Gasification of Blended Feedstocks with Carbon Capture and Sequestration to Achieve Low Carbon Intensity Hydrogen

Presented at the 2024 FECM/NETL Spring R&D Project Review Meeting, Pittsburgh, PA on April 24, 2024

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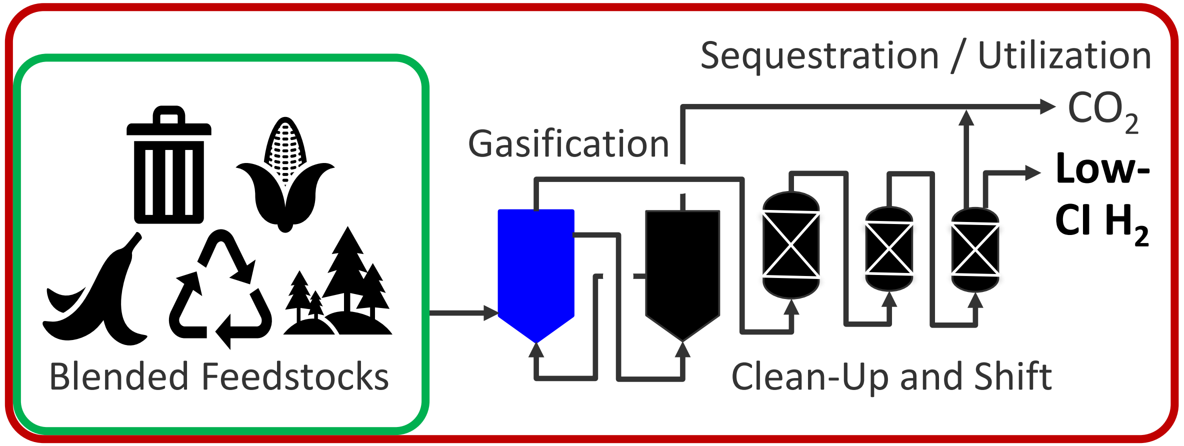
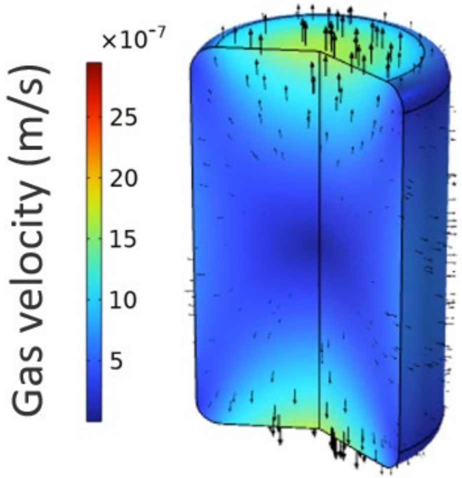
Low-CI H_2 via Gasification of Blended Feedstocks

Year-1 Project Scope (Mike Talmadge-PI)



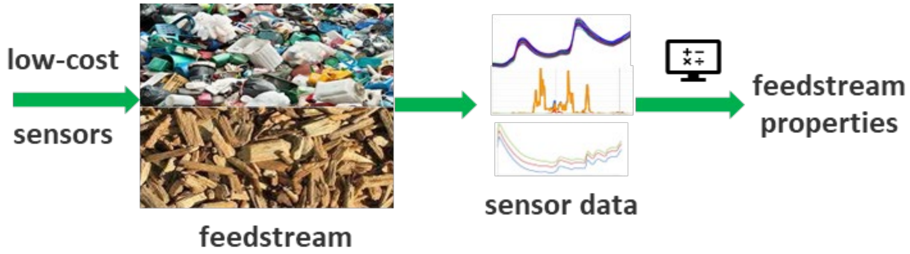
Meso- & Particle-Scale Modelling (Peter Ciesielski)

Detailed particle models will be applied to capture feedstock-specific behavior and intra-particle heat and mass transfer. Results will be applied to reactor-scale simulations to enable scale-up analysis , deployment, and optimization.



Real-Time Feedstock Characterization (Ed Wolfrum)

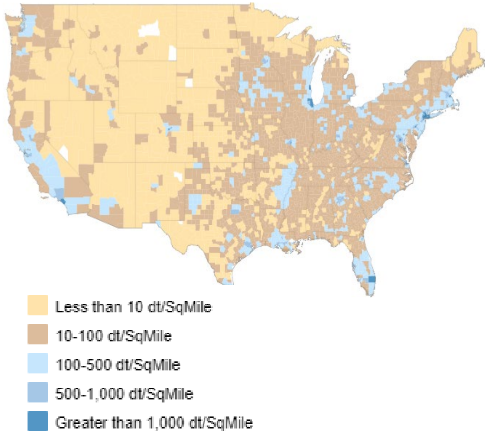
Develop report on SOT and R&D needs for real-time material attribute measurement tools based on imaging and non-imaging spectroscopy. Verify the hypothesis that a low-cost system design is feasible and identify partners for next steps.



Resource & Pathway Analysis (Gary Grim/Anelia Milbrandt)

Quantify and map domestic resources and identify co-location opportunities with existing infrastructure.

Apply pathway models to explore impact of scale, technology, and feedstocks on overall economic and sustainably metrics.



2016 Billion Ton Update Waste Resource Map

Real-Time Feedstock Characterization

Real-Time Feedstock Characterization

Real-Time Feedstock Characterization Allows Feed-Forward Gasifier Control

Mixed biomass and MSW feedstocks have heterogeneous chemical attributes that can make real-time, feed-forward control of gasifiers extremely challenging.

Key Hypothesis

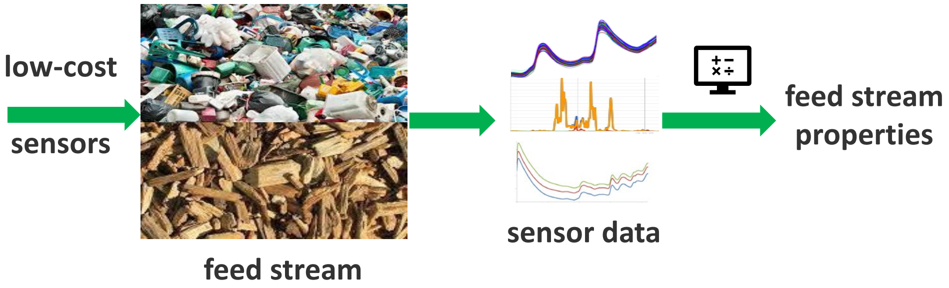
- **Minimal set** of attribute data needed to characterize biomass and MSW streams
  - Biomass/MSW fractions
  - Bulk moisture content
  - Bulk inorganic content & speciation
  - Material size & morphology
- Combination of **low-cost sensors** for data collection
  - Predict attributes of mixed feed stream
  - HHV, fixed/volatile carbon

Work Plan

- Survey current technologies for real-time material attribute measurement tools based on imaging and non-imaging spectroscopy.
- Test the key hypothesis that a low-cost system is feasible and identify specific areas that require technology development.

