Joint Stanford-Berkeley Carbon Capture and Sequestration Workshop

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www.lbl.gov/dir/eih/ccs/
Conclusions

• There will be many ideas that turn CO$_2$ into money, but not many of these will have any noticeable impact on global CO$_2$ levels (quote from Sally Benson)

• Yes we would like to generate as many options as possible, but we also need these ideas but we need to ensure that we can provide a feedback what the research targets will be if employed on a global scale

• A gigaton is beyond comprehension; evaluating targets is a research topic that includes economical and sociological impacts

• The targets depend on how the world will look like in 30 years;
  • a 50% reduction of total CO$_2$ emissions is sufficient
  • zero CO$_2$ emissions
  • negative emissions
What to do with a GIGATON of CO₂?

Abhoyjit S. Bhowm (EPRI):

Let’s convert CO₂ into “Dreamium™”

www.TwentyThousandMinusThreeAppsOfDreamium.com
## Making Dreamium™

<table>
<thead>
<tr>
<th>Rank</th>
<th>Chemical</th>
<th>2002 Production</th>
<th>Estimate +13% for 2007</th>
<th>GWe if equimolar rx with CO2 90% capture</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Mt</td>
<td>Mt</td>
<td>Gmol</td>
</tr>
<tr>
<td>1</td>
<td>Sulfuric Acid</td>
<td>36.65</td>
<td>41.54</td>
<td>423.54</td>
</tr>
<tr>
<td>2</td>
<td>Nitrogen</td>
<td>30.75</td>
<td>14.67</td>
<td>1244.65</td>
</tr>
<tr>
<td>3</td>
<td>Ethylene</td>
<td>23.87</td>
<td>26.83</td>
<td>338.44</td>
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<tr>
<td>4</td>
<td>Oxygen</td>
<td>22.04</td>
<td>24.98</td>
<td>560.27</td>
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<tr>
<td>5</td>
<td>Lime</td>
<td>16.42</td>
<td>20.57</td>
<td>372.24</td>
</tr>
<tr>
<td>6</td>
<td>Polyethylene</td>
<td>16.05</td>
<td>18.20</td>
<td>588.91</td>
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<tr>
<td>7</td>
<td>Propylene</td>
<td>14.43</td>
<td>16.36</td>
<td>360.27</td>
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<tr>
<td>8</td>
<td>Ammonia, Anhydrous</td>
<td>13.23</td>
<td>14.88</td>
<td>379.51</td>
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<tr>
<td>9</td>
<td>Chlorine</td>
<td>11.33</td>
<td>12.91</td>
<td>182.02</td>
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<tr>
<td>10</td>
<td>Phosphoric Acid</td>
<td>10.01</td>
<td>11.26</td>
<td>125.06</td>
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<tr>
<td>95</td>
<td>Sodium Bicarbonate</td>
<td>2.54</td>
<td>0.64</td>
<td>7.24</td>
</tr>
<tr>
<td>96</td>
<td>Cyclammones</td>
<td>2.54</td>
<td>0.64</td>
<td>6.19</td>
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<tr>
<td>97</td>
<td>Propylene Glycol</td>
<td>2.55</td>
<td>0.60</td>
<td>7.92</td>
</tr>
<tr>
<td>98</td>
<td>Phthalic Anhydride</td>
<td>2.53</td>
<td>0.60</td>
<td>4.03</td>
</tr>
<tr>
<td>99</td>
<td>Sodium Sulfate</td>
<td>3.54</td>
<td>0.64</td>
<td>4.08</td>
</tr>
<tr>
<td>100</td>
<td>Potassium Hydroxide</td>
<td>3.47</td>
<td>0.64</td>
<td>9.55</td>
</tr>
</tbody>
</table>

**Global top 100 chemicals production total ~ 0.5 Gt/yr; CO₂ Emissions ~ 30 Gt/yr**

A + CO₂ → ACO₂

Limited supplies of A & limited sales of ACO₂

Must regenerate A or produce A with CO₂ constraints for 335 GWe US coal power

*Source: American Chemistry Council*
GIGATON!

• **Useless options: Geological sequestration:**
  • there is the space for a gigaton and it is more or less proven technologies

• **Useful options: none at the gigaton scale!**

• ... but, with an increasing cost of producing CO$_2$ there will an increasing number of niche applications below the gigaton scale ...

