Modelling overview for CO$_2$ storage

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Why Modeling?

The ultimate goal is risk management which will rely on models & surface/atmosphere monitoring
CO2 Storage Workflow

Pre-Operation Phase
- Site Selection
- Site Characterization (SCP)
- Field Design
- Site Preparation
- Site Construction
- Injection
- Monitoring (M&V)
- Site Retirement Programme (SRP)
- Transfer of Liabilities

Operation Phase
- Permitting
- ~ 3-5 year

Post-Injection Phase
- ~ 10-50 years
- Transfer of Liabilities
- ~ 100+ years

Performance Management & Risk Control System
- Communication and Public Acceptance
- NEGLIGIBLE: Safe to proceed
- ACCEPTABLE: Proceed carefully, with continuous improvement
- UNDESIRABLE: Demonstrate ALARP before proceeding
- NON-OPERABLE: Evacuate the zone and/or area/country
- IN TOLERABLE: Do not take this risk

Likelihood
- Possible
- Unlikely
- Improbable
- Probable
- Likely
- Serious
- Major
- Catastrophic
- Multi-Catastrophic

Severity
- Light
- Moderate
- Serious
- Catastrophic
- Multi-Catastrophic

White arrow indicates decreasing risk

Red
- Prevention

Blue
- Mitigation

Yellow
- Control Measures

Green
- Red

Black
- Non-operable

Green
- Transfer of Liabilities
Role of Modeling in Performance (Risk) Management

Performance & Risk Assessment
- Functions / Stakes
  - Capacity
  - Injectivity
  - Containment

Risk Mitigation
- Actions
  - Cost
  - Environment
  - Health & Security
  - Image

Characterization
- Modeling

Tools & Technologies
- Monitoring
  - Design (prevention)
- Remediation
CO₂ Storage Site Modeling Workflow

Data input
Information management
GIS database

Calibration
History match
Post processing
Presentation

Surface imaging
Mapping
EM survey interpretation

Log interpretation
Well correlation
Surface identification
Surface/subsurface interaction

Data analysis
Facies modelling
Fault modelling
Fracture modelling
Hydrodynamic test analysis

3D flow simulation
Geochemistry
Geomechanics

3D Geological model
3D Property model of the Reservoir and the Overburden

Uncertainty analysis
Upscaling processes
Reservoir and Aquifer property population
Modeling is everywhere in CO2 storage

> Constant iterative process: measurements vs modeling
  → as initial conditions
  → (re) calibration
  → predictive / fault detection

> At all phases: site selection/characterization, operation, closure, all providing relevant info to ensure model non-divergence

*could have been from Mr de La Palice
Modeling Activity (Network or else): everybody wants it!

- IEA GHG ExCo: identification of the need
- IEA GHG Networks: see questionnaire
- Public Authorities: models as part of the regulatory framework
- Public: when all will be closed/unaccessible, almost only models will provide the answer
Outline

1. Modelling is key for CO2 storage implementation
2. Modelling is very complex
3. Modelling examples
4. Previous initiatives of code comparison
5. Additional efforts needed
6. Towards a IEA GHG modelling network?
1- Modelling is key for CO2 storage implementation

> Top Necessity for:
  - Assessing the geological framework
  - Assessing storage capacity, injectivity, integrity (caprock, faults, wells), risks (leakage, ground movement), impacts
  - Advising monitoring (mutual impetus)

> Only dynamic modelling enables practical conclusions

> Modelling will have a top importance in regulatory and legal frameworks
e.g. draft EC Directive on CO2 geological storage (23/01/2008)
Draft EC Directive on CO2 storage
Annex 1 CRITERIA FOR THE CHARACTERISATION AND ASSESSMENT OF STORAGE SITES

> **Step 1: Data collection**

  - Sufficient data shall be accumulated to construct a *volumetric and dynamic three-dimensional (3-D)-earth model* for the storage site and storage complex.

