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 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

U.S. DOE/NETL

Statement of Problem

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

Project Objectives

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

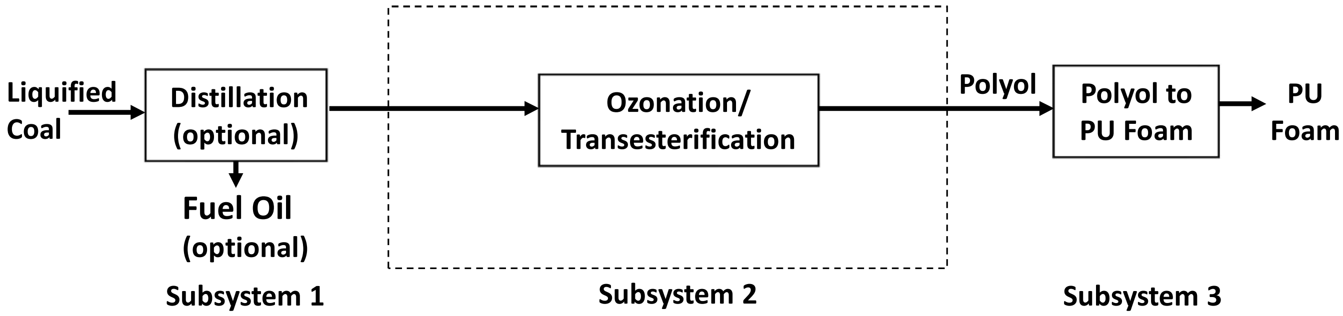
- Confirm a high rate of return compared to petroleum-based, solid PU foam products
- Determine the PU foam properties to establish a market value and demand for these high-value solid products
- Develop a process scale-up and commercialization plan
- Advance the coal-liquids-to-polyols process to TRL 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 products

Proposed Technology



- Coal is turned to liquids using Battelle's proven CTL technology based on use of bio-based solvents, with optional fuel-oil byproduct; also applicable to coal-pyrolysis feedstocks
- The coal-derived liquids are treated via ozonation/transesterification to create polyols in Subsystem 2; project focus is to determine performance advantages over industrial polyols
- In Subsystem 3, polyols are converted to PU-foam products, which typically sell for over $5,000/MT

