Computational Challenges in Geological Storage of Carbon Dioxide

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Three Main Points

1. CCS is necessary for 'Clean Coal'
2. CCS simulations controlled by computational limitations.
3. Large parametric uncertainties dominate the problem.
Outline

• Overview of the Carbon Problem
• Geological Storage and Leakage Estimation
• Computational limitations and model simplifications
• Example Application
• Conclusions
The Carbon Problem

>650,000 years
CO₂ Emissions

Current Global Emissions: ~30 Gt CO₂/yr ≈ 8 Gt C/yr
Projected Emissions (2059): ~60 Gt CO₂/yr ≈16 Gt C/yr
Stabilization Wedges

Billions of Tons Carbon Dioxide Emitted per Year

1 Wedge = 25 Gt C

Interim Goal

16 GtC/y

Eight “wedges”

How to Achieve One Wedge

1. Increase fuel efficiency of 2 billion cars from 30 mpg to 60 mpg.
2. Replace 1,400 large-scale coal power plants with natural gas plants.
3. Add twice today’s nuclear power, replacing coal.
4. Install CCS at 800 large-scale coal power plants.
5. Drive 2 billion cars on Ethanol, using one-sixth of cropland worldwide.
7. Increase Wind Power 25-fold, displacing coal.
How to Achieve One Wedge

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"We conclude that CO₂ capture and sequestration (CCS) is the critical enabling technology that would reduce CO₂ emissions significantly while also allowing coal to meet the world's pressing energy needs." (The Future of Coal, MIT, 2007)
Carbon Capture and Storage

- Current Number of Coal Plants Worldwide: 2,200

- Rate of building in China: 1-2 per week.

- Rate of building in US: <10 per year

- Potential number of wedges from CCS: 3 to 5.

- All projections of carbon reductions include a significant fraction from CCS.

- We need to understand the many aspects of CCS.
Storage in Deep Saline Aquifers

- Injected Supercritical CO$_2$:
  - Slightly miscible with brine (*solubility limit* ~4%)
  - Less dense than brine (*density ratio* 0.25 to 0.75)
  - Less viscous than brine (*viscosity ratio* 0.2 to 0.02)
  - Water can evaporate into (dry) CO$_2$.

- Geochemistry, Geomechanics, Nonisothermal, …
Standard Governing Equations

- Mass balance for component \( i \) in phase \( \alpha \):

\[
\frac{\partial}{\partial t} \left( \rho_\alpha \varphi S^\alpha \omega_i^\alpha \right) + \nabla \cdot \left( \rho_\alpha \mathbf{q}_\alpha \omega_i^\alpha \right) - \nabla \cdot \rho_\alpha \varphi \mathbf{D}_i^\alpha \cdot \nabla \omega_i^\alpha = F_i^\alpha
\]

- Geochemical Reactions:

\[
\begin{align*}
CO_2(g) & \leftrightarrow CO_2(aq) \\
CO_2(aq) + H_2O & \leftrightarrow H_2CO_3(aq) \\
H_2CO_3(aq) & \leftrightarrow H^+(aq) + HCO_3^-(aq) \\
HCO_3^-(aq) & \leftrightarrow H^+(aq) + CO_3^{2-}(aq)
\end{align*}
\]

- Geomechanics

- Non-isothermal Effects

- Monitoring, Inverse Problems, …
Equations of State

\[ \omega_{CO_2}^B = \omega_{CO_2}^B \left( p_\alpha, T_\alpha, \omega_{salt}^B \right) \]

\[ \mu_\alpha = \mu_\alpha \left( p_\alpha, T_\alpha, \omega_i^\alpha \right) \]

\[ \rho_\alpha = \rho_\alpha \left( p_\alpha, T_\alpha, \omega_i^\alpha \right) \]
Plume of Injected CO$_2$
Worldwide Density of Oil and Gas Wells

Number of Wells Drilled per ~10,000 km²

1 - 100  100 - 300  300 - 1,000  1,000 - 4,400  4,400 - 23,400  23,400 - 61,000  No Wells/Data

From IPCC SRCCS, 2005
Injection and Leakage

- How to model this system?
- Domain Size: 1,000 km²
- Leakage Pathways: 0.001 m².
- Flow Properties along well highly uncertain.
- Possible Material Degradation.

