Transport and Dispersion Processes for CO_2 in the Unsaturated Zone and Surface Layer

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Introduction and Motivation

- Injection of CO_2 into deep geologic formations involves risk that CO_2 will migrate away from primary target.
- We are carrying out research on CO_2 transport for:

  (1) assessment of health, safety, and environmental (HSE) risk;

  (2) development of sequestration verification approaches (instrumentation requirements and monitoring strategies).

  - CO_2 seepage flux and near-surface concentration are risk drivers.

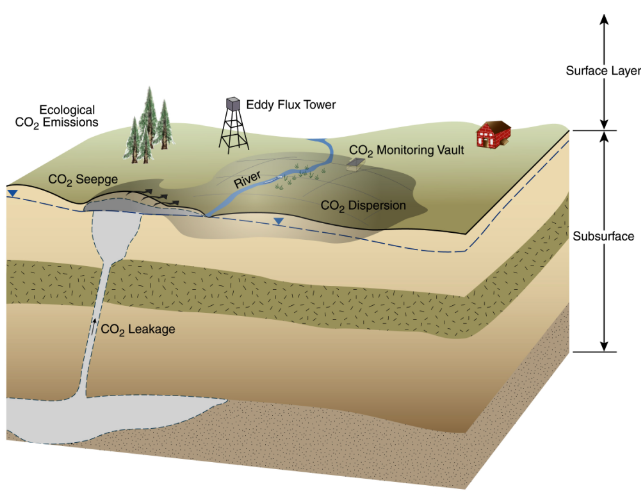
Approach:

Coupled subsurface-surface layer simulation to estimate CO_2 fluxes and concentrations

Outline

- Terminology.
- Leakage and seepage processes.
- Seepage case studies.
- Process modeling.
- Physical properties.
- Unsaturated Zone (UZ) simulations.
- Coupled UZ–surface layer simulations.
- Conclusions.

Leakage and Seepage from Geologic Carbon Sequestration Sites



Terminology

- Leakage = CO_2 migration away from primary sequestration target.
- Seepage = CO_2 transport out of the ground into the atmosphere or into surface water.
- Leakage/Seepage can be diffusive and/or advective.
- Dispersion = CO_2 dilution by advective and diffusive processes.
  - —Hydrodynamic dispersion in subsurface.
  - —Atmospheric dispersion above ground.
- Surface layer = bottom 1/10 of the atmospheric boundary layer.

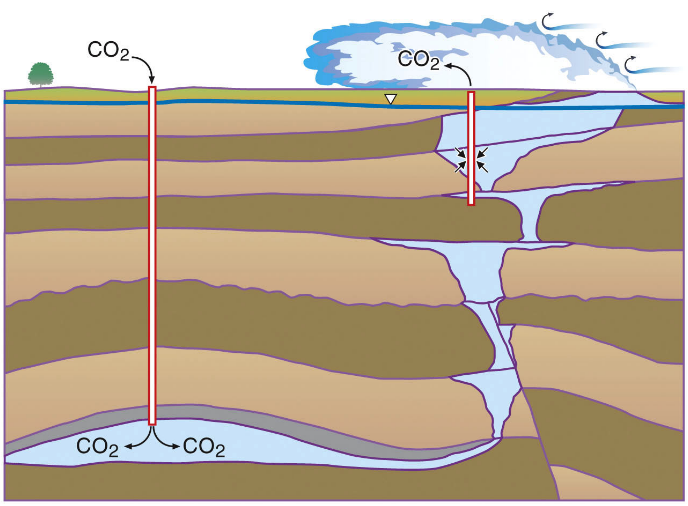
How Will CO_2 Leak?

- Upward buoyancy driving force for CO_2 is present in saturated rock. Geothermal gradient ensures positive (upward) buoyancy force.
- The length scale for leaking CO_2 increases:
  - —Buoyant CO_2 will spread out laterally against permeability barriers.
  - —CO_2 decompresses as it migrates upwards.
- Permeability is a scale-dependent property. Higher-k pathways more likely to be found by a larger buoyant and spreading plume.

How Will CO_2 Seep?

- CO_2 will convectively seep by upward buoyant flow if no unsaturated zone.
- CO_2 will advectively seep if there is a continuous source from the saturated zone.
- CO_2 will diffusively seep if concentrations exceed soil and ambient air concentrations.