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

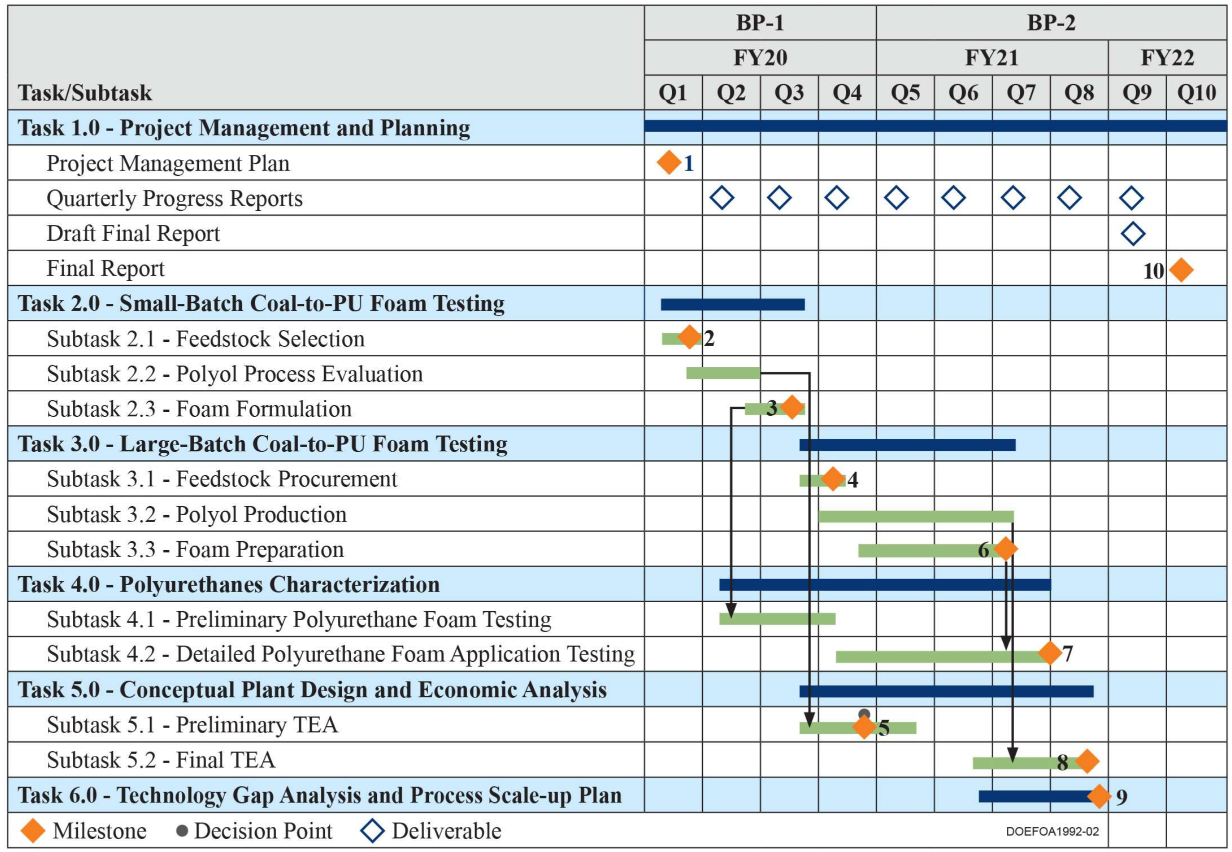
Technology Benchmarking

- 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

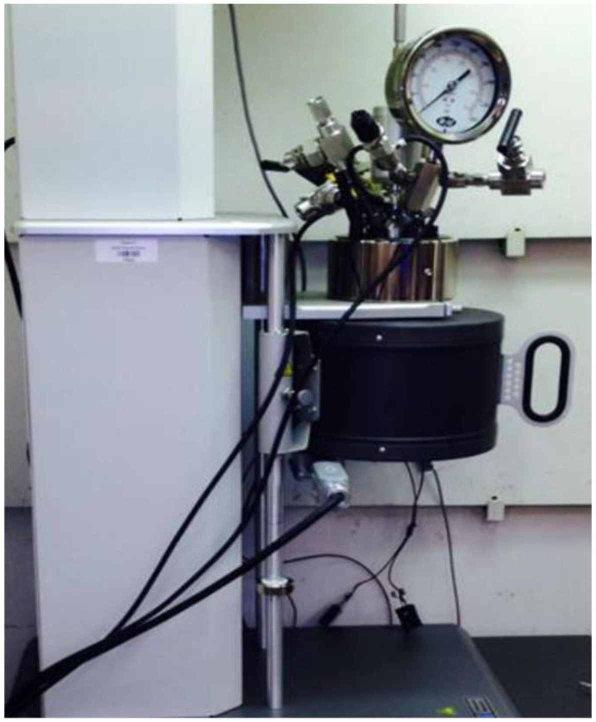
Project Plan

- Oct 1, 2019 start date
- Task 2 and Subtasks 3.1, 4.1, and 5.1-complete
- Subtasks 3.2, 3.3, 4.2, and 5.2 in progress
- ~2 months behind, due to COVID-19 restrictions



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
- Liquefaction of Western (Wyoming) coal was 79%.