> **Step 2: Computerised simulation of the storage complex**

  - Using the data collected in Step 1, a *three-dimensional static geological earth model* shall be built using computer reservoir simulators.
  - The *uncertainty* associated with each of the parameters used to build the model shall be assessed by developing a range of scenarios for each parameter and calculating the appropriate confidence limits. Any *uncertainty* associated with the model itself shall also be assessed.
> **Step 3: Security, sensitivity & hazard characterisation**

- Security characterisation shall be based on dynamic modelling, comprising a variety of timestep simulations of CO2 injection into the storage site using the *three-dimensional static geological earth model(s)* in the computerised storage complex simulator constructed under Step 2.

- Multiple simulations shall be undertaken to identify the sensitivity of the assessment to assumptions made about particular parameters. The simulations shall be based on altering parameters in the *static geological earth model(s)*, and changing rate functions and assumptions in the dynamic modelling exercise. Any significant sensitivity shall be taken into account in the risk assessment.

> **Step 4: Risk assessment**

- The risk characterisation shall be conducted based on the hazard (step 3), exposure and effects assessment.

- It shall include an assessment of the sources of uncertainty.
Draft EC Directive on CO2 storage

Annex 2 CRITERIA FOR ESTABLISHING AND UPDATING THE MONITORING PLAN

• The data collected from the monitoring shall be collated. The observed results shall be compared with the behaviour predicted in dynamic simulation of the 3-D-pressure-volume and saturation behaviour undertaken in the context of the security characterisation pursuant to Article 4 and Annex I Step 3.

• Where there is a significant deviation between the observed and the predicted behaviour, the 3-D-model shall be recalibrated to reflect the observed behaviour.

• Where new CO2 sources, pathways and flux rates are identified as a result of history matching and model recalibration, the monitoring plan shall be updated accordingly.

• Post-closure monitoring shall be based on the information collected and modelled during the implementation of the monitoring plan.
1- Modelling is Key for CO2 storage implementation

But « how confident are we in the modelling results we are generating for CCS projects? »

(Quotation from Risk Assessment network)
2- Modelling is very complex

- Large timescale range of interest: from hours to thousands of years
- Large spatial scales of interest: from cms to tens of kms
- Various compartments: reservoir, caprock, overburden, faults, wells, surface
- Natural heterogeneities, poor knowledge of the subsurface
- Various dynamic (& coupled) processes: Fluid flow – Geochemistry – Thermics – Geomechanics – Microbiology
- Uncertainty and sensitivity
- Site specificity
Only modelling can address such complex issues for enabling to make predictions

- Numerical & Analytical approaches
- Need for efficient computing algorithms and machines
- Conceptual modelling is very important
- Mutidisciplinary teams are needed (all fields of geosciences, mathematics, computer sciences)

But real data is necessary for model calibration and benchmarking

- Lab & Field experiments
- Field monitoring
- Comparison analytical / numerical models
- Comparison between various numerical codes
3- Modelling examples

To illustrate why we need models, how complex they are, why we should improve them to increase confidence

- Static geological model
- Fluid flow
- Chemical reactivity
- Geomechanical behaviour
- CO2 leakage through a well – analytical model
Weyburn Geological Model (Phase 1)
Rhaetian sandstone reservoir in France (Lorraine)

Quality index of the sandstone, based on porosity and permeability (good for storage over 5)
3D model of CO₂ injection in K12-B
(Audigane et al. 2007, AAPG special publication on Carbon Dioxide Sequestration in Geological Media)

- Enhanced Gas Recovery scenario envisaged
- CO₂ can flush CH₄ through permeable regions of the reservoir
- 10 kg/s injection
  - K12-B6
- 2 x 1 kg/s production
  - K12-B1 and K12-B5

After 10 years of CO₂ injection and CH₄ recovery
Modelling chemical reactivity: 4 cases

> **CO₂ fate in the reservoir:**
  - 2D flow and geochemical modelling, Sleipner
  - Toughreact

> **Caprock integrity:**
  - 1D diffusive model, Sleipner
  - PhreeqC

> **Injectivity**
  - 1D radial model from the injection well, Paris basin
  - Toughreact, Scale2000

