A Novel Process for Converting Coal to High-Value Polyurethane Products

DOE/NETL Agreement DE-FE0031795

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Project Overview

Coal to Polyurethane (PU) Foam Products

- Client: DOE/NETL; Cost Share Grant from State of Ohio (OCDO/ODSA)
- Project Team: Battelle, mterra, and MLB Molded Urethane Products
- Project Manager: Dr. Satya Chauhan (Battelle)
- Period of Performance: 2 years; from 10/1/2019 to 9/30/2021
- Convert coal-derived liquids to high-value polyurethane foam

Statement of Problem

- Increase utilization of coal through new applications
- Produce high-value solid products from coal via direct liquefaction of coal
  - Bituminous coal
  - Western coal
- Need conversion processes to efficiently improve value proposition of coal

Project Objectives

Demonstrate a novel coal-to-PU foam process at bench-scale and establish a straightforward path to near-term commercial production

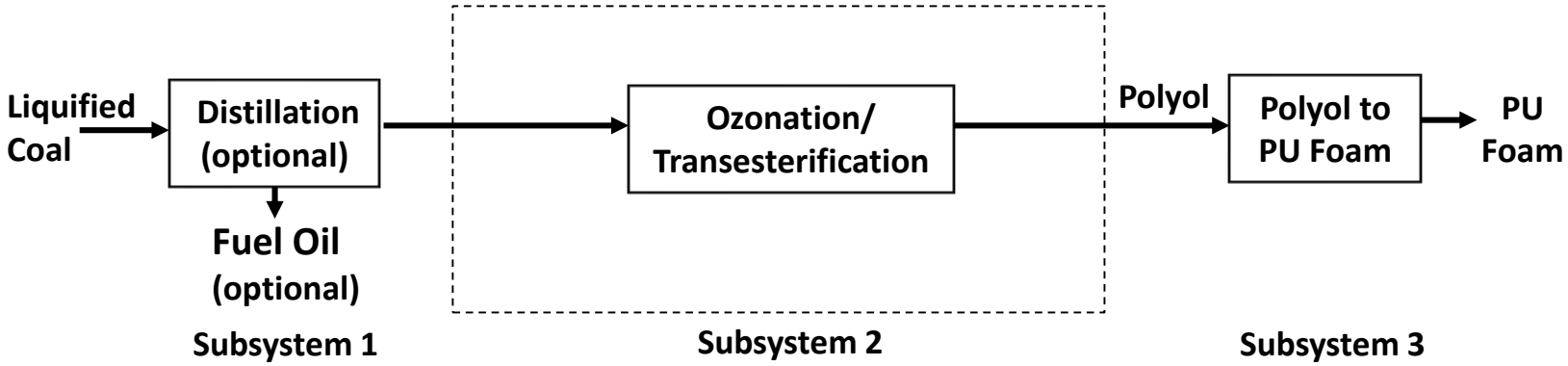
- Confirm a high rate of return compared to petroleum-based, solid PU foam products
- Determine the PU foam properties to establish a market value and demand for these high-value solid products
- Develop a process scale-up and commercialization plan
- Advance the coal-liquids-to-polyols process to TRL 5 from the current TRL 3
- Promote the use of coal in the face of environmental regulations

Alignment With DOE Objectives

Areas of Interest (AOI)

- Advanced technology aligns with AOI 2-Producing High-Value Solid Products from Domestic U.S. Coal
  - 2A-Laboratory testing of technologies for making high-value solid products from coal
  - 2B-Continuous process testing of technologies for high-value solid products from coal
- Project aimed at producing polyols (primay component in PU foams) with typical value ~$2000/Metric Tonne (MT)
- Can utilize various feedstocks
  - Coal liquefaction products
  - Bituminous or sub-bituminous coal

