Why worry about complex fuels?

[Graph showing world energy supply by source from 1971 to 2019.]


World Coal Consumption
(megatons/yr)

[Graph showing global coal consumption by region from 2000 to 2024.]

https://www.iea.org/reports/coal-2021
Power Plants in the US
(2019)

https://www.visualcapitalist.com/mapped-every-power-plant-in-the-united-states/

IPP Slides
Figure 1. Summary of coal structure information in a hypothetical coal molecule. 
From Solomon and coworkers (1985)

Figure 2. Cracking of hypothetical coal molecule during thermal decomposition.
**Fuel Characterization**

Where are...graphite...oil...peat...biomass?

![Coal Band Diagram](chart.png)

**TABLE 1** Classification of Coals by Rank

<table>
<thead>
<tr>
<th>Class</th>
<th>Group</th>
<th>Fixed carbon limits (%) (dry, mineral-matter-free basis)</th>
<th>Volatile matter limits (%) (dry, mineral-matter-free basis)</th>
<th>Calorific value limits (Btu/lb) (moist, mineral-matter-free basis)</th>
<th>Agglomerating character</th>
</tr>
</thead>
<tbody>
<tr>
<td>I. Anthracite</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1. Meta-anthracite</td>
<td>98</td>
<td>2</td>
<td></td>
<td></td>
<td>nonagglomerating</td>
</tr>
<tr>
<td>2. Anthracite</td>
<td>92</td>
<td>2</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3. Semianthracite</td>
<td>86</td>
<td>8</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>II. Bituminous</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1. Low volatile bituminous coal</td>
<td>78</td>
<td>14</td>
<td>22</td>
<td></td>
<td>nonagglomerating</td>
</tr>
<tr>
<td>2. Medium volatile bituminous coal</td>
<td>69</td>
<td>22</td>
<td>31</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3. High volatile A bituminous coal</td>
<td>—</td>
<td>31</td>
<td>14,000</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4. High volatile B bituminous coal</td>
<td>—</td>
<td>14,000</td>
<td>13,000</td>
<td></td>
<td></td>
</tr>
<tr>
<td>5. High volatile C bituminous coal</td>
<td>—</td>
<td>13,000</td>
<td>11,500</td>
<td></td>
<td></td>
</tr>
<tr>
<td>III. Subbituminous</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1. Subbituminous A coal</td>
<td>—</td>
<td>—</td>
<td>10,500</td>
<td></td>
<td>nonagglomerating</td>
</tr>
<tr>
<td>2. Subbituminous B coal</td>
<td>—</td>
<td>—</td>
<td>9,500</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3. Subbituminous C coal</td>
<td>—</td>
<td>—</td>
<td>8,300</td>
<td></td>
<td></td>
</tr>
<tr>
<td>IV. Lignite</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1. Lignite A</td>
<td>—</td>
<td>—</td>
<td>6,300</td>
<td></td>
<td>nonagglomerating</td>
</tr>
<tr>
<td>2. Lignite B</td>
<td>—</td>
<td>—</td>
<td>—</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
### Terminology

- **High heating value**
  - Calculated using $\text{H}_2\text{O (liq)}$ as product

- **Low heating value**
  - Calculated using $\text{H}_2\text{O (gas)}$ as product

- **Heating value** = $-\Delta H_c$
  - i.e., heating value is positive, but heat of reaction is negative
  - Table B.1 lists the high heating value
    - Actually $\Delta H_c$ corresponding to the high heating value

### Coal Combustion

- **Coal Composition (as rec’d)**
  - 4.49% ash
  - 4.63% H$_2$O(liq)
- **Coal Composition (wt% daf)**
  - 80.69% C
  - 5.78% H
  - 11.58% O
  - 1.57% N
  - 0.37% S
- **High Heating Value**
  - 13,280 Btu/lb (as rec’d)
  - 14,613 (daf)
- **Air**
- **Boiler**
- **Particulate Collector**
- **Flue Gas Desulfurizer**
- **Stack**

Diagram showing the flow of coal, air, boiler, particulate collector, flue gas desulfurizer, and stack.
Heat Balance

Strategy

• Get $n_{\text{air},\text{stoich}}$ from elemental composition of coal
• Find $n_{O_2,\text{in}}$ and $n_{N_2,\text{in}}$
• Find $n_{i,\text{out}}$ for all gas species
• Find $m_{i,\text{out}}$ for all solids

• If path method used:

$$
\dot{Q} = \Delta H = m_{\text{coal}} \Delta H_{\text{comb,25^\circ C}} + (m_{\text{moist}} + m_{H_2O,\text{comb}}) \Delta H_{\text{vap,25^\circ C}} + \sum n_i \left[ \frac{1000}{25^\circ C} C_p dT \right]_{\text{products}}
$$

10^6 \text{ lbm/hr of coal 25^\circ C}

6\% \text{ excess air 25^\circ C}

What is the energy balance equation?