Deliverables

- A State-of-Technology (SOT) report defining:
  - Identify minimal set of sensors required.
  - Define detailed work plan including a schematic sensor design, proposed experimental plan, computational work.



Key Sensing Modalities In Commercial On-line Sensing

- Machine Vision (e.g., cameras)
- Vibrational Spectroscopy
  - Near-infrared (NIR, 1D), and Hyperspectral Imaging (HSI, 2D)
- Elemental Spectroscopy
  - Laser-induced breakdown spectroscopy (LIBS)

Commercial Systems and Recent DOE Investments

- Large number of systems for real-time sensing/sortation in waste management industry – over 80 different commercial systems from multiple vendors.
- BETO & FECM have made recent investments in real-time characterization of MSW and MSW/biomass/fossil mixtures (e.g., NCSU, Lehigh, ERCO, INL/GTI).

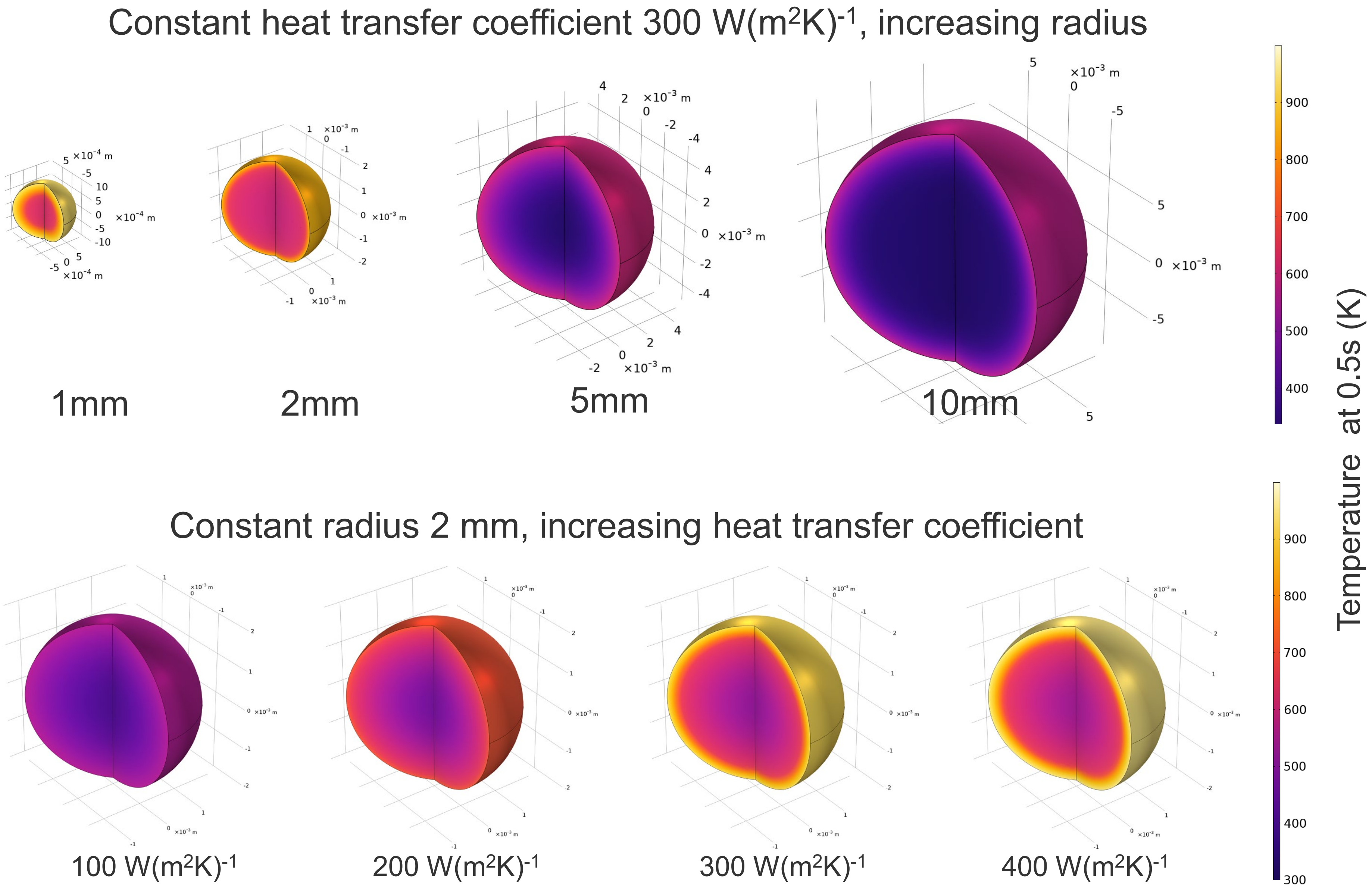
Key Takeaways

- Sensing & sortation **technologies will get better and cheaper** in the future, and the application of MSW systems to biomass/MSW/fossil waste is unlikely to be a major technology hurdle.
- Considerable investments continue to be made in **machine learning** and artificial intelligence associated with on-line sensing. Associated intellectual property (IP) and data sets are not published.
- NREL and NETL researchers will collaborate on generating well-curated datasets using multiple sensing modalities of well-characterized mixtures of biomass/MSW/fossil waste. **Publish data sets** on NETL's Energy Data Exchange (EDX) https://edx.netl.doe.gov/