CO_2 Leakage, Seepage, and Dispersion



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Case Studies: Seeping Gases

- Numerous examples of seeping gases exist.
  - Natural gas vents and blow holes (e.g., Rio Vista, ca. 1900).
  - Trace hydrocarbon gases above oil fields (e.g., Las Animas Arch, KS-CO).
  - Natural gas seeps (e.g., Santa Barbara Channel, CA).
  - Accidental natural gas storage releases, lateral migration, and escape through abandoned wells (e.g., Hutchinson, KS, Leroy Gas Storage, WY).

Process Modeling Approach

- T2CA (TOUGH2 for CO_2 and Air)
  - water, brine, CO_2, gas tracer, air, heat.
  - real gas properties for ρ and μ.
  - Henry's Law for solubility.
  - Subsurface and surface layer domains.
  - 3-D integral finite difference method.

- Surface Layer
  - Logarithmic velocity profile (passive flow).
  - Pasquill-Gifford and Smagorinski Model dispersivities.
  - Subsurface and surface layer are coupled.

Near-Surface CO_2 Density and Viscosity

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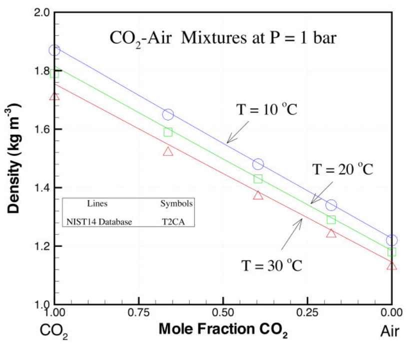

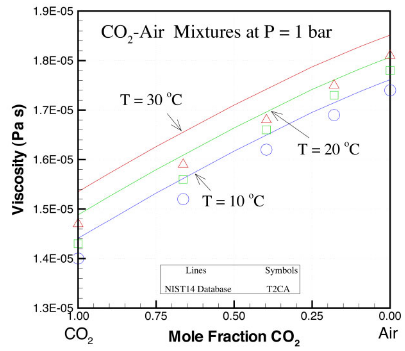

T2CA density and viscosity models agree to
within 5% of NIST14 Database values.

Gas Solubility in Water

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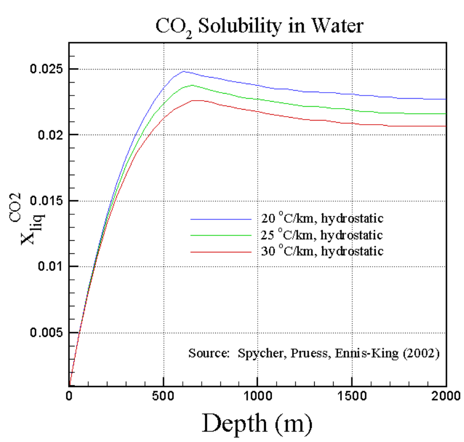

T = 25 °C, 1 atm

<u>Solubility</u> (mol L^{-1})

N_2	**0.68 x 10^{-3}**
O_2	**1.4 x 10^{-3}**
CO_2	**32. x 10^{-3}**

CO_2 is approx. 50x more soluble than air in water.

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CO_2 Migration Through 30 m of Unsaturated Zone with Infiltration 10 cm yr^{-1}

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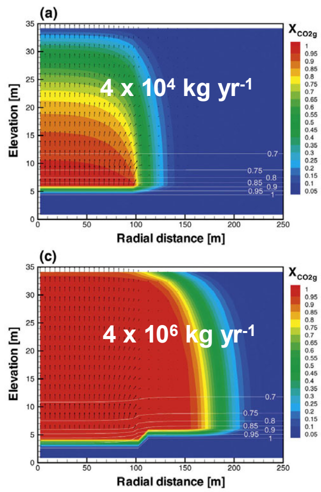

CO_2 mass fraction in the unsaturated zone for various CO_2 leakage flow rates.