> **Wellbore integrity**
  - 1D diffusive model across cement
  - Toughreact
The Sleipner CO$_2$ storage project
2D model of CO$_2$ injection at Sleipner
(Audigane et al., Am. J. of Sc., Sept. 2007)

> 184 m thick reservoir formation with alternance of sand layers and shale layers
> Vertical 2D mesh with a cylindrical geometrical configuration, centered around an injection point located 155 m beneath the top
> Mesh: 22 layers in the vertical and 52 cells in the radial direction with logarithmic progression
CO\(_2\) migration after 25 years of injection

(Audigane et al., Am. J. of Sc.. Sept. 2007)

Concentration of supercritical CO\(_2\) in the reservoir
Note the accumulations under the Shale layers

Amount of dissolved CO\(_2\) in the water (mass fraction)
- Above the injection point maximum saturation is reached
- At the edges we see lower saturation ranges
Effects of CO$_2$ dissolution after 25 years of injection

(Audigane et al., Am. J. of Sc., Sept. 2007)

pH change of the water due to CO$_2$ dissolution. However pH doesn’t decrease below 5.13, due to buffering by calcite dissolution.

Calcite dissolution (mol/kg$^3$) in the acid water. The dissolution of calcite is less pronounced in the shales than in the sands. However some calcite precipitates below each shale layer at the interface between the CO$_2$ saturated brine and the initial brine, due to mixing of different waters in these regions.
CO$_2$ migration after 50 years with injection only in the first 25 years

Concentration of supercritical CO$_2$ in the reservoir
Note how almost all CO$_2$ has moved to the top of the reservoir

Amount of dissolved CO$_2$ in the water (mass fraction)
Similar, but after 1000 years …

(Audigane et al., Am. J. of Sc., Sept. 2007)

Concentration of supercritical CO$_2$ in the reservoir

Amount of dissolved CO$_2$ in the water (mass fraction)
Note that brine with dissolved CO$_2$ migrates downward as it is approximately 10 kg/m$^3$ denser than brine without CO$_2$. 
... After 2000 years ...

(Audigane et al., Am. J. of Sc., Sept. 2007)

Concentration of supercritical CO$_2$ in the reservoir

Note how almost all CO$_2$ has dissolved already. The CO$_2$ plume extends to a maximum radius of 2,000 m around the injection well.

Amount of dissolved CO$_2$ in the water (mass fraction)

Note convection induced by density gradients
… After 5000 years …

(Audigane et al., Am. J. of Sc., Sept. 2007)

Concentration of supercritical CO$_2$ in the reservoir
Note how almost all CO$_2$ has dissolved already.

Amount of dissolved CO$_2$ in the water (mass fraction)
And finally after 10000 years

(Audigane et al., Am. J. of Sc., Sept. 2007)

All supercritical CO$_2$ has dissolved, there is no more free CO$_2$ in the reservoir

Amount of dissolved CO$_2$ in the water (mass fraction)
Dissolved CO$_2$ accumulates at the bottom of the reservoir with a lateral extent of 4.5 km around the injection well
Dissolution of CO$_2$ increases the acidity of the brine, but is buffered by carbonate dissolution. Maximum decrease of pH is 5.13.

(Audigane et al., Am. J. of Sc., Sept. 2007)
Total amounts of carbon dioxide present as a free (supercritical) gas phase, dissolved in the aqueous phase, and trapped in carbonated minerals (dawsonite mainly). Dissolution trapping plays a major role in the long term, while mineral trapping is minor at Sleipner.
Long term predictions of caprock reactivity at Sleipner
(Gaus et al., 2005, Chem. Geol., 217, 319-337)

> **Approach taken**

- 1D-reactive diffusion modelling (kinetics included)
- PHREEQC2.8 code
Porosity and diffusion profiles after 3000 years

**Porosity change profile**

- Porosity decrease limited to lowest 2 m

**Diffusion profile**

- Diffusion « delayed » due to reactions

Porosity decrease (%)