Meso- and Particle-Scale Modelling

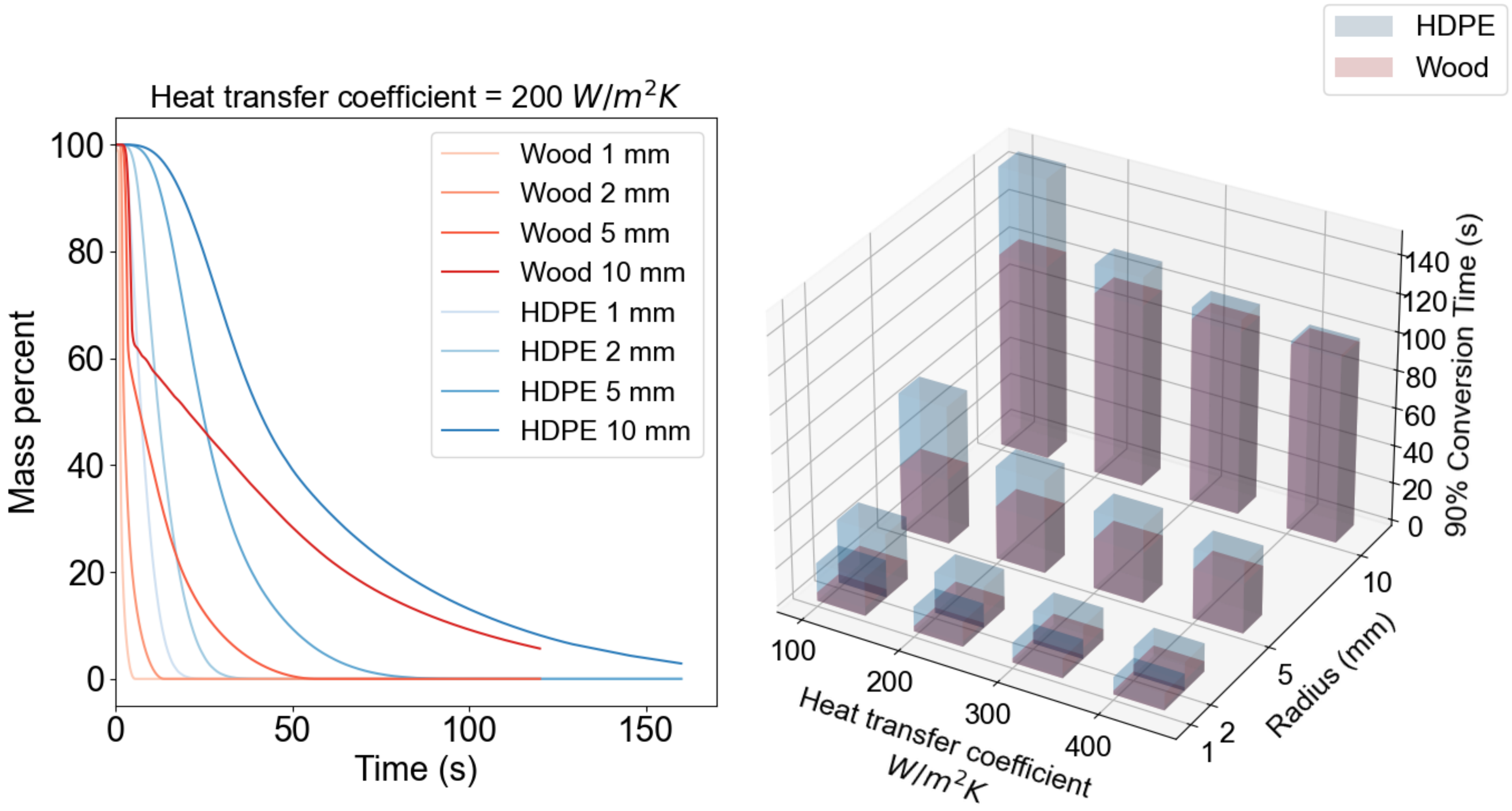
Snapshots of Parametric Sweep Simulations

- Finite Element Simulations developed in Comsol.
- Parameterized based on particle size, shape, composition, and physical properties (e.g, density, thermal conductivity, porosity, etc.).
- Internal heat and mass transport are coupled to conversion kinetics.
- Spherical models are shown but arbitrary shapes may also be simulated.
- Effective heating and conversion rates vary substantially as a function of feedstock particle characteristics.



Predicted Conversion with Varying Particle Properties

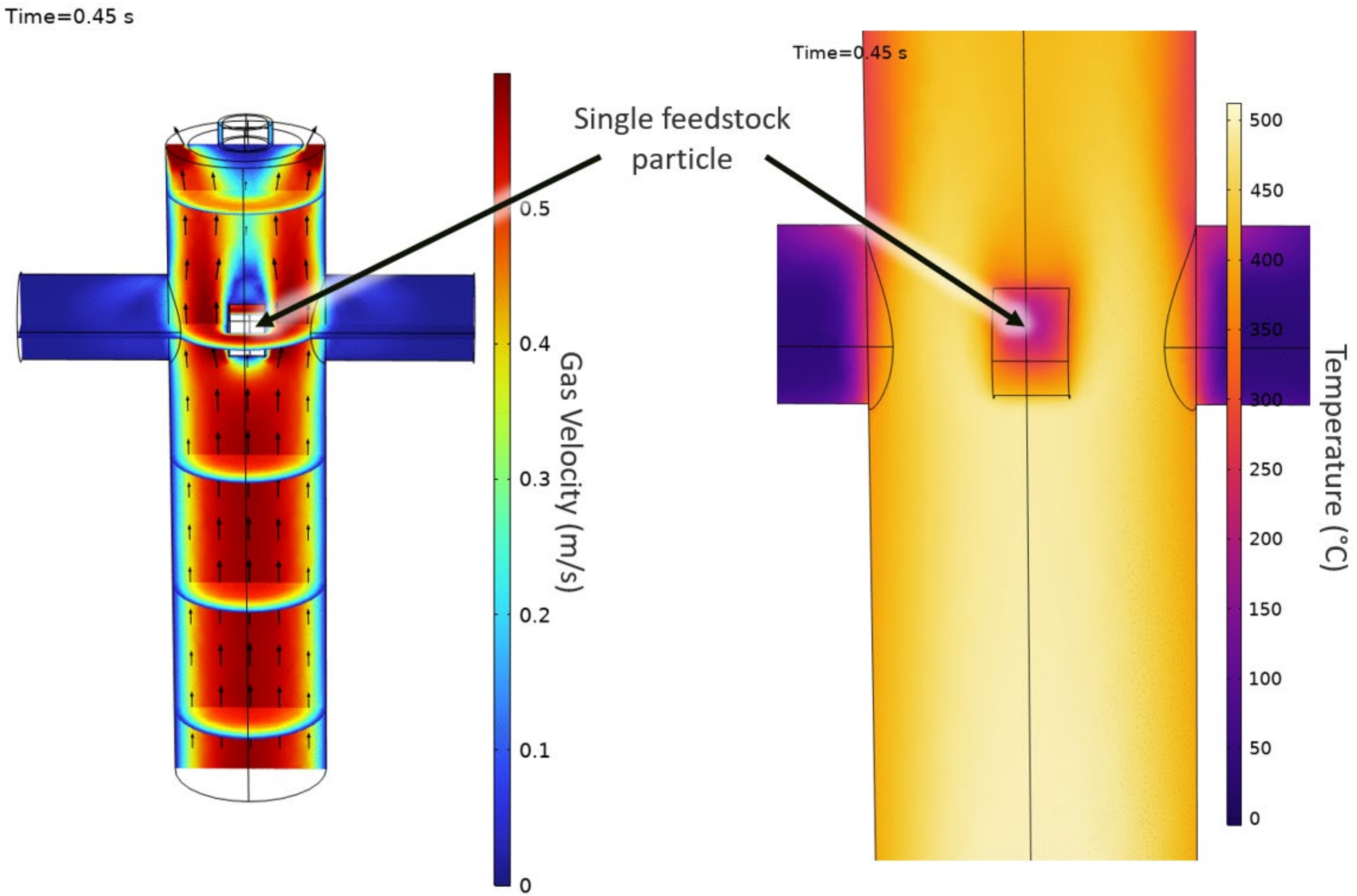
- Predicted conversion times for varying particle composition, size, and heat transfer coefficient.
- Particles consisting of wood and HDPE were simulated.
- Mixed composition (e.g., pelletized MSW) can also be modeled.
- Conversion times, product distributions, and heat and mass flux were computed from each simulation.
- Complete summary of these results will be included in quarterly report.