(From Duguid, 2006)
Numerical Modeling

Standard Simulations
- Need grid refinement around each well
- Need vertical resolution for multiple layers
- Minimum of hundreds of millions of grid cells.

Computational Options
- Upscale parameters in grid blocks with wells (*Gasda and Celia, 2005*)
- Local grid refinement / Local time stepping (*Gasda, 2007*)
- Dual-media approach around wells (*Gasda, 2007*)
- Simplified governing equations (*Nordbotten, Celia, …*)
Possible Simplifications

1. Macroscopic Sharp Interface
2. Vertical Equilibrium (structured vertical velocity)
3. Separation of Time Scales (focus on early time)
   a) Ignore bulk geochemistry
   b) Ignore non-isothermal effects

$$\phi(1 - S^\text{res}_B) \frac{\partial h}{\partial t} + \frac{\partial}{\partial x}\left[\bar{q}^C_x\right] + \frac{\partial}{\partial y}\left[\bar{q}^C_y\right] = -q^C_{\text{leak}}$$

$$\phi(1 - S^\text{res}_B) \frac{\partial (H-h)}{\partial t} + \frac{\partial}{\partial x}\left[\bar{q}^B_x\right] + \frac{\partial}{\partial y}\left[\bar{q}^B_y\right] = q^B_{\text{leak}}$$

$$\bar{q}^C = -h \frac{k k_{rel}^C (1 - S^\text{res}_B)}{\mu_C} \left(\nabla p_{\text{bot}} - \rho_B g \nabla H - (\Delta \rho) g \nabla h + \rho_C g \nabla z_{\text{top}}\right)$$

$$\bar{q}^B = -(H-h) \frac{k}{\mu_B} \left(\nabla p_{\text{bot}} + \rho_B g \nabla z_{\text{bot}}\right)$$
Numerical Solutions

Solve for $p(x,y,t)$, $h(x,y,t)$
Possible Simplifications

4. Locally constant fluid properties
5. Large-scale layering and concentrated leakage pathways dominate
6. Parameter uncertainty is important
7. Formations are horizontal and homogeneous
Analytical Solution

\[ \Gamma \equiv \frac{2\pi \Delta \rho g k \lambda_w H^2}{Q_{in}} \]
\[ \tau \equiv \frac{Q_{in} t}{2\pi H \phi (1 - S_{res})} \]
\[ \lambda_1 \equiv \frac{\lambda_c}{\lambda_w}, \quad \lambda_2 \equiv \frac{\lambda_{cw}}{\lambda_w}, \quad \vartheta \equiv \frac{\rho_{cw} - \rho_c}{\rho_w - \rho_{cw}} \]
\[ h' \equiv \frac{h}{H}, \quad i' \equiv \frac{i}{H} \]
\[ \chi \equiv \frac{r^2}{\tau} \]

(From Nordbotten and Celia, *JFM*, 2006; See Celia and Nordbotten, 2009)
Similarity Solution: Simplified

When $\Gamma < 0.5$:

$$h'(\chi) = \frac{h(\chi)}{H} = \frac{1}{\lambda - 1} \left( \sqrt{\frac{2\lambda}{\chi}} - 1 \right)$$

$$\chi_{\text{min}} = \frac{2}{\lambda}$$

$$\chi_{\text{max}} = 2\lambda$$

(From Nordbotten and Celia, *JFM*, 2006)
A Semi-analytical Model

1. Injection Plume, Secondary Plumes and Pressure Fields: Similarity Solution (*Nordbotten and Celia, JFM, 2006*)

2. Leakage Dynamics: Multi-phase Darcy Flow along Leaky Well Segments (*Nordbotten et al., ES&T, 2005, 2008*)

3. Upconing around Leaky Wells (*Nordbotten and Celia, WRR, 2006*)

4. Grid-free solutions: We can now solve 50 years of injection over 2,500 km², 12 layers, and 1,200 wells in about 10 minutes.