Proposed Technology



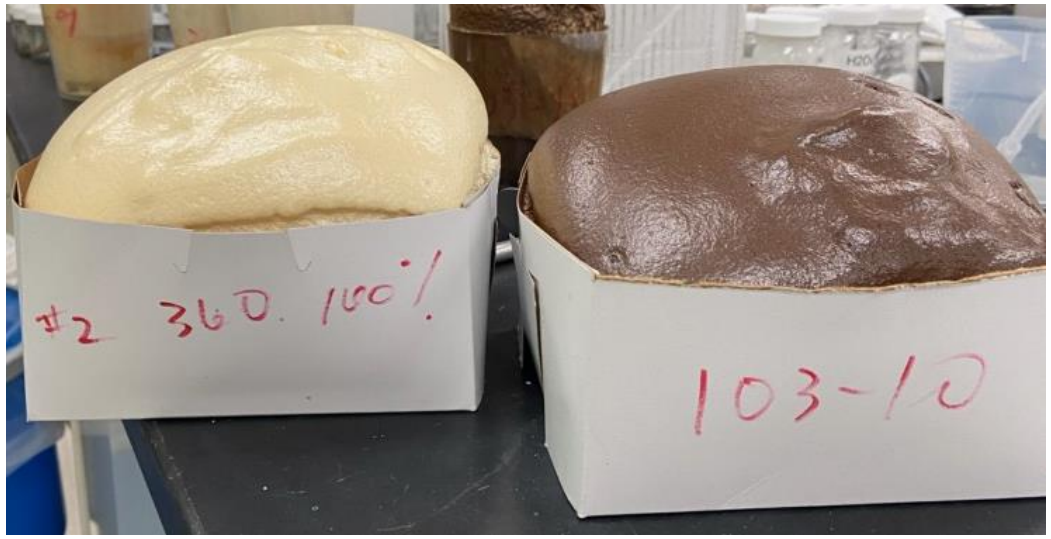
- Coal is turned to liquids using Battelle's proven CTL technology based on use of bio-based solvents; optional fuel-oil byproduct
- The coal-derived liquids are treated via ozonation/transesterification to create polyols for making PU-foam products, which typically sell for over $5,000/MT; this Subsystem 2 is the only one needing development
- Determine performance advantages versus industrial polyols; expect good mechanical performance due to aromatic content of coal

Project Starting Status

- Technology Readiness Level (TRL) 3
  - Proof of concept Demonstrated
  - Filed patent application
- Current target for feedstock
  - Direct coal-liquefaction liquids and its fractions
- Solvent ozonation
- Transesterification step
  - Short-chain polyols