- Results will be analyzed with ML methods to obtain sub-grid models provided to the MFIX team to capture feedstock effects at the reactor scale.

Next Steps: Model Validation and Improved Kinetics

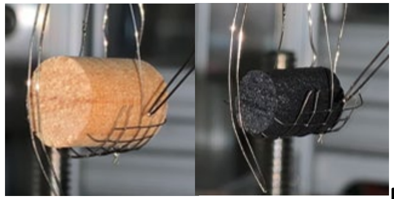
- Kinetic models for specific plastic species developed by NETL will be implemented.
- Particle models will be validated by experiments using NREL's Single Particle Reactor.
- This will leverage models previously developed for the Single Particle Reactor.
- This will enable robust validation for particles of varying size, shape, and composition.

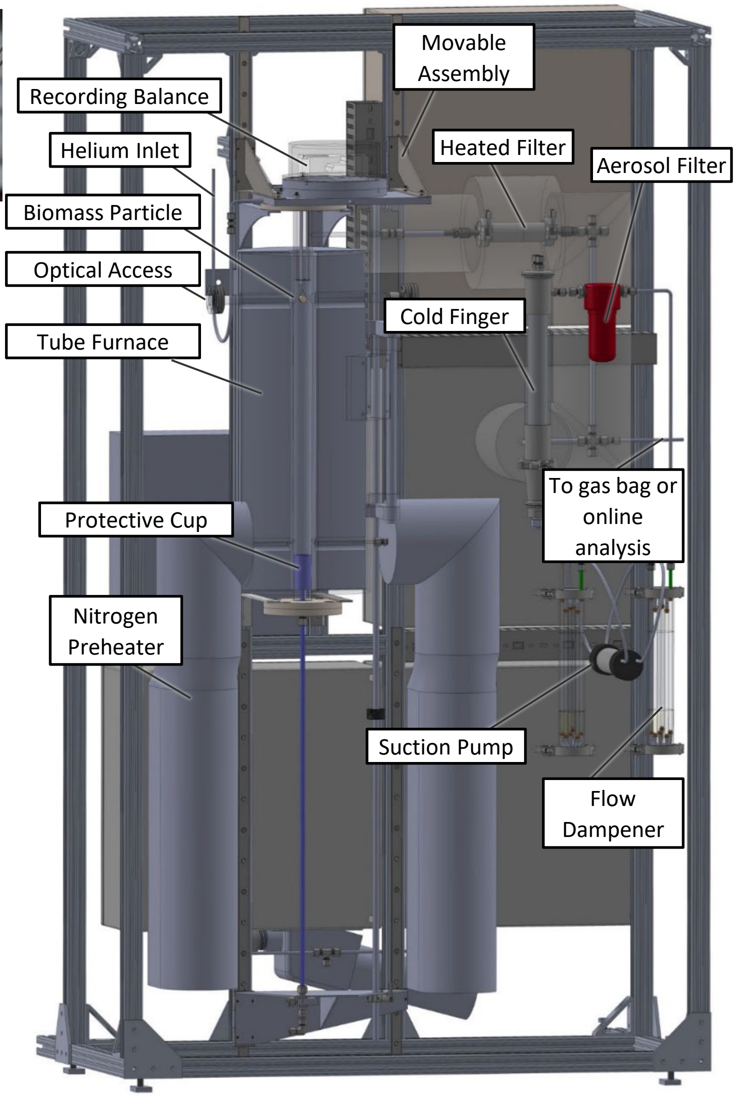


- Simulations of NREL's Single Particle Reactor are shown. Reactor previously developed for pyrolysis experiments and will be modified to simulate gasification for validation of intra-particle heat and mass transport.

Single Particle Reactor:
Filling Gaps in Experimental Space and Enabling Model Parameterization

Custom thermogravimetric analyzer (TGA) with high heating rate and gas flows for high throughput generation of single particle reactor data to enable model development.





Description:

Single particle reactor enables the study of pyrolysis (and gasification) on single particle with mass up to 2 g, temperatures up to 800˚C, heating rates of 50˚C/s, and mass loss resolution of 1 mg with analysis of evolved vapors.

Value Added:

Enables experimental validations of single particle models which inform industry on effects of particle size, shape, and particle size-distributions on reaction kinetics. Capable of increased throughput of roughly 10x from current systems (furnace remains heated between samples), enabling iterative collaboration between modelers and experimentalists.

Industry Impact:

Feedstock providers and industry partners benefit from Improved modeling of changes in material attributes and operating conditions. Goal to increase confidence and decrease timelines for scale-up. Provides unique visual component, allowing direct observation of particle cracking, pellet explosion, and change in radius with temperature.

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Resource and Facility Siting Analysis

Resource and Facility Siting Analysis

Objective: Apply geospatial methods to integrate resource data and visualize promising regions for low-carbon hydrogen production from waste feedstocks.

Technical Approach:

- Define analysis criteria
  - Resource Availability
  - Infrastructure Considerations
  - Market Favorability
- Conduct individual analyses
- Conduct an integrated analysis
- Incorporate techno-economic analysis (TEA) for next phase of siting analysis.

Source: ESRI

Waste Resources

- Siting production facilities close to feedstock:
  - Minimizes costs and carbon intensity impact from resource transportation.
- Waste resource categories:
  - Ag harvesting residues (corn, wheat, sorghum, oats, and barley).
  - Forest residues (primary mill and logging residues).
  - MSW-derived feedstocks (paper-rich and plastic portions).
  - Future supply (energy crops, ag and forest projections from the Billion Ton Study).

Figures on resource maps have been removed from the presentation as the analysis results are not yet published. Publication is targeted for end of fiscal year 2024.

Infrastructure Considerations

- Existing infrastructure:
  - Transmission infrastructure (H_2 and CO_2 pipelines)
  - Sites with co-location opportunities (pellet mills, sawmills, pulp/paper mills, and landfills)
- Proximity to carbon storage sites:
  - Oil and gas reservoirs
  - Unmined coal seams
  - Deep saline reservoirs
- Utilizing existing infrastructure can reduce capital investments.
- Proximity to carbon storage simplifies logistics and costs of sequestration.

Figures on resource maps have been removed from the presentation as the analysis results are not yet published. Publication is targeted for end of fiscal year 2024.

Market Favorability

- Industrial facilities associated with hydrogen consumption
  - Current H_2 Consumers:
    - Petroleum refineries
    - Ammonia plants
    - Methanol production plants
  - Potential H_2 Consumers:
    - Steel plants
    - Natural gas plants
    - Electronics manufacturing
    - Cement plants
- Industry is projected to drive most of the clean H2 demand until 2030.
- Per McKinsey & Company (2024), mobility in maritime, aviation, and trucking could drive industry by 2050.
- Mobility sites include ports, airports, truck stops, bus stops.

