Dispersion of CO2 in the water column

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**CO₂ under seabed storage and challenge: Leakage prediction and risk management**

**The Sleipner field**

CO₂ Treatment and Injection

**Potential Escape Mechanisms**

- A. CO₂ gas pressure exceeds capillary pressure & escapes through siliciclastites
- B. Free CO₂ escapes through *a* gas cap rock into higher aquifer
- C. CO₂ escapes through gas cap rock into higher aquifer
- D. Injected CO₂ migrates up dip, increases reservoir pressure & permeability of fault
- E. CO₂ escapes via natural leakage from CO₂ / water interface & transports it out of closure
- F. Injected CO₂ dissolves CO₂ at CO₂ / water interface & transports it out of closure
- G. Dissolved CO₂ escapes to atmosphere or ocean

**Remedial Measures**

- A. Extract & purify ground-water
- B. Extract & purify ground-water
- C. Remove CO₂ & re-inject elsewhere
- D. Lower injection rates or pressures
- E. Plugging well with cement
- F. Infrasound & re-inject CO₂
- G. Infrasound & re-inject CO₂

**CO₂ leakage mechanisms** (IPCC SRP on CCS, Chapter 5, 2005)

**Morphology of Sea Urchin Larva** (Kurihara & Shirayama, 2004)
Model Synthesis (WP2 + WP6.3 of QICS)

WP 1 RISCS

WP 2.3 L-B sediment dispersion

WP 2.1 and 2.2: Bubble / plume dispersion

WP 2.5 Fine scale hydrodynamics FSPOLCOMS / FVCOM

POLCOMS 1.8km resolution shelf model

Set of exposure scenarios at epicentre, locality and region

CO2 propagation

physics

Use these to drive 1D ERSEM

System impact
I. Background

II. Modelling of CO$_2$ dispersion in a small-scale ocean
   a) Dynamics of CO$_2$ drop/bubble in seawater
      • Numerical models developed
      • Model calibration with observation data from Lab. and small scale field Exp.
   b) Model application: Dispersion of Leaked CO2 from North seabed

III. Summary and suggestions
Background

Under seabed:
- Multi-fluid/phase
- Porous media, stratification
- Interface actions (fluids and fluid/solids)

Sediments:
- CO2 hydrate formation

Ocean:
- Turbulent boundary layer
- Multi-fluid plume
- Stratification, free surface
- Bubble/drop dynamics
- Chemical/Bio-impacts

Sea surface
Sediments layer (hydrate formable)
Cap rock
Geo-formations
CO2 solution plumes
CO2 plume under seabed
CO2 leaked to ocean

Saline water reservoirs

Produced oil or gas
Injected CO2
Stored CO2
Scales and the roles of ocean turbulence on dispersions of leaked CO$_2$ in the ocean

Background energy spectra from Wood, Science 1999
Theory and methodology for two-phase small-scale turbulent ocean model

Large-scale information from Boundaries:
- Mean properties \((X,t)\)
- Turbulent properties at \(K > K_f\)

Inside of small-scale ocean:
- N-S based 3-D unsteady Governing Eq.s for CO2 & seawater
- Forced-dissipative Energy cascade theories
- Adjusted by observation spectrum

Data analysis
Field Obs. Data
Governing Eq.s of two-fluid small-scale turbulent ocean

**Governing Eq.s of Seawater**

\[
\begin{align*}
\frac{\partial \rho}{\partial t} + \frac{\partial \rho \hat{u}_i}{\partial x_i} &= \dot{w}_{dco} \\
\frac{\partial \rho \hat{u}_i}{\partial t} + \frac{\partial \rho \hat{u}_i \hat{u}_j}{\partial x_j} &= -\frac{\partial \hat{p}}{\partial x_i} + \frac{\partial D_{ij}}{\partial x_i} + (\rho - \rho_0) g_i \\
&\quad + (\hat{F}_d) + F_f \delta_{ij} \\
\frac{\partial \hat{p}}{\partial x} &= \frac{\partial P^*}{\partial x} - \rho_0 g_i \\
\frac{\partial \rho \hat{\phi}}{\partial t} + \frac{\partial \rho \hat{\phi} \hat{u}_i}{\partial x_i} &= \frac{\partial}{\partial x_i} (\rho D_{\phi}) + \frac{\partial \rho \hat{q}_i}{\partial x_i} + \dot{w}_{dco} \delta_{ij}
\end{align*}
\]