• ... and these find a “scientific dessert”

• ... who in its scientific right might would be working on something as unexciting as CO$_2$?
Stage of CCS component technologies

<table>
<thead>
<tr>
<th>Stage of development</th>
<th>Concept</th>
<th>Lab testing</th>
<th>Demonstration</th>
<th>Commercial refinements needed</th>
<th>Commercial</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Membranes</td>
<td>Potential future breakthrough technologies</td>
<td>First projects are coming online now</td>
<td>Component technologies are mature; integrated platform to be proven</td>
<td>Several projects are operational (e.g., Weyburn (Canada)). EU has limited EOR potential</td>
</tr>
<tr>
<td></td>
<td>Chemical looping</td>
<td>Oxy-fuel</td>
<td>Post-combustion Pre-combustion</td>
<td>Depleted oil and gas fields</td>
<td>CO₂-EOR</td>
</tr>
<tr>
<td></td>
<td></td>
<td>CO₂-EGR</td>
<td>Saline aquifers</td>
<td>Transport off-shore</td>
<td>Transport On-shore</td>
</tr>
</tbody>
</table>

Sleipner (Norway) field has been operational for around 10 years

Have been used for seasonal gas storage for decades

US has existing CO₂ pipeline network of more than 5000 kilometers

Source: Interviews; Team analysis

Successful CCS involves two aspects: capture and storage.

**Capture** is currently considered to be the most **expensive** part of CCS.

**Geologic storage** involves **uncertainties** and risks when considered at full scale.
The aim of this EFRC is to develop new strategies and materials that allow for energy efficient selective capture or separation of CO$_2$ from gas mixtures based on molecule-specific chemical interactions.

**RESEARCH PLAN AND DIRECTIONS**

Capture of CO$_2$ from gas mixtures requires the molecular control offered by nanoscience to tailor-make those materials exhibiting exactly the right adsorption and diffusion selectivity to enable an economic separation process. Characterization methods and computational tools will be developed to guide and support this quest.
Integrating Carbon Capture R&D

Needs to work in < 5 years

Pilot Power plant With CCS
Engineering
Materials

NETL
Optimizing known concepts

Needs to work in 10, 15, and 25 years

1000 US Power Plants

Pilot Power plant With CCS
Engineering
Materials

NETL
Developing new concepts

EFRC
**In-silico Process Development**

- Configurational-Bias Monte Carlo simulations
  - Sorption isotherms
    - Ideal Adsorbed Solution Theory
      - Maxwell-Stefan diffusivities
        - Maxwell-Stefan theory for Zeolite Diffusion
          - Equations of continuity of mass and momentum
            - Permeation fluxes across membranes; Breakthrough curves in packed bed adsorbers
  - Molecular Dynamics Simulations; Transition State theory
    - Ideal Adsorbed Solution Theory
      - Maxwell-Stefan diffusivities
        - Maxwell-Stefan theory for Zeolite Diffusion
          - Equations of continuity of mass and momentum
            - Permeation fluxes across membranes; Breakthrough curves in packed bed adsorbers
  - Kinetic Monte Carlo simulations
    - Mixture diffusion
Scientific questions related to CO$_2$

• Conversion of CO$_2$: upgrading or downgrading
  • Upgrading: we need a source of energy (sun)
  • biological sequestration: how to improve the efficiency
  • chemical conversion

• Downgrading: we need to improve the kinetics (if geologically stored CO$_2$ becomes limestone in less than 10,000 years)
The Splitting of CO₂ – Conversion to the simplest potential fuel

2 CO₂ = 2 CO + O₂

- Only scheme that produces a fuel (CO) and O₂, and recycles CO₂.
- E₀ = -1.33 V Only 0.1 V more energetic than H₂O splitting.
- Still have to deal with the hardest part of H₂O splitting: O₂ evolution.
- CO₂ + 2 H⁺ + 2 e⁻ = CO + H₂O, E₀ = -0.1 V (NHE)
- O₂ + 4 H⁺ + 4 e⁻ = 2 H₂O, E₀ = +1.23 V (NHE)
- CO can be converted to H₂ and “synthesis gas” by “water gas shift”: CO + H₂O = CO₂ + H₂; to gasoline by “Fischer-Tropsch” process; to ethanol by microbial process (Lanza Tech (NZ)).

(source: Kubiak UCSD, 2009)
If you increase PV efficiency from ca. 20% to 30% (a gigantic step), you increase $\eta_{\text{overall}}$ by 50%.

Current efficiencies are already pretty good.

If you increase TOF from 1s$^{-1}$ to 1000s$^{-1}$ (in the catalyst limited regime), you increase efficiency by a thousand-fold.

Catalyst TOF is the highest gain parameter in the overall efficiency of solar to chemical energy conversion.

(source: Kubiak UCSD, 2009)
Solar capture, conversion, and electro-catalysis (Re catalyst)

Solar panel, voltage control, bulk electrolysis cell

Photochemical CO$_2$ Splitting:
CO observed by GC (32 mL/h)
4% overall efficiency (sunlight)

(source: Kubiak UCSD, 2009)
PV Operating Point

- 70 mA at 0.041 m² working electrode

(source: Kubiak UCSD, 2009)
Biological Carbon Capture and Fixation in Bacterial Microcompartments

Cheryl Kerfeld
US Dept of Energy, Joint Genome Institute
Dept of Plant & Microbial Biology, UC Berkeley
Integrated solutions
Sequestration can give a lot of salt water

Source: Christer Jansson (LBNL)
Integrated solutions

CO$_2$ as cushion gas for energy storage

Source: Curt Oldenburg (LBNL)
Recommendation

Generate Options

Evaluate Options