Depth (m)

Dissolved CO2 (mol/kg)

Depth (m)

Diffusion only

diffusion + reactions

**3000 years**

IEA GHG R&D Joint Network Meeting, New York, June 11-13, 2008
CO$_2$ injectivity

André et al., 2007, En. Conv. Mgmt., Volume 48, Issue 6, 1782-1797

Evaluate the geochemical reactivity induced by injection of SC-CO$_2$ in the Dogger limestone, Paris basin

- **Injection of dry & pure supercritical CO$_2$**
  - TOUGHREACT based on TOUGH2 – (Xu et al. 2004) (LBNL)

- **Near-well dry out and desiccation phenomenon with high salinity**
  - SCALE2000 (Azaroual et al. 2003) (BRGM)
Changes over time at 1 meter distance from the well
\((\text{CO}_2 \text{ injection rate: } 10 \text{ kg/s} = 0.3 \text{ Mt/y})\)

Three periods identified:
- Single phase: brine
- Two phases
- Single phase: supercritical \(\text{CO}_2\) (dry out)

Out of the Debye Hückel Formalism: Ionic Strength >0.5

USE OF SCALE2000
To calculate correct Index of Saturation for precipitated minerals
Chemical changes function of distance from the injection well after 10 years of injection ($\text{CO}_2$ injection rate: 10 kg/s = 0.3 Mt/y)

**Mono phase (SC-CO2)**
- Dry out
- Evaporite precipitation (CaSO4, NaCl)

**Two phases (SC-CO2 + liquid)**
- Acidification
- Mineral dissolution (Calcite)

**Mono phase (liquid)**
- Initial phase conditions

Dry-out zone a few meters around the injection well
Various mineral precipitation and dissolution processes that impact on injectivity
Modelling CO$_2$ reactivity with well cements
(Jacquemet 2007)

> New research domain

> Example:

1D diffusion of dissolved CO$_2$ into the cement at 500 bar and 150°C and induced geochemical reactions

> Further developments under progress
Mineralogical & porosity changes after 2 months of cement alteration

**Perspectives:**
- Coupling with mechanics
- Chemistry feedback on diffusivity

IEA GHG R&D Joint Network Meeting, New York, June 11-13, 2008
Conclusions on the modelling of chemical reactivity

> Multiple modelling approaches are needed to assess the chemical impact of CO₂ storage

> During the last 15 years, geochemical and coupled geochemical and flow modelling have made large progress

> Still large uncertainties due to:
  - the complexity of the various processes involved
  - insufficient site-specific geochemical data acquisition (rock and fluid samples for precise mineralogy, salinity, detailed fluid chemistry, etc.),
  - insufficient site-specific hydrodynamic data acquisition (porosity, permeability, dispersivity, laws Kr-Pc relative permeability - capillary pressure, etc.)
  - heterogeneities

> New research areas:
  - Impact of impurities co-injected with CO₂ (e.g. O₂, N₂, NO, SO₂, H₂S)
  - Links geochemistry-geomechanics
  - Pore scale modelling to simulate wormhole formation
Geomechanical modelling

> Determination of the maximum injection pressure, in order to preserve the integrity of the caprock while optimising the CO2 injection rate

> Modelling of fault reactivation and induced leakage or ground movement

> Assessment of the Impact of a seismic event on a storage site (application to Total pilot at Lacq)

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**Evolution of the effective stress with injection pressure**

**Crack density function of injection pressure**

- **Injection pressure:** 15 MPa during 30 years
CO2 leakage scenario through a well (Wertz, 2008)

CO2 in a free water column

1-D analytical Model

• Assumptions:
  • Static and Stationary flow
  • CO2 thermally balanced by water
  • Geothermal gradient 3°C/100m, 10bar/100m
  • Darcy Flow in the seal due to overpressure
  • Bubble and slug flow models in the well
  • Velocity $V(\text{CO}_2)$ depends on:
    • density $\rho_{\text{CO}_2}(P, T)$
    • interfacial tension $\sigma_{\text{CO}_2/brine}(P, T)$,
    • gas volume fraction $x$
CO2 leakage scenario through a well (Wertz, 2008)