Technology Benchmarking

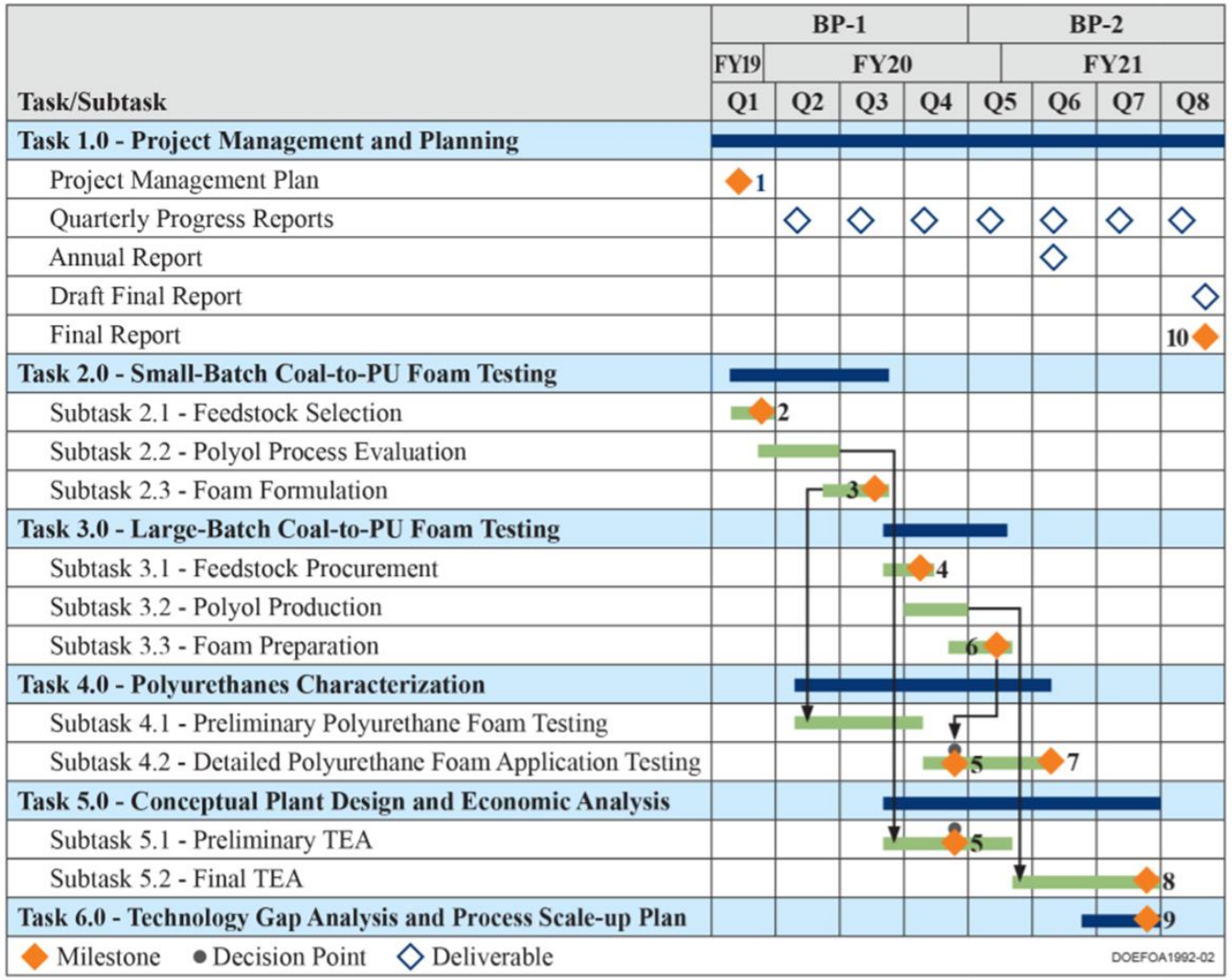
- Successful benchmarks
  - PU foam properties
    - Reactivity
    - Density
    - Compression at break
  - Polyol properties
    - Typical hydroxyl value range
    - Viscosity
    - Density



- Currently benchmarking versus industrial standard Huntsman SG-360
  - Hydroxyl value=360
  - Sucrose/Glycerol initiated polyether polyol
  - Viscosity ~3500 cps at 25C
  - Density 1.06 g/cm^3