Figures on resource maps have been removed from the presentation as the analysis results are not yet published. Publication is targeted for end of fiscal year 2024.

Integrated Siting Analysis

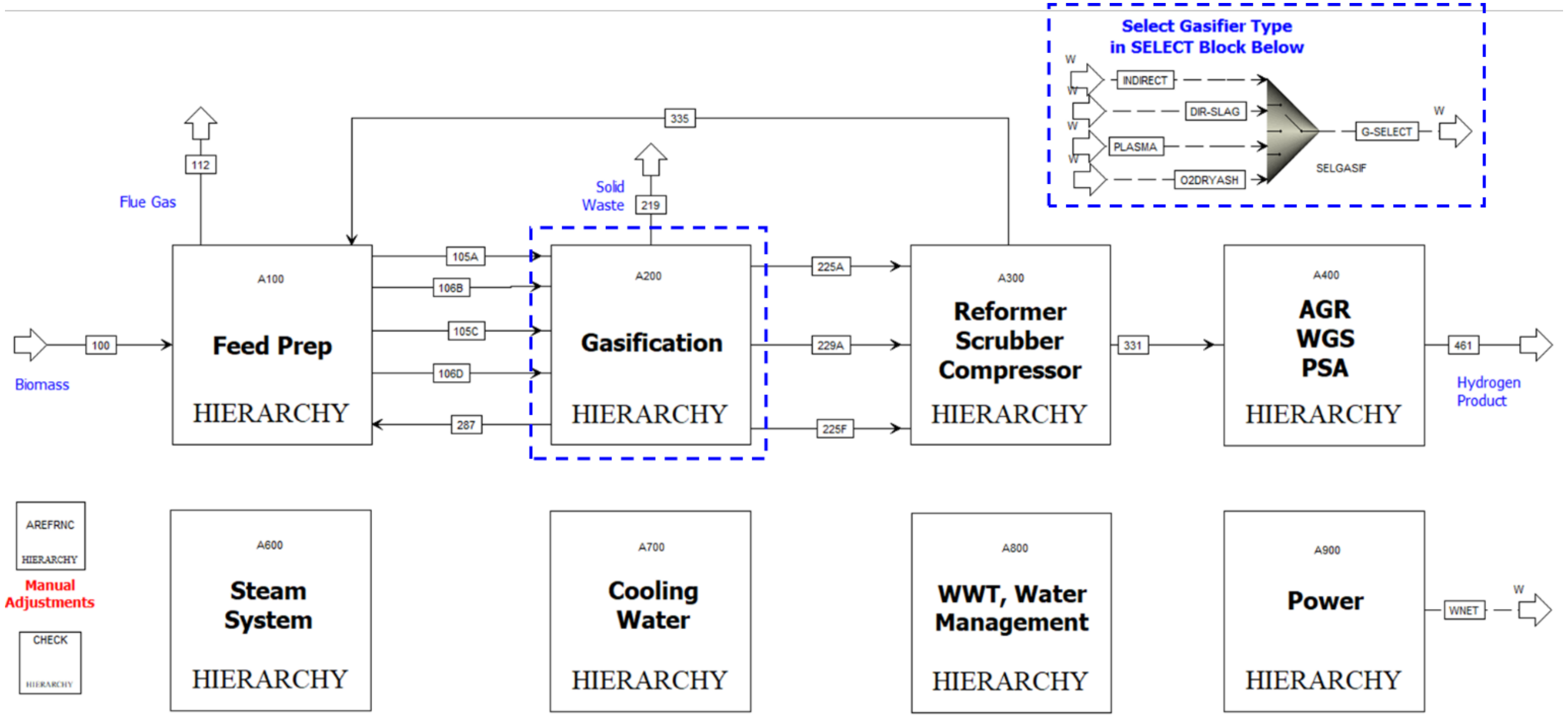
- Combines the main output of the previous analyses to visualize:
  - Areas of intersection for various factors which aids in identifying hot spots
  - Areas of interest not seen as significant if independently observed
- Current approach is overlay with equal representation of inputs
- Potential approach is to apply weighted overlay in which we assign ranks and weights for each individual input and let the model determine areas of interest
- Incorporate techno-economic analysis (TEA) for next phase of siting analysis.

Figures on resource maps have been removed from the presentation as the analysis results are not yet published. Publication is targeted for end of fiscal year 2024.

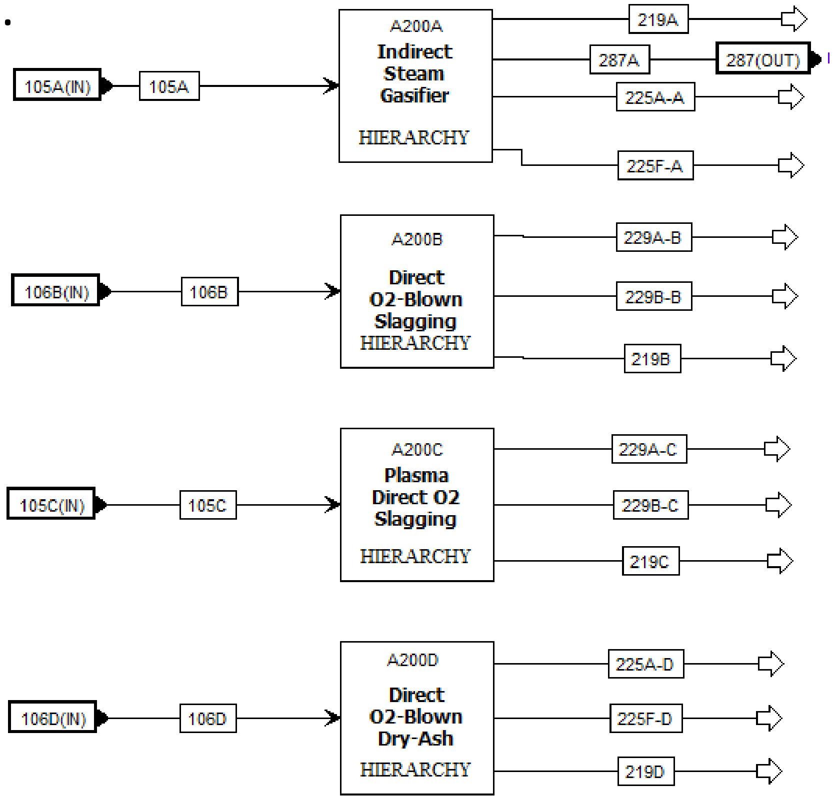
Pathway Analysis

Innovative Development in Gasification Process Modeling

- Developed Aspen Plus model with four gasification technologies.
- NREL historical models applied for steam-blown (indirect) and oxygen-blown (direct) technologies.
- Investigated and implemented oxygen-blown, plasma gasification (requires validations).
- Enables comparative analysis for different families of gasification technologies.
- Demonstrated models with multiple feedstocks (correlations for biomass).
- Leveraged FCIC work on gasification of biomass and alternate feedstocks.



