What is the greatest hazard associated with continued use of gasoline and/or coal?
Using Hazard Information to Evaluate Technical Performance

"Yes! I found it...Now I have to remember what I need it for..."

Class 13 - Marty Mulvihill
What is the point of considering hazard anyway?

- Move beyond single metrics for performance, since we live in multi-dimensional space.
- Help make informed decisions.
- Avoid unnecessary hazards and risks.
- Develop robust precautions.

Green Chemistry is unique among various movements and trends in science and engineering because it considers hazard.
Outline for assignment and presentation next Monday

1. Our process is ____ the main steps are___.
   – Show overview of process
2. This process is attractive because....
   – Highlight differentiating factors
3. We considered the following potential impacts _____ because _____.
   – Show hazard tables
4. Key areas for future research
   – More data/research is needed to make x improvement or validate x claim.
5. Summary the main technology and impact drivers are_____ the main barriers are _____.
Types of Hazards

• **Immediate Hazards:** known and quantifiable (Acute Health, Explosively, etc.)

• **Characterized Chronic Hazards:** Known and quantifiable, but not personal. (Known Carcinogen, PM 2.5, etc.)

“India's breakneck pace of industrialization is causing a public health crisis with 80-120,000 premature deaths and 20m new asthma cases a year due to air pollution from coal power plants, a Greenpeace report warns.” - Guardian 3/11/13

• **Suspected Hazards:** Not easily quantifiable (Global Warming, Endocrine Disruptions, Data Gaps.)
Organizing and Comparing Hazards

• How the heck to you compare things with different units?
  
  – *Reference or Complementary compounds* (compare you emissions for x with gasoline emissions of x)
  
  – *Relative Severity* (compare all of the potential emissions from your process and decide which are the most concerning)
    • Hazard only approach (GreenScreen)
    • Hazard + Exposure (Risk and LCA)
Global Warming: Reference Compound gCO$_2$e (e=equivalents) for transportation

<table>
<thead>
<tr>
<th>Fuel</th>
<th>Pathway</th>
<th>gCO$_2$e Direct</th>
<th>gCO$_2$e indirect</th>
<th>gCO$_2$e total</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gasoline</td>
<td>Ave. CA Crude, CA refined.</td>
<td>95.9</td>
<td>0</td>
<td>95.9</td>
</tr>
<tr>
<td>Ethanol</td>
<td>Midwest Ave</td>
<td>69.4</td>
<td>30</td>
<td>99.4</td>
</tr>
<tr>
<td>Ethanol</td>
<td>CA Ave</td>
<td>65.66</td>
<td>30</td>
<td>95.66</td>
</tr>
<tr>
<td>Ethanol</td>
<td>CA Dry Mill, Wet Process</td>
<td>50.7</td>
<td>30</td>
<td>80.7</td>
</tr>
<tr>
<td>CNG</td>
<td>US produces, CA compress</td>
<td>68</td>
<td>0</td>
<td>68</td>
</tr>
<tr>
<td>CNG</td>
<td>Landfill gas, pipeline quality, CA compress</td>
<td>11.3</td>
<td>0</td>
<td>11.3</td>
</tr>
<tr>
<td>Electricity</td>
<td>CA Ave</td>
<td>124.1</td>
<td>0</td>
<td>124.1</td>
</tr>
</tbody>
</table>
Other Important Pollutants for consideration using reference compounds/sources:

- PM 10/2.5
- SOx
- NOx


California air resources board.

**Note:** These are not normalized per unit energy, they are CA wide emissions values.

These are all regulated and so there is a driver for data collection.

It is also hard to differentiate at times, since the standards will dictate emissions levels.
Hazards through out the lifecycle

The goal of the Hazard Tables is to help prioritize and compare the other chemical hazards that occur at other stages in the life cycle.

CO$_2$, SO$_x$, NO$_x$, PM all from the use phase...
## Hazard Tables

<table>
<thead>
<tr>
<th>ID</th>
<th>Reactivity</th>
<th>Flammability</th>
<th>Corrosivity</th>
<th>Explosivity</th>
<th>Acute toxicity (LD50)</th>
<th>Irritation (eye or skin)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Carcinogen / mutagen</td>
<td>Reproductive</td>
<td>Developmental (teratogenicity)</td>
<td>Neurotoxicity</td>
<td>Endocrine disruption</td>
<td>Respiratory effects</td>
</tr>
<tr>
<td></td>
<td>Persistence</td>
<td>Bioaccumulation</td>
<td>Acute aquatic toxicity (ecoindicator species)</td>
<td>Mobility</td>
<td>Other Ecotoxicity</td>
<td>Other Health</td>
</tr>
</tbody>
</table>


## GreenScreen Organization of Hazard Traits

### 18 Hazard Endpoints

<table>
<thead>
<tr>
<th>Human Health Group I</th>
<th>Human Health Group II and II*</th>
<th>Environmental Toxicity &amp; Fate</th>
<th>Physical Hazards</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carcinogenicity</td>
<td>Acute Toxicity</td>
<td>Acute Aquatic Toxicity</td>
<td>Reactivity</td>
</tr>
<tr>
<td>Mutagenicity &amp; Genotoxicity</td>
<td>Systemic Toxicity &amp; Organ Effects</td>
<td>Chronic Aquatic Toxicity</td>
<td>Flammability</td>
</tr>
<tr>
<td>Reproductive Toxicity</td>
<td>Neurotoxicity</td>
<td>Other Ecotoxicity Studies when available</td>
<td></td>
</tr>
<tr>
<td>Developmental Toxicity</td>
<td>Skin Sensitization</td>
<td>Persistence</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Respiratory Sensitization</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Endocrine Activity</td>
<td>Skin Irritation</td>
<td>Bioaccumulation</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Eye Irritation</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Weight the hazards relative to standards and data.