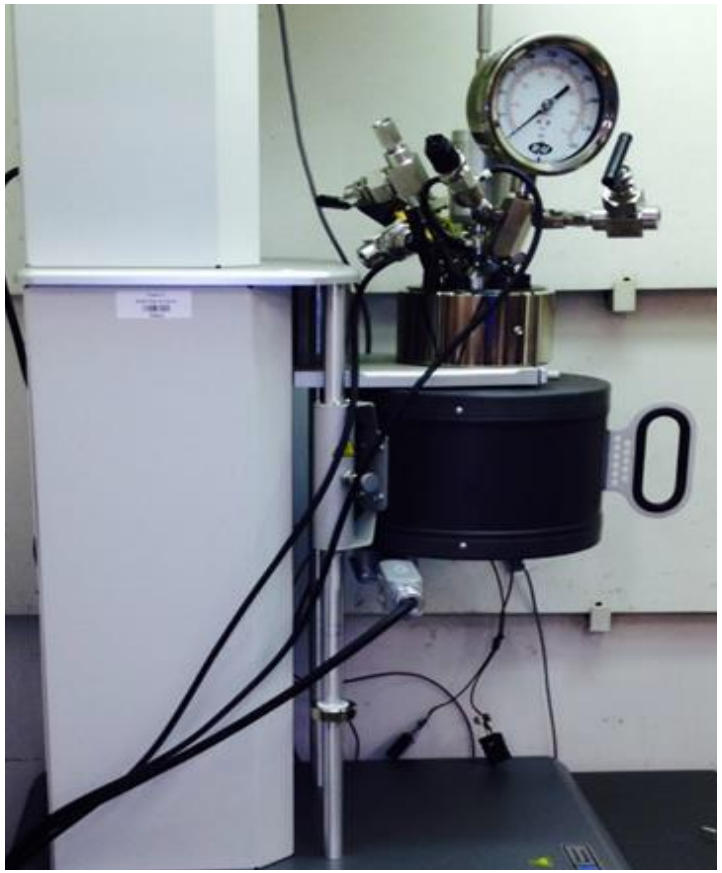
Project Plan

- Oct 1, 2019 start date
- Task 2-complete
- Tasks 3, 4, and 5 in progress
- 1-2 months behind, due to COVID-19 restrictions
- Back on schedule by end of Q5



Results for Coal Liquefaction

- Consider ≥80% solubilization of coal as successful
- 18 tests on Ohio(Middle Kittaning) coal, with 80-89% solubilization at various proportions of coal-liquids recycle for slurrying coal
- Tests on Western (Wyoming) coal completed; results are in progress