**Governing Eq.s of CO_2 plume**

\[
\begin{align*}
\frac{\partial \hat{n}_a}{\partial t} + \frac{\partial \hat{n}_a \hat{u}_0}{\partial x} &= \hat{q}_{dn} \\
\frac{\partial \hat{\alpha}}{\partial t} + \frac{\partial \hat{\alpha} \hat{u}_0}{\partial x} &= \hat{q}_{d\alpha} - \dot{w}_{dco} / \rho \\
\frac{\partial \rho \hat{u}_a}{\partial t} + \frac{\partial \rho \hat{u}_a \hat{u}_0}{\partial x} &= \frac{\partial \rho \hat{\tau}_i}{\partial x} + \hat{\alpha} (\rho - \rho_0) g - (\hat{F}_{\text{eco}})
\end{align*}
\]

Coupled by source terms highlighted by underlines, which are the models of CO2 droplet/bubbles, LES turbulent model and density change model of CO2 solution.
Example of reconstruction of small-scale turbulent ocean

(Chen et al, Direct and Large-Eddy Simulation, 2005)

Modeling prediction of turbulent kinetic energy (TKE in \( \text{m}^2\text{s}^{-2} \)) distribution on a horizontal section at depth of 750 m (Keahole case)

Experimental data obtained by CREIPI at Keahole Pt. Offing (19°43.324N; 156°04.806W)
An integrated model of CO$_2$ droplet/bubble leaked from seabed

a) Sub-model of CO2 properties
   • CO2 solubility
   • CO2 phase diagram

b) Sub-model of individual CO2 droplet/bubble
   • Momentum exchange sub-model
   • Mass transfer sub-model
CO₂ Phase diagram

- PG < 4.56 MPa
- TG > 9.1°C
- Ps > 7.39 Ma
- Ts > 31.5°C

- CO₂ Gas
- CO₂ Hydrate
- Liquid CO₂ in deep saline formations
- Supercritical CO₂
Governing Eq.s of a Drop/Bubble in seawater

Momentum exchange Eq.

\[
\frac{du_r}{dt} = \frac{\rho_s}{\rho_c} \left( (1.0 - \frac{\rho_c}{\rho_s}) g - \frac{3u_r^2}{4D} C_d \right) - u_r \frac{d \ln(m_c)}{dt}
\]

Mass Eq.

\[
\frac{dd_e}{dt} = -\frac{1}{\rho_c} \left( \frac{d_e}{3} \frac{d \rho_c}{dt} + 2k(C_s - C_0) \right)
\]

- \( u_r \): slip velocity
- \( d_e \): equivalent diameter of bubble
- \( C_s \): solubility
- \( \rho \): density

Key Parameters:
- \( k \): mass transfer coefficient
- \( C_s \): CO\(_2\) solubility
- \( C_d \): drag coefficient

Shape (spherical or deformed) & interfaces (solid, liquid, and gas to water)
Model validation: CO₂ droplet in deep ocean

Droplet dissolving modeling vs data
(Chen et al., JGR 2005 and field Exp data by P. Brewer et al, EST, 2003)

Droplet velocity modeling vs data
(Nikolaus et al. EST, 2008)
Model validation: CO\textsubscript{2} bubble in shallow ocean

ADCP backscatter showing bottom “flares” (red signal) at Salt Dome Juist, north sea. CO\textsubscript{2} bubble size (de) 4 – 8 mm. (F. Daniel et al, University of Kiel, to be published by JGR)

Numerical simulation of CO\textsubscript{2} bubbles leaked from seabed (Chen et al, GHGT-9, 2008)
Model validation: Field Exp of direct injection of LCO2 into the ocean