\[
Q_{well} \propto K_{well} k(S_\alpha)(\frac{p_1 - p_2}{H} - \rho \alpha g)
\]
Study Area around Edmonton – Wabamun Lake
Leakage: Nordegg Formation

![Leakage: Nordegg Formation](image)
Recent Developments

- High-performance Implementation (Elsa)
  - Complete re-implementation of code in C++
  - Highly modular, very efficient

- Expanded Physics in Semi-analytical Model
  - Diffuse leakage of brine through caprock formations
  - Improved similarity solutions for low flow rates

- User-friendly Interfaces
  - Web-based interface for simple systems
  - Multiple formats for input

- Separate numerical sharp-interface code (VESA)
- Hybrid numerical-analytical multi-scale models.
Concluding Remarks

• Simplified models can be reasonable because:
  – Buoyancy provides strong vertical segregation
  – Risk of leakage is maximum during injection period
  – Large uncertainties in critical leakage parameters limit utility of detailed fine-scale simulation

• Fully coupled detailed models are appropriate for:
  – Fine resolution along critical leakage pathways
  – Computational upscaling for bulk parameters
  – Basic Science

• Important practical questions require practical models \(\Rightarrow\) Hybrid multi-scale models.
Thank You!


## Layer Properties

<table>
<thead>
<tr>
<th>Aquifer Name</th>
<th>Depth [m]</th>
<th>Thickness [m]</th>
<th>Permeability [mD]</th>
<th># Wells</th>
<th>Max Inj Rate [Mt/year]</th>
<th>Wells reached by CO₂ plume</th>
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<tbody>
<tr>
<td>Belly River</td>
<td>729</td>
<td>56</td>
<td>86</td>
<td>1237</td>
<td>2.8</td>
<td>197</td>
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<td>Cardium</td>
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<td>15</td>
<td>7</td>
<td>1155</td>
<td>0.1</td>
<td>23</td>
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<td>Viking</td>
<td>1288</td>
<td>30</td>
<td>53</td>
<td>900</td>
<td>1.7</td>
<td>200</td>
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<tr>
<td>Mannville</td>
<td>1462</td>
<td>65</td>
<td>7</td>
<td>895</td>
<td>1.0</td>
<td>43</td>
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<tr>
<td>Nordegg/Banff</td>
<td>1538</td>
<td>80</td>
<td>4</td>
<td>733</td>
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<tr>
<td>Wabamun</td>
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<td>160</td>
<td>4</td>
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<td>1</td>
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<tr>
<td>Nisku</td>
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<td>72</td>
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<td>Keg River</td>
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<td>22</td>
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<td>14</td>
<td>16</td>
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<tr>
<td>Basal Sandstone</td>
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<td>38</td>
<td>23</td>
<td>1</td>
<td>2.6</td>
<td>1</td>
</tr>
</tbody>
</table>
Effective Well Permeability

- **Fully Random:**
  - Bi-modal lognormal distribution
  - Vertical correlation structure

- **Soft Data and Well Scoring System:**
  - Watson and Bachu (2008) well scores
  - Conditional probability distribution

- **Direct Measurements:**
  - Approach of Gasda et al. (2008) and Crow et al. (2008)
  - We are beginning to integrate these into our modeling framework
Leakage: Basal Sandstone

Baseline sandstone

\[ \log_{10} \text{fractional mass to surface} \]
Leakage: Nisku Formation

![Graph showing distribution of log10 fractional mass to surface for Nisku Formation. The graph has two modes, indicated by different colors, showing the distribution of data points.]