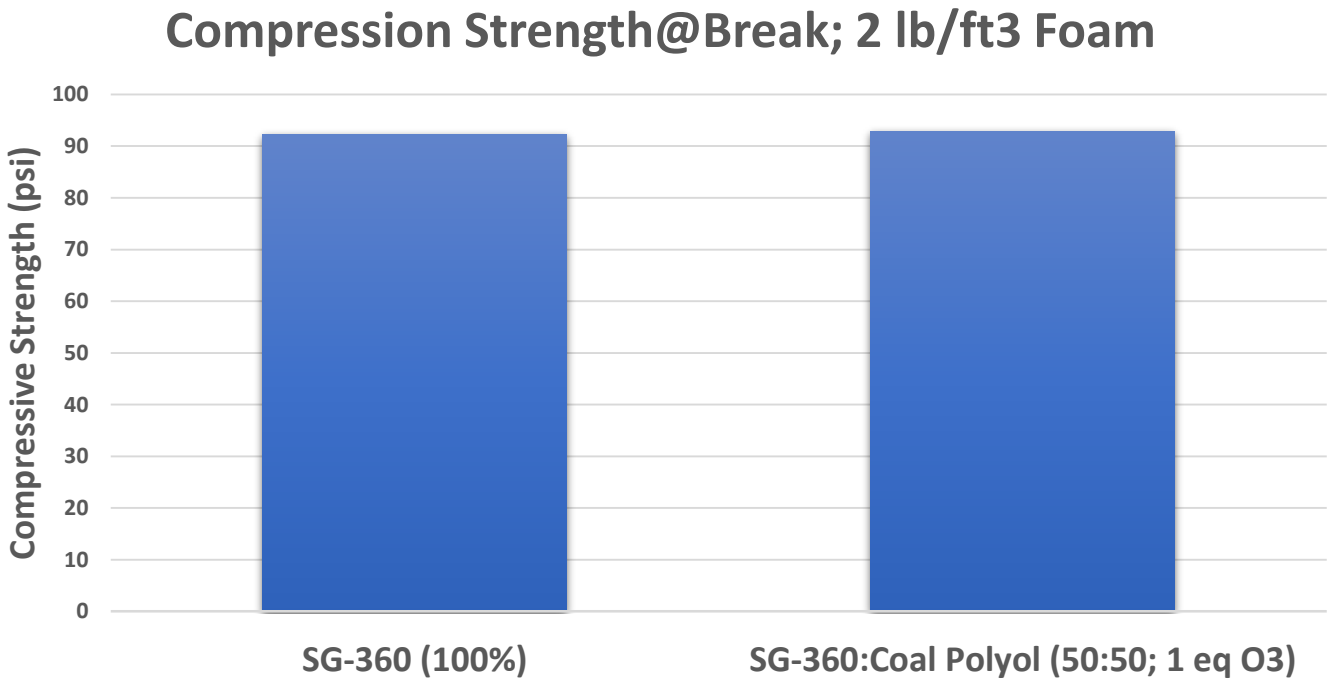


Polyol Formation

- Main ozonolysis step parameters
  - 1 equivalent (eq)
  - 2 eq
  - Temperature
  - Residence time
- Transesterification with
  - C3 polyols
  - Other primary polyols
- 28 Polyols produced to date
- Found 1 eq ozone to be acceptable for polyol formation

Initial Results on Foam Properties

- Evaluation of foams from19 coal-derived polyols complete
- Evaluation of foams from 9 additional polyols in progress
- Results compared to Standard SG-360 polyol
- Performed 2 levels of SG-360 replacement
  - 50%
  - 100%
- Multiple coal-derived polyols gave good performance
- 1 eq ozone is adequate



Current Scale-Up Activities

- Bench scale will utilize Metler RC-1 reactor
- Initially 1-kg continuous stirred tank, batch reactor
  - Obtain heat data
  - Test up to 3-hr reaction time
- Switch to continuous after batch

  @ ~0.3 Kg/hr
- Polyol formation run via batch transesterification

Preliminary Technoeconomic Analysis

- Assumed a coal-derived polyol production plant capacity of 162 MT/day at 6.5% of US PU foam demand
- Current selling price of SG-360 polyol estimated at ~$1.00/lb
- Assumed coal-derived polyol selling price of $0.80/lb
- Estimated Return on Investment (ROI): 24%

Go/No-Go Criteria Met

Success Criteria

- ≥80% of liquified coal can be converted to polyols: Achieved 80-89%
- The properties of at least one coal-derived PU foam are acceptable for higher value (over $5,000/MT) foams: Achieved
- The return on investment (ROI) is at least 12%/year; Estimated at 24%

Market Benefits

- Worldwide PU foam market is over $80 billion/year
- US PU foam market ~ $20 billion/year
- Advantageous properties through use of coal-as demonstrated in prior work
  - Satisfying the US demand for PU foam for insulation consume 4,000 MT per day (1.3 million MT/yr) of coal; 5.2 million MT/yr for worldwide PU foam demand
- PU foam is widely produced and used in USA, and this project has support from mterra and MLB Molded Plastics
- Coverts low cost coal to high value PU foam (solid) products
- Fixes fossil-based carbon in solid products, reducing carbon footprint
- Known conversion chemistry from other higher priced feedstocks
- Drop-in replacement of current PU components

Path To Market

- Several potential commercialization partners identified
  - Producer of coal-derived polyols
  - Manufacturers of rigid and/or flexible foams
- Easiest path to market is partner with foam-formulators to assess product performance for drop-in replacement

Courtesy: MLB; http://mlbproducts.net/mlb5_009.htm

Conclusions

- Demonstrated the feasibility of converting coal to polyurethane (PU) foam, meeting the Go/No Go criteria of at least 80% conversion of coal carbon to PU foam carbon with a high (24%) return on investment (ROI)
- Process seems applicable to both bituminuous and sub-bituminous coals
- Produced 28 polyols from coal, using various test conditions, including duplicates
- Foams from coal initially determined to have performance equivalent to industrial standard
- Bench-scale, continuous system ready to scale-up the coal-to-polyol process to TRL 5
- Project discussions with two potential commercialization partners have been quite positive; open to other potential partners

Acknowledgements

- Cost share provided by Ohio Coal Development Office (OCDO)
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