CO2 rising Velocity for different initial gas volume fraction

- Transition from supercritical to gas phase
- Transition bubble flow to slug flow

CO2 leakage scenario through a well (Wertz, 2008)
CO2 leakage scenario through a well (Wertz, 2008)

CO2 rising time model

CO2 first dissolves into the water before next bubbles continue to rise

depth risen by CO2 Front, m

Time, h

0 5 10 15 20 25 30 35 40 45 50

0 5 10 15 20 25 30 35 40 45 50

Xi=0.14
Xi=0.12
Xi=0.1
Xi=0.08
Xi=0.06
Xi=0.04
Xi=0.02
Xi=0.01
Xi=0.005
Xi=0.002
Xi=0.001

CO2 leakage scenario through a well (Wertz, 2008)
Conclusions:

• Analytical model is faster, and physically easy to describe

• Analytical and numerical models are complementary:
  • while some codes can fail at the phase transition, analytical models can foresee it and find a workaround
  • making analytical and numerical models converge to a similar solution strengthens the confidence in the solution.
4- Previous initiatives of code comparison

> 2002 Workshop at LBNL, Berkeley, USA: Inter-comparison of numerical simulation codes for geologic disposal of CO2 report (reported in Pruess et al. 2004)
  “Code intercomparison builds confidence in numerical simulation models for geologic disposal of CO2”

> 2008 Workshop at University of Stuttgart, Germany: Numerical Models for Carbon Dioxide Storage in Geological Formations (report to be issued)
LBNL code intercomparison exercise (2002)

> Participants:

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<tr>
<th>Research Institute</th>
<th>Code(s)</th>
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<tr>
<td>LBNL, USA</td>
<td>TOUGH2 Family</td>
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<tr>
<td>University of Stuttgart, Germany</td>
<td>MUFTE_UG</td>
</tr>
<tr>
<td>CSIRO Petroleum, Australia</td>
<td>TOUGH2/ECO2</td>
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<tr>
<td>IFP, France</td>
<td>SIMUSCOPP</td>
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<td>University of Stanford, USA</td>
<td>NON BAPTISE</td>
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<td>Alberta Research Council (ARC), Canada</td>
<td>GEM</td>
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<td>LANL, USA</td>
<td>FLOTRAN, ECLIPSE 300</td>
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<td>LLNL, USA</td>
<td>NUFT</td>
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<tr>
<td>Industrial Research Limited (IRL), NZ</td>
<td>CHEM-TOUGH</td>
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<tr>
<td>PNNL, USA</td>
<td>STOMP</td>
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> 8 very simplified exercises (1D, 2D radial, schematic & homogeneous media) that probed advective and diffusive mass transport in multiphase conditions, with partitioning of CO2 between gas and aqueous phases; two problems also involved solid minerals and oil phases.

> broad agreement in most areas; bugs corrected, some unexpl. discrepancies

> also points out sensitivities to fluid properties and discretization approaches that need further study.

> It is hoped that future code intercomparisons will address coupled processes in fully 3D heterogeneous media, constrained by actual field observations.
### Univ. of Stuttgart code intercomparison exercise (2008)

#### Participants:

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<tr>
<td>University of Bergen/Princeton, Norvège/USA</td>
<td>Semi-analytical solutions</td>
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<td>University of Texas/Austin, USA</td>
<td>IPARS-CO2</td>
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<td>IFP Rueil Malmaison, France</td>
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<td>RWTH Aachen, Germany</td>
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<td>Schlumberger Carbon Services, Paris</td>
<td>ECLIPSE 300</td>
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<td>University of Stanford, UK</td>
<td>GPRS</td>
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- 3 exercises: focused on fluid flow and numerical aspects, 3D geometries
- some big discrepancies that need to be further analysed (discretization, numerical algorithm, etc.)
5- Additional efforts needed

