Attractiveness of Wyoming Powder River Basin (PRB) coal as a valuable resource from which to manufacture non-energy and fuel products.

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Coal to Non Energy & BTU Products
The possibilities are vast!

Some of these chemicals and materials can only economically come from coal!

Reference: US Geological Survey

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The Coal Refinery
Adding Premium Value Beyond Energy Value

Current Product Slate

Petrochemicals
- Olefins
- Acetyls
- Alcohols
- Aromatics
- Asphalt

Coal chemicals
- Gasoline
- Diesel
- Naptha
- Aromatics
- Base Oil & Lubes

Common Product Families

New Carbon Product Solutions

New Carbon Conversion Solutions

Coal Intermediate Products
- Petrochemicals
- Acetyls
- Alcohols
- Aromatics
- Asphalt
- Carbon Fiber
- Carboxylates
- Aerogels
- Graphene
- Building materials
- Needle Coke

Investment in Carbon Engineering

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Summary of Coal Conversion…TODAY

- Some specialty chemical products today are derived only from coal.

- Unlike crude oil, coal is not readily fractionatable.

- Coal constituent polycyclic hydrocarbons readily react and polymerize.

- Understanding conversion behavior – thermal impacts on molecular chemistry is crucial to exploit coal’s ‘hidden’ value.
Existing Approaches

Pyrolysis
Coal is converted using high temperature decomposition.

Advantage: (1) Can aggressively and deliberately breakdown coal into intermediate liquids and solids that are convertible into valuable products

Disadvantage: (1) Reduced O₂ atmosphere – needs H₂ or CH₄ gasses

Gasification
Coal is blown with oxygen and steam (water vapor), while heated (pressurized).

Advantage: (1) Turn coal into multi-use feedstock i.e. syngas

Disadvantage: (1) Managing – separating the CO₂ is costly
(2) Converting to chemicals is energy intensive & costly
(3) Requires air separation unit for pure oxygen

Coal Liquefaction
Coal converted to liquids by hydrogen addition

Advantage: (1) Multiple Product Yields
(2) Possible – Hedge Against crude oil!

Disadvantage: (1) Qualities generally poor for chemicals
(2) CO₂ production challenge
(3) Consumes large volumes of water and/or hydrogen
## Coal Differences

<table>
<thead>
<tr>
<th>Ultimate Analysis</th>
<th>HV Bituminous</th>
<th>Sub-Bituminous</th>
<th>Lignite</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wt% Dry</td>
<td>Illinois #6, IL</td>
<td>PRB, WY</td>
<td>Beulah-Zap, ND</td>
</tr>
<tr>
<td>Carbon</td>
<td>71.72</td>
<td>69.21</td>
<td>61.88</td>
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<tr>
<td>Hydrogen</td>
<td>5.06</td>
<td>4.70</td>
<td>4.29</td>
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<tr>
<td>Nitrogen</td>
<td>1.41</td>
<td>0.89</td>
<td>0.98</td>
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<tr>
<td>Sulfur</td>
<td>2.82</td>
<td>0.30</td>
<td>0.98</td>
</tr>
<tr>
<td>Chlorine</td>
<td>0.33</td>
<td>0.03</td>
<td>0.00</td>
</tr>
<tr>
<td>Oxygen</td>
<td>7.75</td>
<td>18.67</td>
<td>16.44</td>
</tr>
<tr>
<td>Ash</td>
<td>10.91</td>
<td>6.20</td>
<td>15.43</td>
</tr>
<tr>
<td>Moisture, wt%</td>
<td>11.72</td>
<td>27.42</td>
<td>36.08</td>
</tr>
</tbody>
</table>

NETL, Detailed Coal Specifications, January, 2012

### High Oxygen in PRB

- Liquid and solid products have significant oxygen
- Can make oxygenated products such as phenols, xylenols, etc.
- Investigating how to keep oxygen in liquids and solids rather than expel it as CO2
- New Opportunities !!!
Coal Fed Refinery Goals & Constraints

Goals

• Product slate worth is > coal BTU value
• Full conversion of primary (PRB) coal feed – maximize liquids production
  • Include other feeds - /gas/LNG/shale oil/biomass feeds in support of this prerequisite

Constraints

• Extraction & complete process use only water extracted from coal
  • Zero effluent discharge & water consumption neutrality
  • PRB coal contains 20% or more water
• Zero or minimal pure stream CO2 emissions
  • Not producing it in the first place?
• Optimal energy consumption
  • Exothermic rather than endothermic processing
• Reject and manage carbon rather than adding hydrogen
  • Differentiate
• Maximize atom utilization and minimize waste
Evaluating Coal Conversion Approaches

Two ways to convert coal

• Thermally
  • Pyrolysis, gasification and liquefaction
• Chemically
  • Solvent extraction (Single phase, Low temperature)

Deciding on coal conversion approaches to pursue

• Considerations
  • oxygen in liquids/solids
  • managing CO2
• Result
  • The best research opportunities are solvent extraction and pyrolysis
Systems & Process Engineering Approaches

Direct and validate technology development strategy

- Atomic balances
  - Know where CHNOS goes; critical for value-added products
- Process flowsheet development
  - Identify processing sequences and unit operations required
  - Identify recycles
  - Identify likely separation and physical properties issues (i.e., azeotropes, LL)
- Identify simulation and process design requirements
  - Parametric studies
  - Extra lab data required
  - Industrial design studies (i.e., realistic recycled gas compositions)
  - Catalyst deactivation studies
  - Greater industrial focus
- Simulation ↔ Experimentation
  - See effects of new data on recycles
  - Identifies key variables for parametric studies
This is an example of how multiple technologies can be integrated into a multi-high volume product, low energy consumption & CO2 emissions complex.
This is an example of how multiple technologies can be integrated into a maximizing high-value chemical production while minimizing CO2 emissions.