Sensitivity of CO_2 Seepage and Soil Gas Concentration to Various UZ Properties

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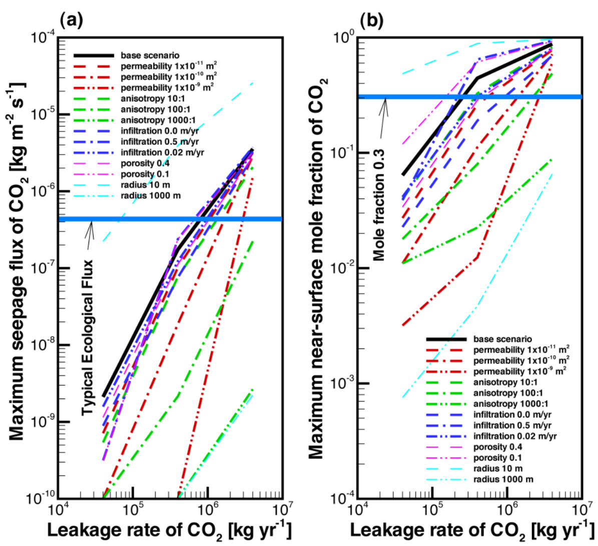
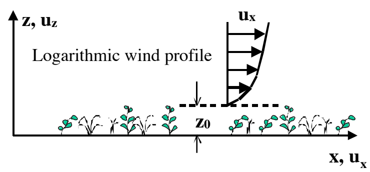


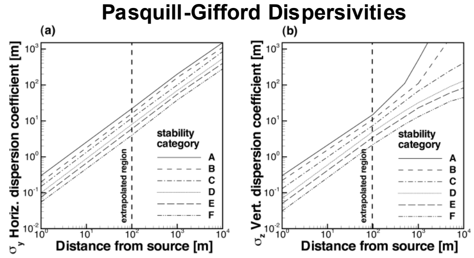
(Oldenburg and Unger, *Vadose Zone Journal*, 2003)

Surface Layer Modeling



$$u_x(z) = \frac{u_*}{k_*}\ln\left(\frac{z}{z_0}\right)$$

Pasquill-Gifford Dispersivities



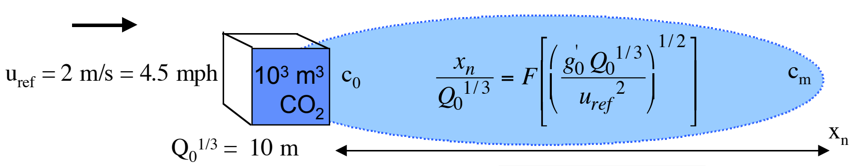
$$\sigma_x^2 = 2D_{xx}t$$
$$\sigma_y^2 = 2D_{yy}t$$
$$\sigma_z^2 = 2D_{zz}t$$

$$D = \frac{l^2}{\sqrt{2}}\left(\frac{\partial u_x}{\partial z} + \frac{\partial u_z}{\partial x}\right) = \frac{l^2}{\sqrt{2}}\frac{u_*}{k^*}\frac{1}{z}$$

Smagorinski Model dispersivities (*l* is a grid-related length scale).

Empirical Correlations of Atmospheric Dispersion of CO_2

(Britter and McQuaid, 1988)



x_n	c_m/c_0
100 m	0.02
200 m	0.008

Empirical results suggest atmospheric dispersion is effective in diluting dense gases over relatively short time and length scales.

However, calm conditions and topographic effects may alter these predictions and require numerical modeling approaches to assess.

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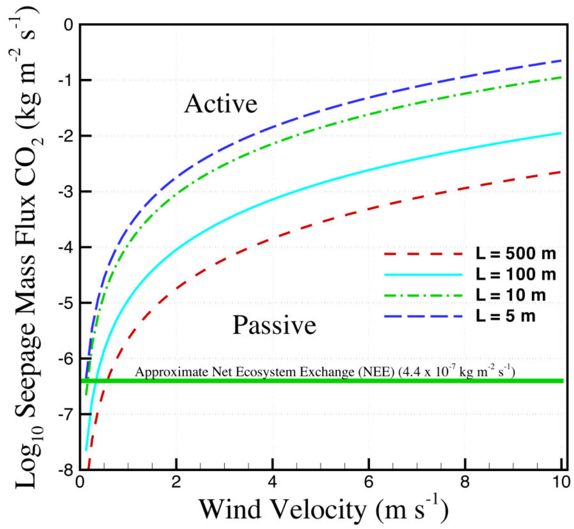
Criterion for Active vs. Passive Dispersion for Various Source Length Scales



