Advanced Reaction Systems

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The objective of the Advanced Reaction Systems Portfolio is to design, develop, and analyze technologies to support the mission of the Gasification Program to enable the use diverse feedstocks to produce hydrogen and other value-added products with net-zero carbon emissions.

Value Proposition: Gasification technologies offer promising opportunities to generate value from waste materials with minimal carbon emissions.
Current Research

Overview

• Task 3: Advanced Reactor Design
• Task 4: Refractory Materials for Multi-Fuel Gasification
• Task 5: Oxygen Integration for Net-Zero Carbon
• Task 7: Process Development to Mature Oxygen Sorbent-Based Technology
• Task 6: Microwave Reactions for Gasification
• Task 8: Gasification of Waste Plastic to Enable a Circular Economy
• Task 13: Hydrogen Production from Gasification Assessment
• Task 14: Syngas Conversion to Industrial Chemicals
Task 3: Advanced Gasifier Design

Overview

• Task Objective: Use Simulation-based Engineering Tools to decarbonize gasification-based processes for production of power, syngas, and hydrogen

• Project Goals:
  • Use CFD simulations to guide commercial scale-up and optimization of a moving-bed gasifier design
    • Application to the proposed University of Alaska, Fairbanks (UAF) modular plant
    • Evaluate gasifier performance for a range of feedstock and operating conditions
    • Optimize operation for production of H₂ with Net-Zero to negative Carbon
    • Evaluate gasifier performance for low-tar application – tar reinjection
  • Evaluate novel fluid bed gasifier performance for mixtures of biomass and waste plastic feedstocks
Task 3: Refractory Materials for Multi-Fuel Gasification

Accomplishments

Current Accomplishments (EY21)

• Simulations were performed on a gasifier with coal/biomass mixtures to determine operating conditions for hydrogen production with net-zero carbon emissions

• Re-Injection of tar into a gasifier was modelled and found to create local regions of high temperature which crack the tar and increase the rates of gasification and char/tar oxidation reactions

• Gasification of Cypress biomass in Sotacarbo’s pilot-scale fluidized air blown experimental reactor (FABER) was simulated and gasification reaction kinetics were developed and validated against experimental results

• A HDPE pyrolysis scheme was developed compatible with CFD applications as the first step in modelling the gasification of waste plastic

Future Accomplishments (EY22 – future)

• Complete the modelling for a pilot-scale fluidized bed gasifier

• Implement the plastic pyrolysis model into existing gasifier models to determine the performance of these systems on a waste plastic feedstock
Task 4: Refractory Materials for Multi-Fuel Gasification

Overview

• Objective: Develop novel refractory materials that enables multi-fuel gasification

• Project Goals:
  • Develop refractories that can withstand gasifier conditions with waste plastics feedstock options
  • Facilitate the use of a carbon-diverse fuel in gasification for production of chemicals, power, and H₂
  • Contribute to a circular economy and net-zero carbon goal by enabling plastic recycling
Accomplishments

Current Accomplishments (EY21)

• Industrial partnerships with Eastman (gasifiers), Allied Mineral Products (castable refractories), HarbisonWalker International (sintered bricks).

• Developed own plastic ash composition database for various plastic types (HDPE, LDPE, PP, PS, PET, etc.) by ashing based on ASTM D5630-13.

• Alumina- and mullite-based refractories were fired against 20% plastic slag; the former tended to degrade while the latter exhibited some resistance.

• Two refractory compositions were successfully identified to be used in mixed coal-biomass modular gasifier environments (up to 100% biomass).

Publications/presentations (EY21)

• Kristin Tippey, Anna Nakano, Jinichiro Nakano, Hugh Thomas, Ömer N. Doğan, Matthew Lambert, and Dana G. Goski, ‘In-operando Interactions of Refractory Materials with Ash/Slag from Mixed Feedstock Gasification,’ was presented at TMS2022, 2/27-3/3, 2022, Anaheim, CA.

• Kristin Tippey, Jinichiro Nakano, Anna Nakano, Hugh Thomas, Ömer N. Doğan, Matthew Lambert, and Dana G. Goski, ‘In-situ observations of alumina- and mullite-based refractory materials interacting with ash in coal-biomass gasification environments,’ was presented at UNITECR2022, 3/15-18, 2022, Chicago, IL.

• A conference proceedings, Kristin Tippey, Jinichiro Nakano, Anna Nakano, Hugh Thomas, Ömer N. Doğan, Matthew Lambert, and Dana G. Goski, ‘In-situ observations of alumina- and mullite-based refractory materials interacting with ash in coal-biomass gasification environments,’ was published in UNITECR2022, 3/15-18, 2022, Chicago, IL.

Future Accomplishments (EY22 – future)

• Establish novel refractory composition that enables sustainable plastics gasification.
Task 5: Oxygen Integration for Net-Zero Carbon

Overview

• Objective: Design a metal oxide carrier material capable of separating oxygen from air and develop a reactor based on NETL developed carrier materials

• Project Goals:
  • Develop a carrier material that can rapidly and reversibly store and release oxygen
  • Create a knowledge base and modelling tool for the optimization of carrier materials
  • Design an oxygen production reactor based on NETL carrier materials

\[
\text{Sr}_{0.75}\text{Ca}_{0.25}\text{FeO}_3 - \delta + \frac{\delta}{2}\text{O}_2 \rightarrow \text{Sr}_{0.75}\text{Ca}_{0.25}\text{FeO}_3
\]
Task 5: Oxygen Integration for Net-Zero Carbon

Accomplishments

Current Accomplishments (EY21)

- Demonstrated ability to control capacity, desorption temperature, and rate through compositional changes
- Designed and tested a carrier with greater than 2 wt% oxygen capacity with rates in excess of 2.0 wt%/min and demonstrated stability over more than 10,000 cycles
- Ellingham diagrams for perovskite carriers have been calculated and experimentally validated
- Preliminary reactor design completed using NETL’s MFiX software

Publications/presentations (EY21)

- Eric J. Popczun, Ting Jia, Sittichai Natesakhawat, Chris M. Marin, Thuy-Duong Nguyen-Phan, Yhua Duan, Jonathan W. Lekse “Investigation of Sr0.7Ca0.3FeO3 Oxygen Carriers with Variable Cobal B-Site Substitution” ChemSusChem 14, 1893-1901.