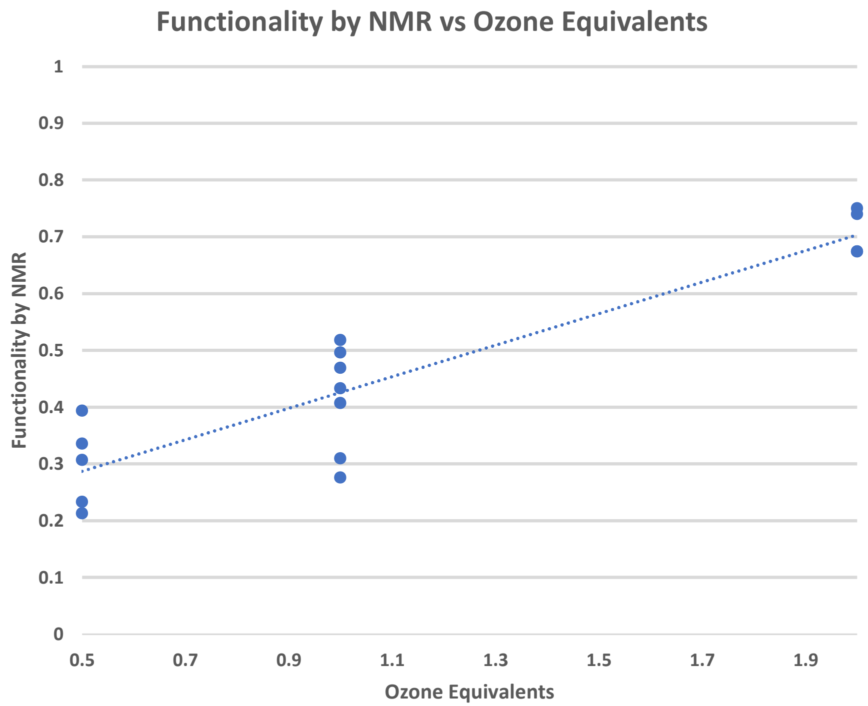


Polyol Formation

- Main ozonolysis step parameters tested
  - Ozone equivalent (eq): 0.5, 1.0, and 2.0
  - Temperature: 15 to 40°C
  - Ozonation Rate (0.5-1; correlates to 6-12 grams O_3/hr)
- Transesterification with
  - C3 polyols
  - Other primary polyols
- 47 Polyols produced to date
  - 28 range-finding tests
    - 2 polyols from western coal; comparable PU foam mechanical properties
  - 19 additional polyols produced as part optimization
- Found 1.0-1.5 eq ozone to be acceptable for polyol formation

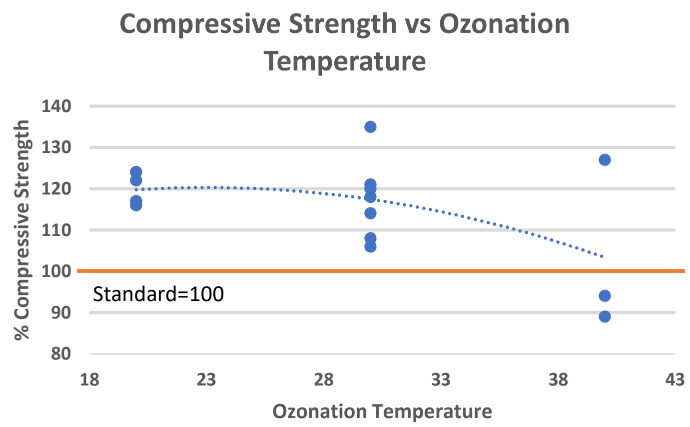
Ozonation Parametric Effects

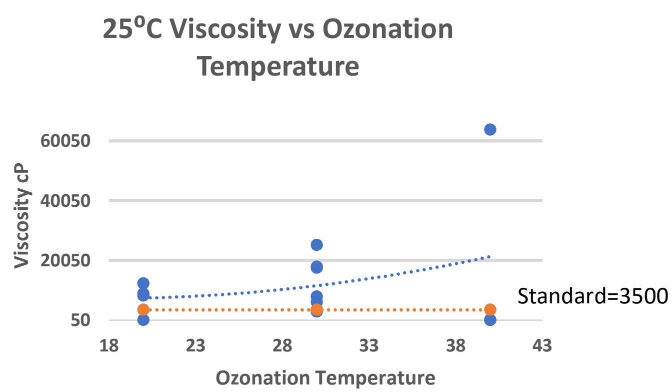
- Ozonation parameters explored
  - Ozone equivalent (eq) based on weight ozone/grams coal liquids
  - Rate at which ozone was delivered
- Effect of increasing eq
  - Increases functionality
  - Most important effect on foam properties
- Ozonation rate
  - Two rates evaluated
  - Minor effect on performance
  - Slower rate had slight improvement in foam properties likely due to uptake



Effect of Ozonation Temperature

- Effect on Foam Compressive strength
  - Lower temp improved performance
  - Optimum temperature: ~30C
- Effect on functionality (checked by NMR)
  - Not as large effect
  - Slight improvement at lower temperature
- Effect on polyols Viscosity
  - Not a major effect
  - Slight improvement on lower and higher from average

