cost of carbon avoided to evaluate cases
- Compare methanol production from carbon refinery to incumbent method of steam methane reforming
- Provide detailed market analysis of coal- and CO_2-related products

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Questions?

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