Future Accomplishments (EY22 – future)

- Develop a machine learning model for carrier materials optimization
Task 7: Process Development to Mature Oxygen Sorbent Technology

Overview

• Objective: To develop a computational model that captures the oxygen storage/release potential of NETL designed materials and to leverage simulation to design a pilot-scale fixed bed, perovskite sorbent oxygen separation reactor.

• Project Goals:
  • Develop a kinetic model that accurately describes the behavior of NETL designed materials
  • Design and validate a reactor model that maximizes oxygen production
  • Use simulation tools to scale the reactor design from bench scale to a pilot-scale reactor system
Accomplishments

Current Accomplishments (EY21)

- NETL scientists ran TGA experiments over a range of $O_2$ gas concentrations and temperatures that were subsequently used to derive the kinetic constants described in the Bulfin model.

- Multiple simulations of $O_2$ absorption and desorption swings at a 50 kg scale were conducted to gain an understanding of how a simple change in reactor mass loading can affect $O_2$ production in a fixed bed device.

- The reactor design was scaled to 100 kg of material and additional simulations were performed and compared to performance at 50 kg.

Publications/presentations (EY21)


Future Accomplishments (EY22 – future)

- A bench scale system is being built to perform steam desorption at the 300 g scale for model validation.

- Optimization of the 50/100 kg reactor including flow rates, thermal management, and swing timings.
Task 6: Microwave Reactions for Co-Gasification of Plastic and Biomass

Overview

• Objective: To investigate microwave reactions of plastic and biomass mixtures, determine the benefits afforded by utilization of microwaves, and design a microwave gasification system.

• Project Benefits:
  • Synergy exists for co-gasification of plastic and biomass, depending on
    ✓ Plastic to biomass ratio
    ✓ Moisture content of biomass
    ✓ Plastic type (HDPE > PP > PS)
    ✓ Temperature
    ✓ Catalysts (Ni based)
  • With increasing PE, PP or PS, syngas yield increases, tar and char decrease, $H_2$ increases

Diagram with various processes and components related to plastic, biomass, and their conversion into energy forms.
Task 6: Microwave Reactions for Co-Gasification of Plastic and Biomass

Accomplishments

Current Accomplishments (EY21)

• Complete gasification and high hydrogen production with mixed plastic and biomass
• High H₂ and CO selectivity with biomass + plastic gasification
• Low H₂ production and incomplete gasification with plastic only (no biomass) – confirming synergy
• MW reduced the reaction time for complete gasification ~15 min for 6g sample

Publications/presentations (EY21)

• P.D. Muley, Y. Wang, J. Hu, D. Shekhawat “Microwave Assisted Heterogeneous catalysis” Catalysis, 2021, 33, 1–37

Future Accomplishments (EY22 – future)

• Test the effect of a gasifying agent (CO/air/Steam) on microwave gasification of biomass and mixed plastics
• Perform a parametric optimization to obtain data for system design
Task 8: Gasification of Waste Plastic to Enable a Circular Economy

Overview

- Objective: To study the thermal gasification of waste plastic to determine syngas yields and compositions and design a machine learning tool to predict reactor performance based on feedstock and operating conditions.

- Project Goals:
  - Determine syngas composition and yield for various plastic and plastic/waste coal/biomass blends
  - Conduct a literature analysis to gather data on emerging trends in plastic recycling
  - Develop a machine learning tool to predict gasification reactor performance

[Images and diagrams related to gasification and reactor schematics]
Accomplishments

Current Accomplishments (EY21)

• Studied the gasification of alternative feedstock of waste plastic and waste coal to generate enhanced H₂/syngas in a drop tube reactor
• Identified key parameters for product composition
  • Temperature
  • Residence time
  • Plastic/H₂O feed ratio
  • Gas environment
    (H₂O, inert gas)
• Analyzed approximately 10,000 papers on plastic recycling/upcycling to explore emerging trends using Big-data tool

Future Accomplishments (EY22 – future)

• Investigate biomass and plastic blends for potential of net-zero carbon emissions
• Continue to develop the machine learning model
Task 13: Hydrogen Production from Gasification Assessment

Overview

• Objective: Support the Gasification Program by developing a reference study for commercial, gasification-based hydrogen production technologies

• Project Goals:
  • Develop reference study for commercial, gasification-based H₂ production technologies
    • Using alternative feedstocks
    • Estimate levelized cost of hydrogen
  • Identify key R&D areas to improve performance and cost of H₂ production technologies
  • Support ongoing and future research by furthering current understanding of the cost and performance of gasification-based H₂ production plants

• Accomplishments:
  • The hydrogen baseline study was completed and is currently being prepared for publication

Acknowledgments

• Acknowledgment
  • This material is based upon work supported by the Department of Energy research under the Gasification Research Program. The research was executed through the NETL Research and Innovation Center’s Advanced Reaction Systems field work proposal. Research performed by Leidos Research Support Team staff was conducted under the RSS contract 89243318CFE000003.

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Conclusion

The Advanced Reaction Systems portfolio supports the Gasification Program by designing and developing technologies and tools to enable modular gasification systems that can convert waste materials into valuable products with net-zero carbon emissions.
Questions?