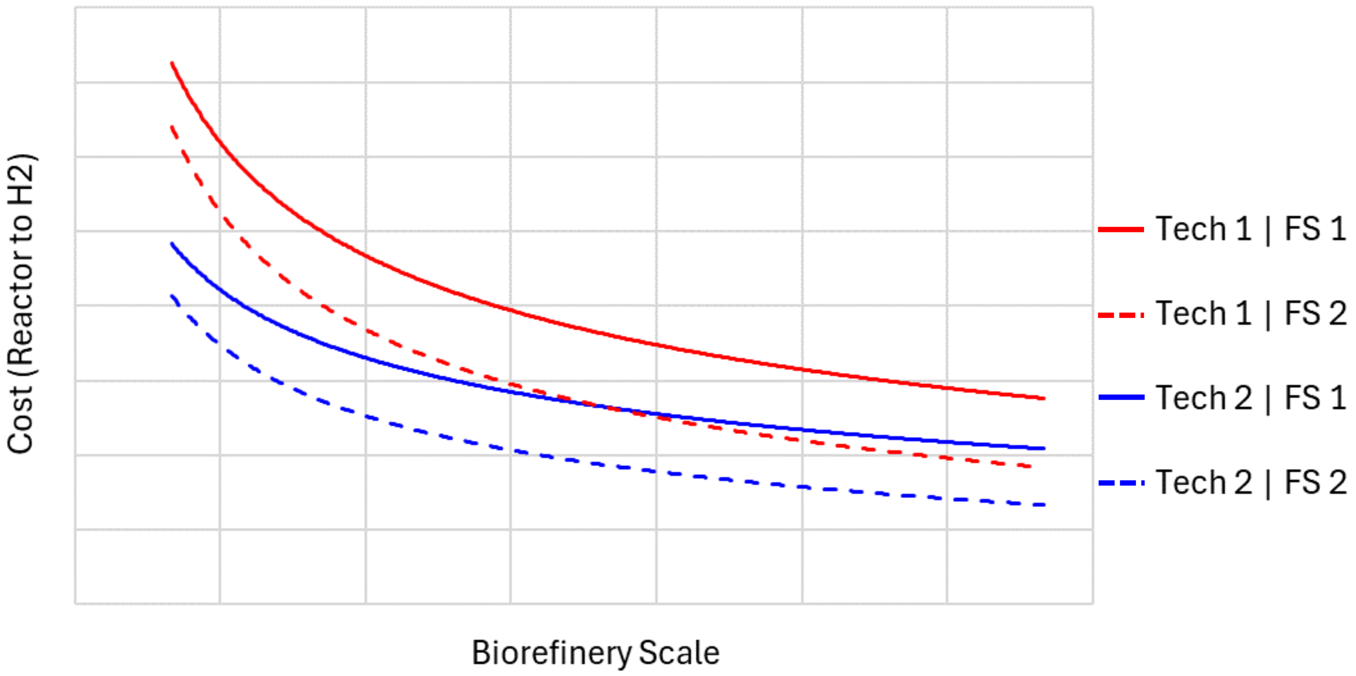
A200: Collection of Gasifiers



Techno-Economic Analysis Updates

- Updated capital cost models to correspond with gasification technologies.
- Added CCS basis for syngas and flue gas.
- Integrated carbon intensity (CI) quantification with TEA framework to enable direct GHG emissions estimates from Aspen Plus outputs (GREET factors).
- Demonstrated integration of Aspen Plus model with TEA and CI quantification with different feedstocks (biomass and MSW) and variable plant scales.

Comparative TEA for Technologies and Feedstocks



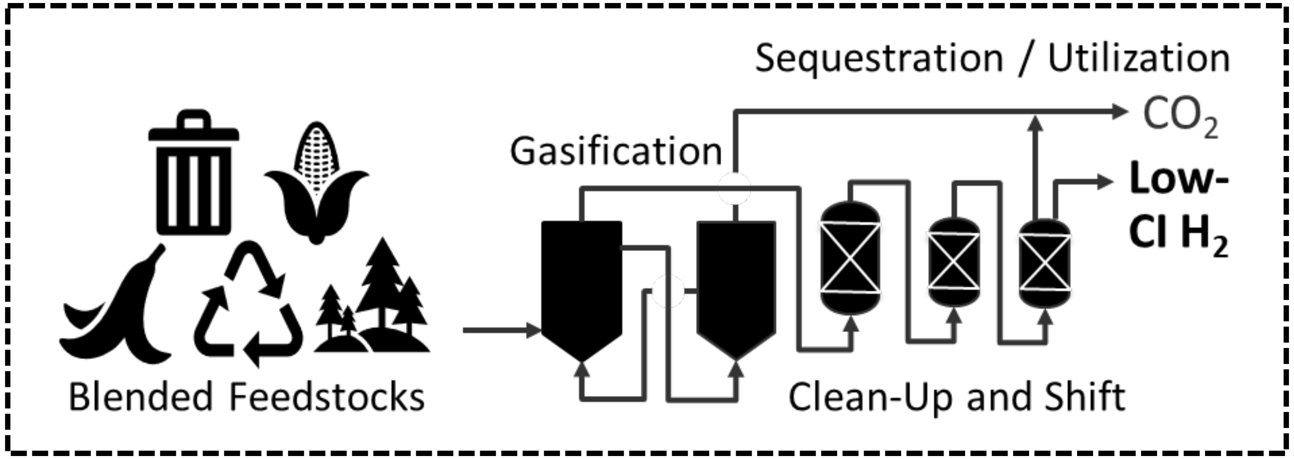
Note: Figure represents an illustrative example of comparative analysis. Model results are not yet reviewed or published.

- TEA framework will connect with resource assessment to perform biorefinery facility siting.
- Coordinate future efforts with NETL in applying results of real-time feedstock characterization, gasifier experiments, and reactor modeling validations to enhance process models.

Future Analysis Objectives

Resource availability and locations.

Low-cost feedstock characterization and pre-processing.



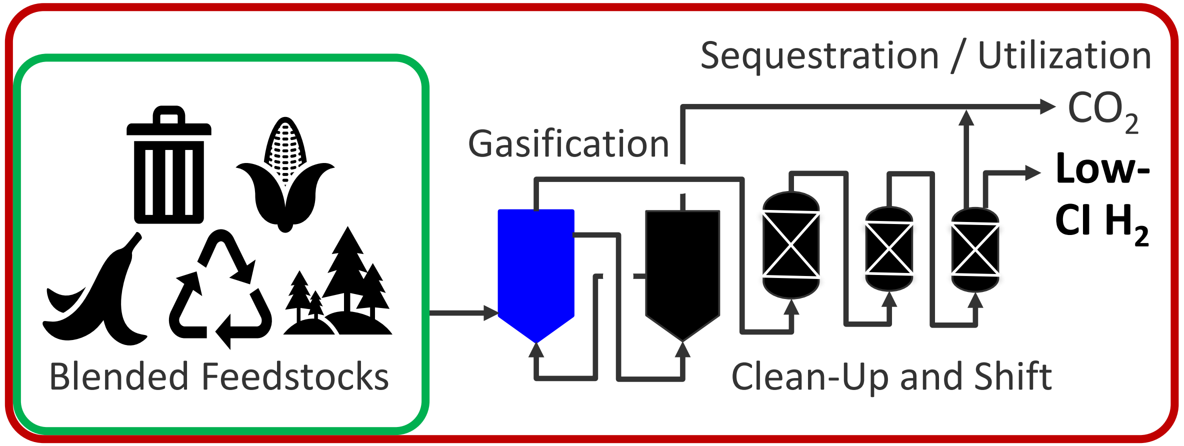
Validated process yields per feedstock.