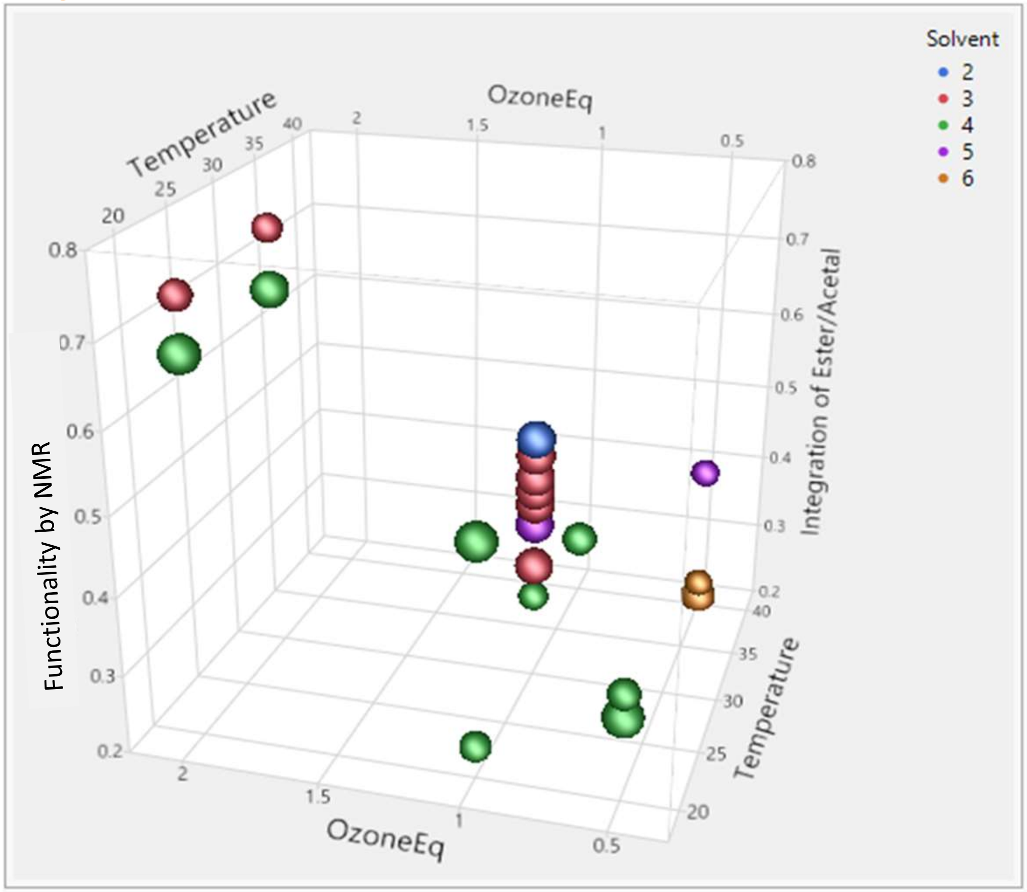




Overall Parametric Performance

Determination from Design of Experiments

- Optimized conditions based on
  - Functionality
  - Foam compressive strength
  - Temperature
  - Ozone equivalents
  - Ozonation rate
- Determined optimal
  - Ozone equivalents=1.5
  - Solvent: C3 to C4
  - Ozonation rate= 0.75 (Rate 1= 29 grams ozone per gram coal liquids)
  - Temperature: 20 to 30°C



Scale-Up to Bench Scale

- Bench scale utilizing Mettler RC-1e calorimeter with HP-50 reactor
- Initially tested at 1 kg/batch; continuous stirred tank, batch reactor
  - Obtained relative heat-of-reaction data
  - Tested up to 16-hr reaction time
- Switching to continuous after batch

  @ ~0.3 Kg/hr (scheduled)
- Polyol formation run via batch transesterification post ozonation

Conceptual Plant Capital Cost

BASIS

- Coal-derived polyol production plant capacity of 170 MT/day
    - 6.5% of US PU foam demand
- Current selling price of SG-360 polyol: $1.00/lb
- Coal-derived polyol selling price: $0.80/lb

CAPITAL COST

- Capital cost escalation: 3.5%/yr
- Construction period: 3 yrs
- Fixed Capital Cost: $34.80M
- Other capital cost: $22.44M
- Total As-Spent Cost (TASC): $70.73M

Estimated Revenue & Operating Cost

NATIONAL ENERGY TECHNOLOGY LABORATORY

Annual Cost Component (con)	Cost or Revenue ($000/yr)
TOTAL RAW MATERIAL COSTS	$50,330
TOTAL LABOR COST	$3,780
TOTAL UTILITY COST	$1,452
EQUIP MAINTENANCE COST	$1,679
TOTAL OPERATING COST	$57,241
TOTAL REVENUE ($0.80/lb)	$97,874

Estimated Rate of Return

Assumptions:

- 3% annual inflation costs and products
- 20 year operating life
- 15 year depreciation, double declining balance
- 2019 costs

Internal Rate of Return (IRR)	Selling Price, $/lb
31%	$0.80
21%	$0.69
16%	$0.64

Met Project Success Criteria

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 30+% at product selling price 20% below current market price

Market Benefits

- Worldwide PU foam market is over $80 billion/year and growing at 10%/yr in 2018
- US PU foam market ~ $20 billion/year with similar growth
- 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

- Exploring potential commercialization partners
  - 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

Concluding Remarks

- Demonstrated the feasibility of converting coal to polyurethane (PU) foam, meeting the success criteria of at least 80% conversion of coal carbon to PU foam carbon with a high (30+%) internal rate of return (IRR)
- Process seems applicable to both bituminous and sub-bituminous coals
- Produced 47 polyols from coal, using various test conditions, including replicates
- 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)
- Commercialization guidance being provided by MLB
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