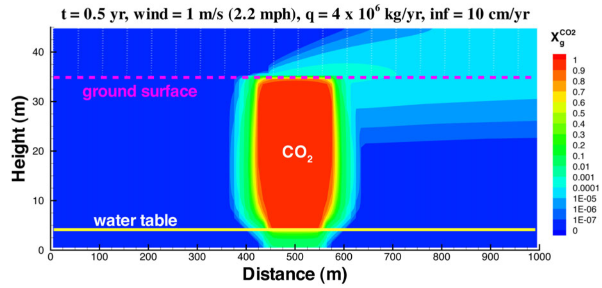
(correlation of Britter and McQuaid, 1988)

Properties of Coupled System

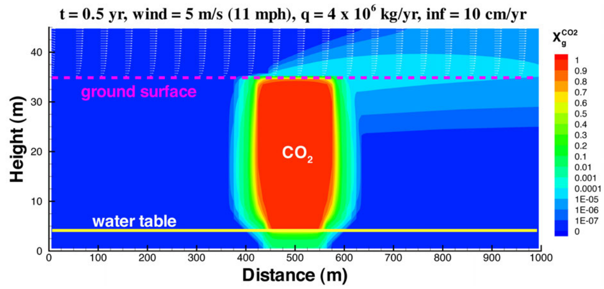
Property	Value
Subsurface	
Permeability ($k_r = k_Z$)	1×10^{-12} m^2
Porosity (ϕ)	0.2
Infiltration rate (i)	10. cm yr^{-1}
Residual water sat. (S_{lr})	0.1
Residual gas sat. (S_{gr})	0.01
van Genuchten (1980) α	1×10^{-4} Pa^{-1}
van Genuchten (1980) m	0.2
Surface Layer	
Friction velocity for $u_x = 1$ m s^{-1}	0.0869 m s^{-1}
Friction velocity for $u_x = 5$ m s^{-1}	0.434 m s^{-1}
Reference height (z_0)	0.10 m
Reference velocity at $z = 10$ m	1 or 5 m s^{-1}

Preliminary T2CA Results

t = 0.5 yr, wind = 1 m/s (2.2 mph), q = 4 x 10^6 kg/yr, inf = 10 cm/yr

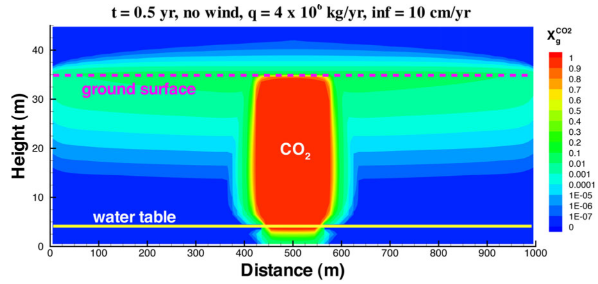


t = 0.5 yr, wind = 5 m/s (11 mph), q = 4 x 10^6 kg/yr, inf = 10 cm/yr

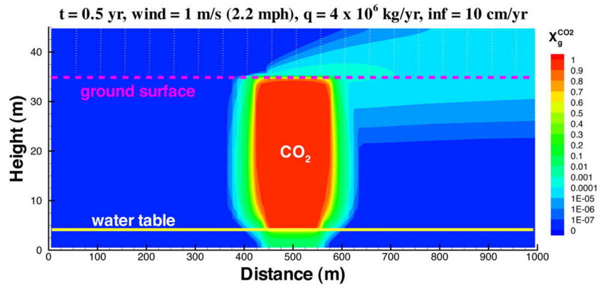


Preliminary T2CA Results

t = 0.5 yr, no wind, q = 4 x 10^6 kg/yr, inf = 10 cm/yr



t = 0.5 yr, wind = 1 m/s (2.2 mph), q = 4 x 10^6 kg/yr, inf = 10 cm/yr



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Conclusions

- Leakage and seepage of gases are common.
- Leakage rate and source area strongly control seepage.
- Although diffuse seepage flux may be small, CO_2 concentrations in shallow soil can be large.
- Unsaturated zone can attenuate small leakage fluxes but should not be counted on to attenuate large CO_2 leakage fluxes.
- Rainwater infiltration returns CO_2 to the subsurface.
- Atmospheric dispersion is effective at diluting gases.
- CO_2 concentrations may be higher in low-lying and stagnant (low-wind) areas.

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Acknowledgments

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