- Location: Monterey Bay (Tubeworm Slump, 36.6417 N, 122.4158 W)

- Motivations:
  - Test new Acoustic Sonar system for monitoring
  - CO2 plume dynamics

- Time: 17 ~ 21, Nov. 2005
CO₂ droplet plume monitored (right top) and (right-bottom) (Brewer & Chen et al, GRL 2006)
Acoustic Detection (top) and modeling (bottom) of CO$_2$ plume at horizontal (Brewer & Chen et al, GRL 2006)
Application example: Dispersion of leaked CO2 from North seabed

- **CO₂ leakage parameters:**
  - Leakage rates: 0.5 kg/s/m²
  - Ocean current: 0.5, 0.05 m/s
  - Initial bubble sizes: 10, 15, 30 mm

- **Leakage site:**
  - North sea (58.53N 0.21E)
  - Leakage depths: 30m, 82m; 150m
CO₂ bubble (left) and CO₂ enriched water plumes at T=1.0hr

Leakage depth: 150m; de=10 mm; Uc = 0.5m/s; CO₂ leakage rate: 0.5kg/m²/s

Along the current (km)
Volume of CO₂ enriched plume with pH changes

<table>
<thead>
<tr>
<th>Case</th>
<th>Leakage depth (m)</th>
<th>Season</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>150M</td>
<td>Summer</td>
</tr>
<tr>
<td>2</td>
<td>150M</td>
<td>Winter</td>
</tr>
<tr>
<td>3</td>
<td>80M</td>
<td>Summer</td>
</tr>
<tr>
<td>4</td>
<td>80M</td>
<td>Winter</td>
</tr>
<tr>
<td>5</td>
<td>30M</td>
<td>Summer</td>
</tr>
<tr>
<td>6</td>
<td>30M</td>
<td>Winter</td>
</tr>
</tbody>
</table>

All cases: $D_e = 15 \text{ mm}; \ U_c = 0.05 \text{ m/s}; \ T = 1.0 \text{ hr};$
## Effects of current, leakage depth, rate and bubble size

<table>
<thead>
<tr>
<th></th>
<th>Max height of seawater plume (m)</th>
<th>Effective volume per unit width of pH Distribution (m²)</th>
<th>Maximum pH change</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Base Case</strong></td>
<td>13.35</td>
<td>24033</td>
<td>1.571</td>
</tr>
<tr>
<td><strong>Ocean current: 0.0 m/s</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Leakage depth: 150m</strong></td>
<td>15.82</td>
<td>4270</td>
<td>2.832</td>
</tr>
<tr>
<td><strong>CO2 leakage rate: 1.0 kg/m²/s</strong></td>
<td>15.41</td>
<td>27730</td>
<td>1.572</td>
</tr>
<tr>
<td><strong>Initial bubble size: 30 mm</strong></td>
<td>14.99</td>
<td>26991</td>
<td>1.854</td>
</tr>
</tbody>
</table>

**Note:** The table values are rounded for clarity.
Summary and suggestions

• Summary:
  – A two-phase model of leaked CO₂ dispersion in small scale turbulent ocean is developed
  – Model is validated by available Lab. and filed observation data from shallow and deep ocean

• Improvements:
  – More field exp data of CO₂ bubble/drop plume
  – Model of CO₂ phase transition (depth 400 – 300m)
  – Model of bubble/drop interactions

• Nesting to the mesoscale model (QICS)

• Development and nesting to the model of CO₂ dispersion through sediments (QICS)
Acknowledgements

- Dr. Peter Brewer of MBARI, USA, for collaboration on CO2 field observations.
- Mr. Jerry Blackford, PML, project leader and modelling collaboration.
- Mr. Marius Dewar, student of Heriot-Watt University, performed the Case studies

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WP 2.5 Physical coupling of fine scale and regional hydrodynamic models

Previously we have resolved ‘events’ at rather coarse scales based on the POLCOMS – ERSEM platform.