Flash Pyrolysis
Integrated Example

hydropyrolysis, dry methane reforming, phenol recovery, HC fractionation, carbidization

Gas Clean-Up

Dry Methane Reforming

Gas Clean-Up

Flash Pyrolysis & Fractionation

Phenol Extraction

Trans-alkylation Hydro Treatment

Hi-Ash Char

Lime

Carbidization

Mixed Gas

Methane / H2

Coal

(co) Methane

NH₃, S

CO₂

Methane
Ethane
Propane

CO₂

CH₄

C₂

C₃

H₂O

Phenol

Benzene
Xylenes
Paraxylene
Polyethylene Terephthalate (PET)

Resins (Pitch, tars), fibers and surfactants

Asphaltenes (asphalts, fibers, cokes)

Syngas

CaC₂ (to acetylene)
Next Steps
Immediate Plan

• Define coal conversion schemes
  • Validate techno-economic viability of Wyoming located coal refineries

• Preserve and Protect Intellectual property
  • 5 Patents filed or in process in FY 2016-17
  • 15 (est.) by end July 2018

• Attract collaborators & investors who want to demonstrate their technology with PRB coal
  • Augment with University of Wyoming Coal Conversion Technologies

• Identify scale & scope of coal refinery
  • Attract investors
Thank You
Example Approach for Determining Products from PRB Coal

**Butadiene, C4 Olefins and Butanes Business: MAN, PAN and derivatives – Phthalic Anhydride (PAN) and derivatives**

### Technical Feasibility:

**Conventional**
- (catalytic oxidation of ortho-xylene)

- **O-Xylene**
  - Catalytic oxidation
  - Phthalic Anhydride
  - Catalytic oxidation

- **Naphthalene**

**Coal Route**
- (catalytic oxidation of naphthalene)

### Market Evaluation:

**PAN derivatives**
- PAN demand growing ~3% pa
- Main use is Plasticisers for PVC
- Carbon fibre growth emerging
- Alkyd resins is an important use:
  - Drying resins based on plant and vegetable oils
  - Non-drying based on glycerol etc.
- Production of UP resins is a minor use

**PAN production**
- Most PAN made from O-X
- Few plants still use naphthalene
- Efficiency, carbon footprint and cost advantage opportunity

### Economic and Product Quality Analysis

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Opportunity Assessment Example:
Chemical Products from Coal Using Flash Pyrolysis

Main Vectors
- CO₂
- Electric Power
- Syngas

Market
- Specification
  - Chemicals
    - Ammonia
    - SC CO₂ for EOR
    - Methanol
    - VCM
    - n-Propanol
    - n-Butanol
    - Acrylic Fibre
    - Adiponitrile
    - Plasticiser Alcohols
    - Propylene
    - Butadiene
    - EG
    - PTA
    - PAN
    - Naphthalene
    - Caustic Soda
    - BTX
    - Benzene
    - Toluene
    - Mixed Xylenes
    - C₆₆- Aromatics
    - Styrene
    - Cumene
    - Para-Xylene
    - HCl (Hydrochloric Acid)

- Value-Added Products
  - Urea
  - Acrylic Fibre
  - Carbon Fibre (2 types)
  - PP Resin
  - PP Fibre
  - PET Resin
  - Polyester Fibre
  - PET Sheet & Preforms
  - Bisphenol A
  - (PVC) Plasticisers
  - PVC Resin
  - UPVC compounds & siding
  - Flexible PVC cpds & sheet

- Commodities
  - Asphalt
  - Electric Power

- By-Products
  - Slag
  - Ashes

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Abstract

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Abstract Submission

COAL SCIENCE

Attractiveness of Wyoming Powder River Basin (PRB) coal as a valuable resource from which to manufacture non-energy and fuel products.

Abstract:

Most recent coal research has largely been on comprehending better ways to deliberately and aggressively destruct coal to extract energy in novel and effective ways, or to produce syngas that can be used to manufacture fuel and non-energy products. Sense, suggests that historic coal research and technology development activities (largely related to coal combustion and high-temperature conversion) are reaching a mature technical state. Set in the context of the USA, the techno-economic viability of implementing such technology solutions is increasingly challenging.

If the latent value in coal is to be truly realized, either as a clean-energy product or as a feedstock to make other carbon based products, rethinking the notion of coal utilization - migrating from rationale that involves aggressive destruction to deliberate decomposition of coal is offered as a basis to rejuvenate utilization. The understanding and comprehension of molecular structure, physics and chemistry of coal, built upon systems engineering concepts, is required to appreciate and identify the huge potential for investing in transformative ground breaking and pioneering research and technology development, recognizably confronting today’s market and technology need challenges and realities.

This presentation, sets out the compelling proposition for rethinking coal as a value proposition, sharing with participant’s recent research and technology development achievements at the University of Wyoming. This research and technology development pursuit is being funded by the State through the Wyoming Carbon Engineering and Science Initiative. The Carbon Engineering and Science initiative, seeks to explore and investigate conversion of Wyoming Powder River Basin (PRB) coal in ways to both sustain coal as a competitive clean energy resource, and create new carbon product markets that can be leveraged to create economic diversification opportunities. Early successful achievements and findings will be used to highlight the value in thinking about coal differently, justifying investment in improved understanding and comprehension of coal science and engineering.