



GHGT-10

## An efficient software framework for performing industrial risk assessment of leakage for geological storage of CO<sub>2</sub>

Mark E. Dobossy<sup>a,b</sup>, Michael A. Celia<sup>a,b</sup>, Jan M. Nordbotten<sup>a,b,c</sup>

<sup>a</sup>*Geological Storage Consultants, LLC, 3794 McAndrews Road, Rosemount, MN USA*

<sup>b</sup>*Department of Civil and Environmental Engineering, Princeton University, Princeton, NJ USA*

<sup>c</sup>*Department of Mathematics, University of Bergen, Bergen Norway*

---

### Abstract

In response to anthropogenic CO<sub>2</sub> emissions, geological storage has emerged as a practical and scalable bridge technology while renewables and other environmentally friendly energy production methods mature. While an attractive solution, geological storage of CO<sub>2</sub> has inherent risk. Two primary concerns are recognized: 1) leakage of CO<sub>2</sub> through caprock imperfections, and 2) brine displacement resulting in contamination of drinking water sources. Three mechanisms for both CO<sub>2</sub> and brine leakage have been identified: diffuse leakage through the caprock, leakage through faults and fractures in the caprock, and finally, leakage through man-made pathways such as abandoned wells from oil and gas exploration. While the first two leakage mechanisms are important, we emphasize the risks associated with the presence of abandoned wells. This is due to the large number and density of wells from a history of oil and gas exploration around the world, and the high degree of uncertainty surrounding the properties of these abandoned wells. With current proposed legislation in both the United States and Europe, a need is emerging for practical assessment of leakage risk. In order to accurately predict leakage of brine and CO<sub>2</sub> from the injection layer, the geological information for the injection site and the location and makeup of the man-made leakage pathways previously alluded to must be taken into account. Unfortunately, both the geology and abandoned well metadata are typically high in uncertainty, which must be accounted for. With such a high number of random variables, the current state of the art is running many realizations of a system, using a Monte Carlo approach. This requires that the underlying solution algorithms be accurate, and efficient. In the past, many researchers in both academia and industry have turned to robust numerical analysis packages used in the oil industry. However, due to the large range of scales important to this problem (domains of tens of kilometers on a side affected by leakage pathways with diameters of tens of centimeters) such modeling techniques become computationally expensive for all but the most basic analysis. A computational model developed at Princeton University, and currently being commercialized by Geological Storage Consultants, LLC has been shown to be efficient with sufficient accuracy to allow for comprehensive risk assessment of CO<sub>2</sub> injection projects. The model allows for mixing solution methods- using computationally expensive algorithms for formations of greater importance (e.g.- the injection formation) and more efficient, simplified algorithms in other areas of the domain. This ability to arbitrarily mix solution methods offers significant flexibility in the design and execution of models. This paper addresses the framework and algorithms used, and illustrates the importance of efficiency and parallelism using the case study of an injection site in Alberta, Canada. We show how the framework can be used for project planning, for risk mitigation (insurance), and for regulatory groups. Finally, the importance of flexible analysis tools that allow for efficient and effective management of computational resources is discussed.

© 2011 Published by Elsevier Ltd. Open access under [CC BY-NC-ND license](http://creativecommons.org/licenses/by-nc-nd/3.0/).

*Keywords:* Geological Storage of CO<sub>2</sub>; Leakage Along Wells; Analytical Models; Risk Assessment; Carbon Capture and Storage;

---

## 1. Introduction

As geological storage of CO<sub>2</sub> has become a serious green house gas mitigation option, international group recommendations, as well as government regulations concerning safe storage strategies are becoming available [1, 2, 3]. These documents outline risks and regulation from varying points of view. For example, the IPCC report adopts a comprehensive view of carbon storage, addressing general environmental concerns applicable to most CCS projects, whereas the US EPA regulations and OSPAR recommendations approach the problem from more specific viewpoints- protecting drinkable ground water, and storage effects on overlying maritime systems respectively. While the viewpoints vary, the underlying message remains the same- it is necessary to address the currently known risks of CO<sub>2</sub> storage long before the drilling of an injection well begins, and to update this risk profile via monitoring, new information, and technology throughout the life of a geological storage project.