The challenge is to resolve the local scale:

Two possible approaches:

Nesting either

200m scale POLCOMS (tried and trusted)
FVCOM model which resolves down to 5m (new technology)
Lab. Exp on CO$_2$/CO$_2$ solution at capillary-scale pours

$\rho_{in}$

$\rho_w$

$\rho_s$

$\rho_c$

$\rho_{out}$

$\varepsilon$: Porosity of geo-formations

$\mu$

$\rho_c < \rho_w < \rho_s$

Geo fluids: saltwater and oil

CO$_2$ water/oil solutions or CO$_2$ hydrate

CO$_2$ (Liquid or supercritical)

Interaction among CO$_2$, CO$_2$ solutions, geo-fluids, geo-grains

Microscope + High speed CCD camera
Preliminary Experiments

CO2 bubble shrinking in a chancel (dini = 2.8mm) at atmosphere pressure and temperature

Challenge: (RA’s work)

- Suitable exp set up with Microscopic system and capillary pressure
- Observation of micro-dissolution (Micro-PIV?)
LBM model of CO$_2$ dispersion and dissolution in pore scale

**Advantage:**
- First principle from Boltzmann distribution
- Direct treatment of interface actions

**Specifics:**
- Physic space – Dimensionless --- LBM space

Distribution function: $f_a(x, e_a, t)$

Macroscopic density: $\rho = \sum_{a=0}^{8} f_a$

Macroscopic velocity: $u = \frac{1}{\rho} \sum_{a=0}^{8} f_a e_a$

\[ f_a(x + e_a \Delta t, t + \Delta t) = f_a(x, t) - \frac{\left[ f_a(x, t) - f_a^{eq}(x, t) \right]}{\tau} \]
Challenge: (RA + PhD)

- CO2/Water system (EOS)
- Dissolution model (no one available)
Preliminary Schedule

• Sept-10 – Sept. 11:
  – Task 2.1
  – Task 2.2 (Small-scale ocean model)
  – Task 2.3 (Preliminary Lab exp: dispersion rate)
  – Task 2.3 LBM: CO2 EOS, interface tension

• Sept 11 – Sept. 12:
  – Task 2.2: Coupling Small-scale ocean and bubble model
  – Task 2.3 Lab exp: dissolution rate
  – Task 2.3 LBM: Dissolution model

• Sept, 12 – Sept. 13
  – Task 2.2: Modelling simulations and nesting to meso-scale model (WP2.5)
  – Task 2.3 Lab exp data analysis and model development
  – Task 2.3 LBM: Coupling dispersion and dissolution and case simulations
III-2. Governing equations for reconstructing a small-scale turbulent ocean
(Chen et al, Tellus, 2003)

a. Forced-dissipative system of small-scale ocean:

\[
\frac{\partial \bar{\rho} \hat{u}_i}{\partial t} + \frac{\partial \bar{\rho} \hat{u}_i \hat{u}_j}{\partial x_j} = -\frac{\partial \bar{\rho}}{\partial x_i} + \frac{\partial D_{ij}}{\partial x_j} + (\bar{\rho} - \rho_0) g_i + (\ddot{F}_d) + F_f \delta_{ij}
\]

**Forced term:**

\[F_f = \bar{\rho} \bar{u}_0'(k, t) / \sum_{k \in k_f} u_0'(k, t) u_0'(k, t) \quad k \in k_f\]

**Dissipative term:**

\[D_{ik} = 2 \rho \nu_t \bar{S}_{ik}\]

b. Structure function turbulent viscosity model

\[F_2^k = 0.25 \times \sum (u_k(x_k) - u_k(x_k - \Delta x_k))^2\]

\[\nu_t^k(x_k, \Delta x_k) = 0.15 C_k^{-3/2} \Delta x_k [F_2^k(x_k, \Delta x_k)]\]
Bubble dynamics in sediments

An X-Ray CT image of a sediment with inter-banded clay and carbonate sand layers and containing (post-collection?) bubbles in both types of sediments (black circles and ellipses).

Bubbles in the sands are spherical away from mud contacts, e.g., as indicated by the red arrow labelled “a” whereas the bubbles in the muds are oblate spheroids, e.g. as indicated by the yellow arrow labelled “b’.