**Chemicals to be Avoided:**
- Characterized harmful to human health group 1 endpoints. (Cancer, Mutagen, Reproductive, Developmental, Endocrine)
  - “harmful” has different thresholds for each group.
- Very Bioaccumulative and Very Persistent
- Or combined PBT

<table>
<thead>
<tr>
<th></th>
<th>Considered Bioaccumulative</th>
<th>Considered Very Bioaccumulative</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bioconcentration factor (BCF)</td>
<td>&gt;= 1,000</td>
<td>&gt; 5,000</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>Considered Persistent</th>
<th>Considered Very Persistent</th>
</tr>
</thead>
<tbody>
<tr>
<td>Half-life in water, soil, and sediment</td>
<td>Half-life &gt;= 2 months (&gt;= 60 days)</td>
<td>Half-life &gt; 6 months (&gt; 180 days)</td>
</tr>
<tr>
<td>Half-life in Air</td>
<td>Half-life &gt; 2 days</td>
<td></td>
</tr>
</tbody>
</table>
Weight the hazards relative to standards and data.

**Chemicals with more acceptable Hazard:**
- Moderate harmful to human health group 1 endpoints. (Cancer, Mutagen, Reproductive, Developmental, Endocrine)
- High group 2 endpoints. (Acute Toxicity, reactivity and irritation)
- Very B/P with moderate tox (Group 1, 2 or Eco).

**Chemical with relatively little Hazard:**
- Moderate harmful to human health group 1 endpoints. (Cancer, Mutagen, Reproductive, Developmental, Endocrine)
- Moderate (Acute Toxicity and irritation)
- Moderate B/P

**Preferred Chemicals:**
- low(Cancer, Mutagen, Reproductive, Developmental, Endocrine)
- low (Acute Toxicity and irritation)
- low B/P
Logic/Assumption behind GreenScreen Ranking

1. High persistence and bioaccumulations increase the life-time risk of chemicals.
2. Chronic hazards are harder to mitigate than acute hazards because of the time lag between exposure and harm.

*Expectations for your evaluation:*

1. **Transparency**-Tell me where the data comes from and what assumptions you are making
   – It is OK to cite others’ protocol (CA air resources board, GreenScreen, EPI Suite, etc.)
2. **A reasonable not comprehensive scope**- Invest your time wisely. Choose substances and endpoints that are representative and help you compare to competing technologies.
## Taking a look at resources

<table>
<thead>
<tr>
<th>Website</th>
<th>Use</th>
</tr>
</thead>
<tbody>
<tr>
<td><a href="http://www.chemspider.com/">http://www.chemspider.com/</a></td>
<td>ID, Acute Hazards, EPI suite calculation, calculated and measured results (All chemical classes)</td>
</tr>
<tr>
<td><a href="http://www.pbtprofiler.net/">http://www.pbtprofiler.net/</a></td>
<td>Persistance, Bioaccumulations and Toxicity overview, Calculation only (Only Organic Chemicals, no metals or surfactants)</td>
</tr>
<tr>
<td><a href="http://www.cdc.gov/NIOSH/">http://www.cdc.gov/NIOSH/</a></td>
<td>Human Health Resource (All Chemical Classes)</td>
</tr>
<tr>
<td><a href="http://chem.sis.nlm.nih.gov/chemidplus/">http://chem.sis.nlm.nih.gov/chemidplus/</a></td>
<td>Both contain compellations of experimental data. Both link to HSDB which summarizes the literature. Interfaces and search criteria are slightly different. (All Chemical Classes)</td>
</tr>
<tr>
<td><a href="http://www.pharosproject.net">www.pharosproject.net</a></td>
<td></td>
</tr>
</tbody>
</table>
What to do next: Finding the data

Ecotox: ChemSpider/EPI Suite will give you your Persistence and Bioaccumulation Values. (days/hours, and BCF unitless, but sometimes expressed as LOG)
Ecotox LC$_{50}$ EC$_{50}$: ToxNet/HSDB/Animal Tox Studies/
EcoTox Values (mg/L)

LD$_{50}$ Values: ToxNet/HSDB/Animal Tox Studies/non-Human Tox Values

Endocrine Disruption: Pharos/Chemical and Material Library/

“Endocrine” you can click for more details.
Remember the Context

1. Our process is ___ the main steps are___.
   – Show overview of process

2. This process is attractive because....
   – Highlight differentiating factors

3. We considered the following potential impacts _____
   because _____.
   – Show hazard tables

4. Key areas for future research
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5. Summary the main technology and impact drivers are____
   the main barriers are ____.
Class Activity: Returning to Process diagrams and determining how to invest remaining resources.

1. Place Chemicals that you have hazard information about in their correct place.

2. Identify where you think difference in hazard may impact over-all sustainability?

3. Summarize the information that you will need to find to differentiate your process from competing processes.