Assessment of the risk of leakage of CO<sub>2</sub> as well as resident brine will be a vital component of proper planning and execution of a storage project. Along with the international group recommendations previously mentioned, several papers have been written discussing risk assessment in regards to geological storage of CO<sub>2</sub> [4,5]. To assess the risk of any system, one must identify potential hazards in the system, the probability of these hazards occurring, define the impact of these mechanisms on the system as a whole, and assess the cost for probable outcomes. For the geological storage of CO<sub>2</sub>, the two most widely recognized hazards are the leakage of CO<sub>2</sub> out of the injection formation, and the displacement of resident brine to subsequent layers in the geological stack. In order to understand the risk of these hazards occurring, one must first define the mechanisms that cause them. The IPCC special report outlines CO<sub>2</sub> leakage pathways as occurring along naturally occurring faults and fractures, as well as along man-made pathways, i.e.- existing abandoned wells. Research is currently being performed to characterize old wells and assign permeability distributions to the materials associated with those wells, in particular well cements [6,7]. With this information gathered, one can then use computer modeling like those in this paper, to determine system-wide responses incorporating uncertain leakage pathways, as well as uncertainty in the site geology. The resulting distribution of outcomes can then be combined with a cost analysis to yield a comprehensive financial risk assessment of a project.

This paper describes a software framework intended for regulators, risk assessors and planners alike. We start by defining what a software framework requires to be applicable to such a wide array of uses, and how our framework possesses these characteristics. Its usefulness is then illustrated through a case study of a hypothetical injection site in the Alberta Basin.

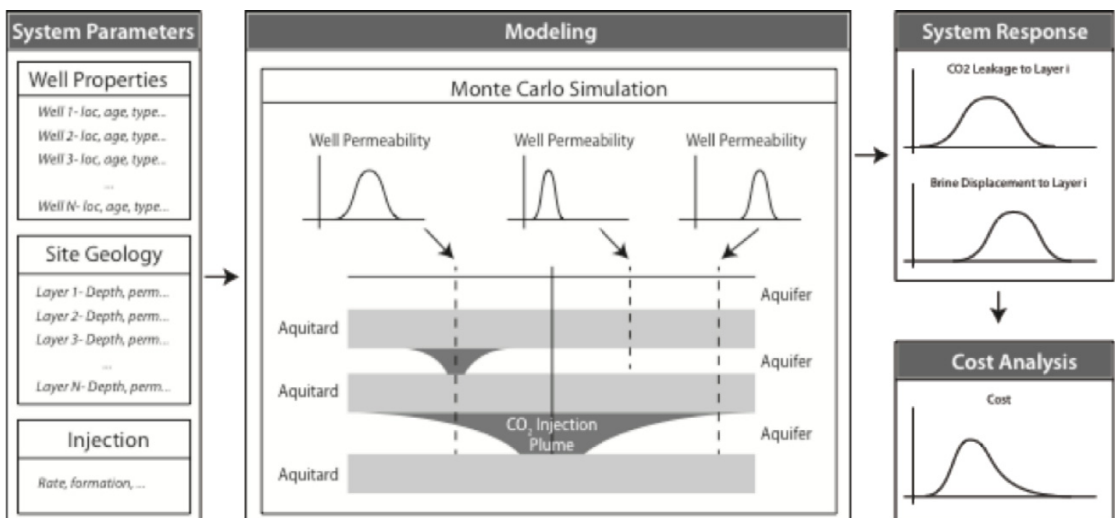


Figure 1: Financial risk assessment of leakage through abandoned wells utilizing Monte Carlo simulation.