Plant economics based on location and scale.

- Validate **yield equations** with experimental data on MSW/mixed feedstocks.
- Incorporate **cost basis** for sorting, feedstock pre-processing, and logistics.
- With NETL teams, develop **biorefinery siting** and **investment strategy** evaluations based on integration of resource analysis, process modeling/TEA, reactor modeling, and feedstock characterization efforts.
- Publish results and engage with **industry stakeholders** on opportunities.

Summary of Next Steps

Year-1 Project Scope (Mike Talmadge-PI)



Meso- & Particle-Scale Modelling (Peter Ciesielski)

- Perform particle scale simulations on different feedstocks and gasifier conditions. Specify residence times and parameterize boundary conditions.
- Generate robust kinetic data on Single Particle Reactor (SPR) for validations of parameterization and reactor modeling with NETL and ORNL.
- Provide sub-grid models for MFIX team.

Real-Time Feedstock Characterization (Ed Wolfrum)

- NREL and NETL researchers will collaborate on generating well-curated datasets using multiple sensing modalities of well-characterized mixtures of biomass/MSW/fossil waste.
- Publish data sets on NETL's Energy Data Exchange (EDX) https://edx.netl.doe.gov/

Resource & Pathway Analysis (Gary Grim/Anelia Milbrandt)

- Work with NETL, NREL, and ORNL teams on validating process models with experimental data.
- Develop biorefinery scenarios to explore TEA/CI with varying scale and feedstock with NETL teams.
- Integrate resource and infrastructure assessments with pathway TEA efforts for gasification biorefinery siting analysis.

Thank you!
Questions?

www.nrel.gov

Thanks to the FECM/NETL team including Katelyn Ballard, Jonathan Lekse, Jai-Woh Kim, Nathan Weiland, Ben Chorpening, Mehrdad Shahnam, Eric Lewis

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Supplemental Content

BP1 Milestone Summary

Task	Milestone	Description	Target Date
2.1	Techno-economic impacts of scale and composition for each gasifier design	Apply models to explore how varying scale impacts key techno-economic parameters by gasifier type. Quantify how different component yields influence overall economics. Develop high-level heuristics on feedstock composition, flowrate, and gasifier design choices. Use data to obtain insights on minimum viable gasifier scale to produce low-carbon H2 with varying feed composition.	Mar-2024
2.2	Low-carbon H_2 production site	Identify promising locations and opportunities for future low-carbon H_2 production. Compatible gasification technology candidates will be identified for subsequent, detailed analysis.	Mar-2024 (Draft in Jan-2024)
3	Construct particle models from feedstock characterization data	Parameterize the models based on compositional analysis, size, and shape distributions provided by the feedstock characterization task.	Mar-2024
4	Define minimal sensor set	Identify the minimally acceptable set of sensors needed to adequately characterize mixed biomass/MSW/fossil feedstock streams in real-time	Mar-2024

Subtask 2.1 Objectives

Subtask 2.1 – Analysis: Baseline Gasification Models

- Apply techno-economic, life cycle, and resource analysis tools.
- Update and baseline existing in-house gasifier models (indirect, direct, high-temp slagging) using harmonized operating assumptions (cost year, design capacity) and available input from other national laboratories (NETL, ORNL).
- Apply models to explore how varying scale impacts key techno-economic parameters (e.g., cost, operability) by gasifier type and will study the impacts of feedstock blending of coal, woody biomass, plastics, MSW, and others through scenario analyses to quantify how different component yields influence overall economics.
- Develop high-level heuristics on feedstock composition, flowrate, and gasifier design.
- Incorporate process/yield data from NETL, FCIC, NREL NRG, Task 3, and Task 4.

Subtask 2.2 Objectives

Subtask 2.2 – Analysis: Low-Carbon H_2 Production Site Identification

- Leverage the tools, assets, and high-resolution geographic data available at NREL's Strategic Energy Analysis Center.
- Quantify and map the domestic availability of sustainable biomass/waste feedstocks.
- Identify opportunities for co-location with existing transportation and storage infrastructure such as CO_2/H_2-compatabile pipelines and geological storage sites.
- Identify key off-take users and consumers.
- A report will summarize the results of these analyses including maps of resource availability, potential H2 production sites based on available resources, infrastructure, market and other factors.