Bernard, P. Boudreau, et al, GRL, 2004
LBM- CO2 dispersion in a channel and a porous media

Bubble rising in a channel (LBM)

T = 0; 900  1700  2500  3500

Wie, W & Chen; to be submitted
I-3. Characteristics of CO₂ droplet & bubble

\[ Eo = \frac{\Delta \rho g d_e^2}{\sigma} \]

Oscillation \( Re > 900; \ We > 2; \ Eo > 0.8 -1.0 \)

- \( \sigma = 0.075 \) (Hirai, RITE-rpt & Yamane, GHGT-5) \( T=2 \sim 5C \)
- \( \sigma = 0.029 \) (LCO2-W, Uchida, RITE-rpt)

Exp \( dv/dh \) (Ozaki et al. JMST, 2001)

Bound for deformation (Clift et al)
Bound for Large-deformation (Clift et al)
For CO₂ under seabed storage, there exists a potential possibility that stored CO₂ could migrate and leak into water column at an engineering scales, which will *alter the local chemical environment*.

Lab. experiments have shown that sustained high concentrations of CO₂ would cause *mortality of ocean organisms*. The effects of leaked CO₂ on marine organisms will have ecosystem consequences.

The chronic effects of leaked CO₂ at an engineering scale on ecosystems over large spatial and long time scales *have not yet been understood (studied?)*.  

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**Challenge:** Marine environmental impacts, risks and risk management
Natural CO₂ plumes in the ocean

CO₂ bubble plume near Panarea, Italy. (Photo by Giorgio Caramanna, Nottingham University, UK)

B: ‘‘Lion chimney,’’ active black smoker vents. E: Liquid CO₂ droplets from the ‘CO₂ lake’ in Southern Okinawa. (Fumio Inagaki et al, PNAS, 2006)
Bio-impact modeling test (deep ocean)
(Activity index of zooplankton without recovering,
Chen et al, JO, 2005)

Bio-impact indicated by an activity index of zooplankton; 1.0: normal; 0.0: the worst

pH plume

Bio-impact indicated by an activity index of zooplankton; 1.0: normal; 0.0: the worst

Mc=0.6kg/s; D₀ =8.0mm
T=100.3 min; Target ocean: Okinawa
Bio-impact modeling test (deep ocean)
(Activity index of zooplankton without recovering)

Chen et al, JO, 2005

Bio-impact indicated by an activity index of zooplankton; 1.0: normal; 0.0: the worst

pH plume

\[ \text{Mc=}0.1\text{kg/s; } D_0=8.0\text{mm} \quad T=100.3\text{ min} \]
I-1. What does the leaked CO2 look like?,
(Dr. Nakajima, NSRI, Japan)
II-a-2. Developed and undeveloped Drop/Bubble models

- **Gas CO$_2$**
  - 
  - **G CO$_2$-seawater** (Clift & Crace, 1978; Bozzano et al. 2000)

- **L/G CO$_2$ phase change??**

- **L$\rightarrow$G CO$_2$-seawater** (Chen et al., *Tellus*, 2003)

- **L-CO$_2$**
  - 
  - **L$\rightarrow$H CO$_2$-seawater** (Clift & Crace, 1978; Chen et al. 2008)

- **L-CO$_2$ + Hydrate**
  -
  - **L$\rightarrow$H CO$_2$-seawater** (Chen et al., *Tellus*, 2003)

Depth

-500m

-800m

Temperature

9°C  12°C
II-a-8: ROV observation of CO$_2$ droplet/bubble transition

Monterey Bay, CA (36.7°N 122.1°W)
Depths: 510m to 380m
The ROV: Ventana
II-a-9. Observation data of CO$_2$ phase transition and dissolution

Rayleigh-Taylor instability:
$\text{d}b = 4.0 - 5.0 \text{ mm}$

a) Droplet at 435 m.
b) A small bubble appeared at 416 m and in-situ time of 12:40:11;
c) & d) Liquid part shaking at in situ time of 12:59:02 and 12:59:29;
e) First breakup of liquid part and formed a coalesce part (top) and a droplet at 13:01:09.
f) Two separated droplet/bubble departed at 13:02:22.
g) Second break up occurred from the liquid part of the coalesce droplet.