> Needs expressed by IEA GHG Wellbore Integrity Network

- Numerical models of wellbore geochemistry and geomechanics need additional development for providing long-term predictions
- Numerical models incorporating realistic permeability distributions for wells are needed to evaluate the leakage potential of fields with multiple wells
- Integrated geomechanical and geochemical experiments/numerical models are needed to capture full range of wellbore behavior
- Long-term numerical modeling grounded in enhanced field and experimental data
5- Additional efforts needed

> Needs expressed by IEA GHG Monitoring Network

- Recognizes the importance of modelling in the various phases of CO2 storage (site investigation, drilling & well testing, storage operation, site closure)
- “The monitoring measurements should be history matched against the predictive flow modelling”
- “The main gap is a lack of a “matrix” presenting the common interests among the three networks and the perspective they are dealt within each individual network. The objective should be to converge to a common outcome. For example, when a CO2 risk pathway is identified, is /are the simulation tools able to calculate it? Which output they provide? How this output can be then translated in probability of occurrence or severity of consequences”.
5- Additional efforts needed

> Needs expressed by IEA GHG Risk Network
  • How confident are we in modelling results?
  • Need for modelling physical/chemical/mechanical phenomena in a way that can be useful for risk assessment

> Needs expressed by ZEP - the European Technology Platform for Zero Emissions Fossil Fuel Power Plant:
  • R&D area: Long-term modelling of CO2 storage in deep saline aquifers: “Modelling is used to characterise both short-term and long-term storage performance in terms of injectivity, capacity, containment, and quantitative estimation of potential leakage. A dedicated project is needed to develop and demonstrate the capacity of models to adequately predict the storage behaviour and CO2 fate. This will increase confidence in the safe implementation of storage sites and will be useful for optimising the injection operations and the short/long term monitoring strategies”.
6- Towards a IEA GHG modelling network?
– Feedback from questionnaire (18 received, 16 with opinion)

FOR (13), e.g.:

• YES. Modelling is a key component of all CCS projects and thus determining best practises in this area would be very useful.

• YES, it is important to create a place where this community can meet, especially to perform benchmarking.

• YES - Definitely. Modelling needs to be performed at several levels, which transcends the scope of the individual networks at present. Our confidence in our ability to model both the small scale and large scale phenomena in the system will be greatly enhanced if we focus effort on this problem and share information that is currently within the domain of the individual network groups.
6- Towards a IEA GHG modelling network?
– Feedback from questionnaire (18 received, 16 with opinion)

> FOR (13), e.g.:

- YES. I think the results of work done in the other networks can feed the modelling to develop better models, but that this topic is a stand alone issue.

- Simulation and modelling is very important for CCS. So, new network should deal with modelling and simulation

- YES, a new network would be useful on this topic … but Modellers shouldn’t be allowed to have more than 2 meetings in a row by themselves! Too susceptible to becoming remote from the “real world”; that is, from addressing issues that matter to other people.
6- Towards a IEA GHG modelling network?
– Feedback from questionnaire (18 received, 16 with opinion)

> AGAINST (2):
  • No. I'd rather see effort put into identifying economic monitoring methods that will work when the plants are at full capacity and the years after abandonment (Tools like InSAR).
  • NO. Modeling is a crosscutting activity that pertains to all the existing networks.

> MAY BE (1):
  • Maybe to some extent
6- Towards a IEA GHG modelling network?

Conclusion is best summarised by one of the answers to the questionnaire:

> “YES, I believe there would be a lot of benefit from a modelling network. Significant components of the practice of CO2 injection and geologic storage can be described only by modelling (e.g., estimated injectivity, injection field design and injection rates, total storage capacity, plume fate and tracking, etc.). Modelling of these technical components will be important in preparing carbon storage permits, and convincing regulators and the public of storage safety and viability. Therefore, a modelling network would contribute to more directly integrating modelling developments with developments in WI, M, and RA, and would also promote accurate, dependable, and practical modelling as applied to permitting and monitoring CO2 geologic storage”.

Schlumberger

brgm