Task 3 Objectives

Task 3.0 – Mesoscale Modeling: Initial Model Selection and Construction

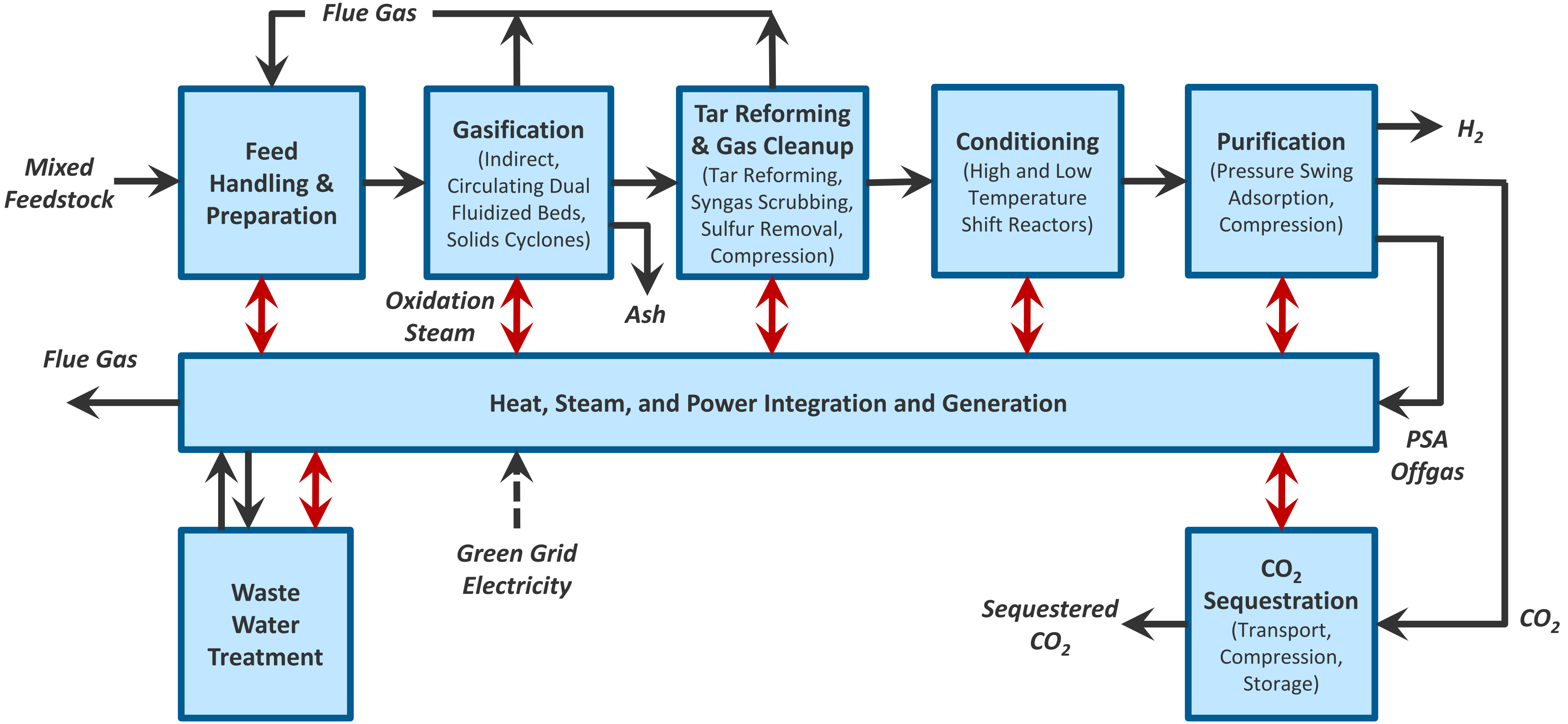
- Simulations performed at the mesoscale, or the scale of single particles, enable detailed treatment of feedstock attributes and their evolution throughout the conversion process.
- Survey available kinetic schemes in literature that are suitable for gasification of blended biomass and MSW feedstocks
- Select best available scheme for both reactor and particle scale simulations
- Construct particle models for components of the blended feedstock.
- Parameterize the models based on compositional analysis, size, and shape distributions provided by the feedstock characterization task.

Task 4 Objectives

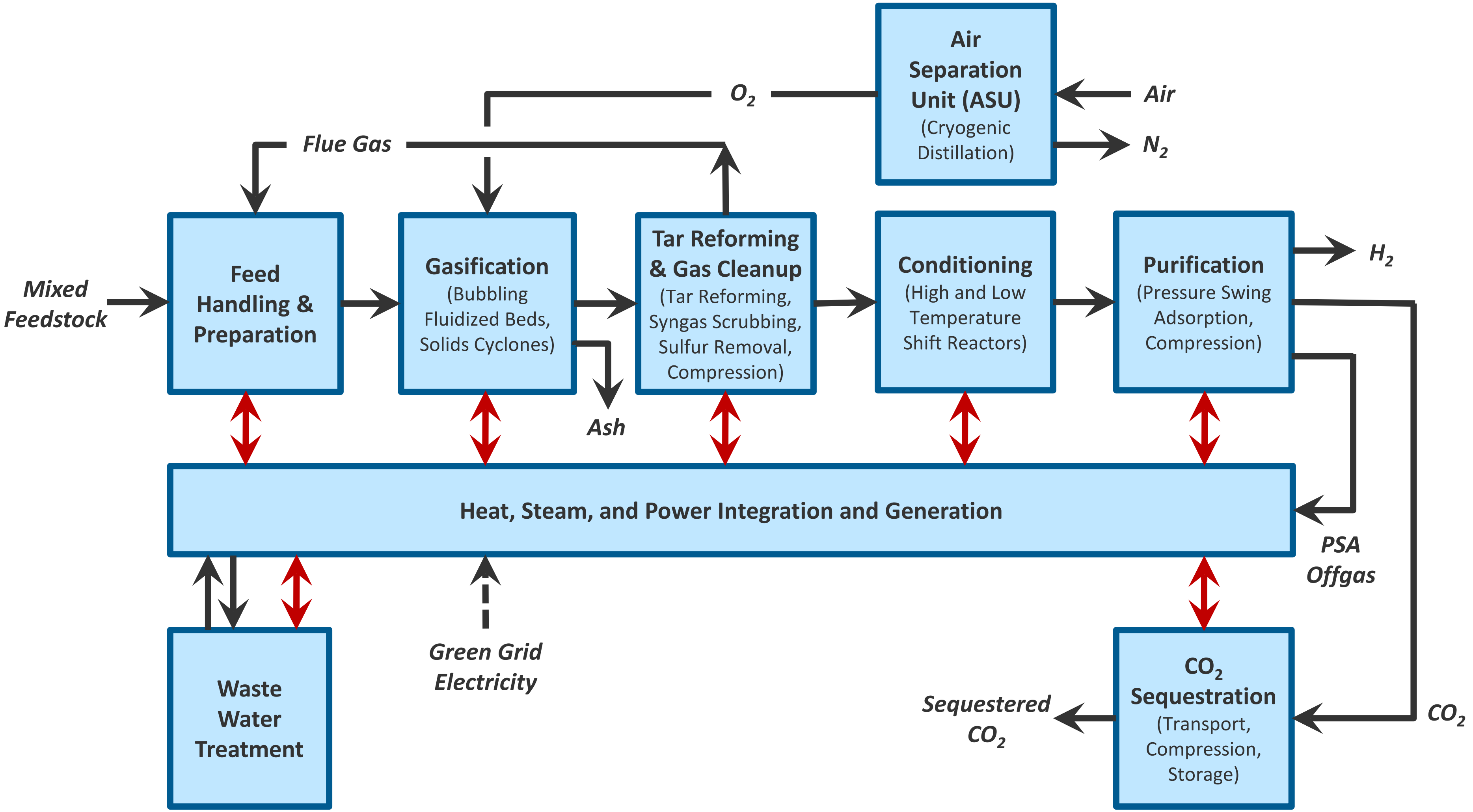
Task 4.0 – Real-Time Feedstock Characterization: SOT Report

- Develop SOT report for real-time material attribute measurement tools based on imaging and non-imaging spectroscopy for biomass and MSW streams, including both individual instruments and commercially available process solutions.
- Gather input from national laboratories, like NETL, on the SOT report, particularly on real-time inorganic characterization. Identify existing capabilities.
- Verify the hypothesis that a low-cost system is feasible.
- Identify specific areas that require technology development.
- Results will inform (1) the minimal set of sensors needed to adequately characterize feedstock mixtures of biomass, MSW and fossil inputs, (2) a detailed work plan for BP2 and BP3 and (3) the identification of specific partners to execute work plan.

Indirect Steam Gasification to H_2 (NREL)



Direct Non-Slagging Gasification to H_2 (NREL)



Direct Slagging Gasification to H_2 (NREL)