Droplet/bubble transition (Chen, B & P. Brewer; GRL to be submitted)
II-a-3. Sub-model of CO$_2$ solubility & phase diagram
II-a-4. \textbf{Cd} for droplet/bubble \hfill (Chen et al, Tellus, 2003 and GHGT9, 2008)

\[ C_d = f (M, Eo, Re, \gamma_\rho) \cdot \left[ \frac{d}{d_e} \right]^2 \]

1). Droplet/Bubble with hydrate film covered:

\[ f(Re) = 24(1 + 0.125Re^{0.72}) / Re \]

\[ \left[ \frac{d}{d_e} \right]^2 = 1.0 + (5.6419 - 8.3484 \times 10^{-3} + 1.4596 \times 10^{-6} Re^2) \times 10^{-4} Re \]

2). Droplet/bubble:

\[ f(M, Eo, Re, \gamma_\rho) = \frac{24}{Re} f_1(Re, \gamma_\rho) \cdot \frac{1 + 12M^{1/3}}{1 + 36M^{1/3}} + f_2(\gamma_\rho) \frac{Eo^{1.5}}{1.4(1 + 30M^{1/6}) + Eo^{1.5}} \]

\[ \left[ \frac{d}{d_e} \right]^2 = \frac{10(1 + 1.3M^{1/6}) + 3.1Eo}{10(1 + 1.3M^{1/6}) + Eo} \]

\[ f_1 = 1 + \gamma_\rho (1.45 - 1.079 \times 10^{-3} Re) \]

\[ f_2 = 1.5617 - 0.8405\gamma_\rho \quad \gamma_\rho = \frac{\rho_C}{\rho_w} \]
II-a-5: Sub-model of CO$_2$ drop/bubble dissolution

**Droplet with hydrate** (Chen et al, 2003):

\[
Sh_e = (2 + 0.69 \text{Re}^{1/2} \text{Sc}^{1/3})(A_{\text{eff}} / A_{\text{eq}})_{sh}
\]

\[
(A_{\text{eff}}/A_{\text{eq}})_{sh} = 1.0 + \text{Re}(4.6707 \times 10^3 \text{Re}^{-1} + 1.4766 \times 10^5 \text{Re}^{-2} ) \times 10^4
\]

**Droplet** (Clift & Crace, 1978):

\[
Sh = \frac{2}{\sqrt{\pi}} \left( 1.0 - (2.89 + \frac{2.15 \lambda^{0.64}}{\text{Re}^{0.5}})^{0.5} (\text{ReSc})^{0.5} \right) \lambda = \frac{\mu_c}{\mu_w}
\]

**Bubble** (Clift & Crace, 1978):

\[
0.0113 \left( \frac{u_d D_f}{0.45 + 0.2d_e} \right)^{0.5} \quad \text{if} \quad d_e \leq 0.5
\]

\[
K = 0.065 D_f^{0.5} \quad \text{if} \quad 0.5 < d_e \leq 1.3
\]

\[
0.0694 d_e^{-1/4} D_f^{0.5} \quad \text{if} \quad 1.3 < d_e
\]
II-a-10. Terminal distance and time of Leaked CO₂ droplet/bubble

**Terminal distance:** the distance rising from leaked depth

**Terminal time:** The time till to completely dissolved
II-b-3. Density change of CO2 solution


The effects of temperature on density ratio
Tasks of WP 2 of QUICS

2.1 Experimental and theoretical study of CO2 dynamics in seawater (HW).
2.2 Development of small-scale two-phase turbulent ocean modelling (HW, PML)
2.3 Parameterisation and modelling of CO2 dispersion in sediments. (HW)
2.4 Biochemical & ecological models of impacts. (PML, NOCS, SAMS)
2.5 Physical coupling of fine scale and regional hydrodynamic models (POL, HW)