See Spreadsheet Example
Heat Balance with Preheated Air

Strategy
• Get \( n_{\text{air,stoich}} \) from elemental composition of coal
• Find \( n_{\text{O}_2,\text{in}} \) and \( n_{\text{N}_2,\text{in}} \)
• Find \( n_{i,\text{out}} \) for all gas species
• Find \( m_{i,\text{out}} \) for all solids
• Use \( \Delta H \) method

\[
\dot{Q} = \Delta H = \sum n_i \dot{H}_i \text{gas, out} + \left( \sum m_i \dot{H}_i \right) \text{solid & liquid, out} - \left( \sum n_i \dot{H}_i \right) \text{in} - \left( \sum m_i \dot{H}_i \right) \text{solid & liquid, in}
\]

Need heat of formation of coal!

Calculation of \( \Delta H_f^0 \) for Coal

• Given:
  – Elemental composition
  – Heating Value (Btu/lbm) … Change to kJ/kg
  – Basis: 1.00 kg of dry, ash-free coal (daf)

• Calculate:
  – Mass of each element (C, H, O, N, S)
  – Moles of each element
  – O\(_2\) requirement to burn each element
    \( \text{C} + \frac{1}{2} \text{O}_2 \Rightarrow \text{CO}_2 \)  O in coal decreases O\(_2\) requirement from air
    \( \text{H} + \frac{1}{4} \text{O}_2 \Rightarrow \frac{1}{2} \text{H}_2\text{O} \text{ (liq)*} \) N in coal goes to N\(_2\)
    \( \text{S} + \frac{1}{2} \text{O}_2 \Rightarrow \text{SO}_2 \)
  – Moles of each product (CO\(_2\), H\(_2\)O, SO\(_2\), O\(_2\), N\(_2\))

\*H\(_2\)O product is liquid if the high heating value is specified!
Calculation of \( \Delta H_f^0 \) for Coal

Energy Balance

\[
Q = H_{products} - H_{reactants} = -Heating\ Value
\]
\[
H_{products} = \sum (n_i \tilde{H}_i)_{products}
\]
\[
H_{reactants} = \sum (n_i \tilde{H}_i)_{reactants}
\]

\( \tilde{H}_{coal} = \Delta H_{f,coal}^0 + \int_{25}\degree C}^{T} C_p,coal dT \)

For heat of formation calculation, reactants and products are at 25\degree C!
- Only need \( \Delta H_{f,products} \), not \( C_p \)'s
Calculation of $\Delta H_f^0$ for Coal (cont.)

- Since we are computing everything at 25°C,
  
  \[
  \hat{H}_i = \Delta H_{f,i}^0 + \int_{25^\circ C}^{25^\circ C} c_p,\text{coal} \, dT
  \]

  \[
  H_{\text{products}} = \sum (n_i \Delta H_{f,i}^0)_{\text{products}}
  \]

  \[
  H_{\text{reactants}} = \sum (n_i \Delta H_{f,i}^0)_{\text{reactants}}
  \]

- And since the gaseous reactant is air, $\Delta H_{f,\text{air}}^0 = 0$

- Therefore:
  
  \[
  -\text{Heating Value} = \sum (n_i \Delta H_{f,i}^0)_{\text{prod}} - m_{\text{coal}} \Delta H_{f,i}^0
  \]

Answer to Special Problem 29.1

\[
\Delta H_{f,\text{coal}}^0 = -3134 \frac{kJ}{kg \text{ of daf coal}}
\]

You will need to know how to get a heat of formation for coal when you do the case study!
Homework: Problem 29.2

Draw schematic

Basis: 1 gmol of methanol

(a) Find % excess air and dew point temperature of the product gas
(b) Find Q₁ and Q₂

Strategy:
(a) 1 mol methanol means 1 mol CO₂ produced, so find n₄₉₄
(b) Find n₀₂ and n₅₂ in outlet stream from yᵢ’s and n₄₉₄
(c) n₅₂ is same in inlet air, so find n₀₂ and hence % excess air
(d) Find Q’s from energy balances