## 2. Computational Modeling framework

A single tool that will assist in the roles of regulation, planning, and risk assessment for geological storage of CO<sub>2</sub> will exhibit three key characteristics. First, it must be computationally efficient; regulators will require simpler general calculations that yield results quickly, while planners and risk assessors will need more comprehensive models that can account for the inherent uncertainty found in geological systems as well as man-made leakage pathways. The ability to run many simulations quickly is key in accounting for this uncertainty. Second, the tools must be flexible. While many of the processes by which one would regulate, plan, and assess risk are related, a modular system that allows the operator to mix and match modeling components tied to their task is vital. Finally, there must be an appropriate level of accuracy for each task. Related to flexibility, the appropriate level of accuracy should be adjustable depending on the task at hand. The software framework discussed here, possesses these three traits.

### *Computational efficiency*

One of the greatest challenges faced by those attempting to accurately model the evolution of an injected CO<sub>2</sub> plume, and the resulting response throughout the simulation domain, is a high degree of system parameter uncertainty. This uncertainty is prevalent in the geological formations of the site, but more importantly in potential known and unknown leakage pathways (both natural and man-made). Perhaps the most appropriate method by which this uncertainty (along with modeling uncertainty) can be accounted for is Monte Carlo simulation. With a high number of random variates realized in any moderate-to-large-scale injection domain, a great number of simulations must be run in order to achieve an acceptable level of error. This is especially true when modeling leakage due to abandoned exploration wells- where the system may contain on the order of thousands of potential pathways, each with its own uncertainties. In order to make the framework efficient enough to run the required number of simulations, each layer is upscaled using vertical integration, greatly reducing the mathematical complexity of the model and in turn reducing the computational requirements. The vertically averaged models were specifically developed to incorporate full characterization of the geological layers, consistent handling of gravitational and capillary forces, leakage through wells and caprocks, and compressibility. This approach can be expanded to also include phase transitions as well as upscaled convective mixing. See Celia and Nordbotten [this conference] for a more complete discussion of these models and the assumptions (and limitations) that underlie them.

The modeling framework developed provides two vertically integrated algorithms by which systems can be simulated- a highly efficient and robust semi-analytical algorithm, and a more flexible, though computationally more intensive finite volume algorithm. The vertically averaged semi-analytical algorithm (Figure 2) models CO<sub>2</sub> plume progression using a self-similar ordinary differential equation (ODE) while a superposition approximation models pressure perturbations throughout the system [8,9]. An assumption of horizontal, homogenous formations is required for the analytical plume solution. The flow of single-phase brine or CO<sub>2</sub>, or a two-phase mixture between aquifers via leaky wells is accomplished through a local upconing solution [10]. The nature of analytical solutions makes them computationally fast and memory-efficient, thus accommodating very large-scale simulations consisting of tens of geological formations and thousands of leakage pathways [11,12,13]. It should be noted that the semi-analytical algorithms are quite scalable- for example, on a modern desktop computer, a system with two permeable formations and a single leaky well takes on the order of hundredths of a second to simulate 50-years of injection, while a system containing 10 permeable formations and 1200 wells takes 3-5 minutes.

In cases where it is not suitable to make the required semi-analytical algorithm assumptions, the software framework provides a vertically averaged numerical model (Figure 3). This numerical algorithm utilizes a finite-volume approximation to implicitly solve for pressure, coupled with an explicit saturation solver (IMPES) [14]. The numerical and semi-analytical models both use the same upconing approach to couple formations through wells. In order to reduce grid resolution as well as time-step size, Peaceman sub-scale pressure corrections are used in grid blocks containing injection or leaky wells. By relaxing the requirement for grid refinement around wells, memory and computation requirements are greatly reduced, and the number of leaky wells that can be practically simulated is significantly increased. The resulting implementation is quite general, allowing for heterogeneity of geological

properties throughout a layer. Additionally, the numerical algorithm implemented models capillary fringe effects in the CO<sub>2</sub> plume and gives the option of diffuse leakage of brine through the cap rock [15].

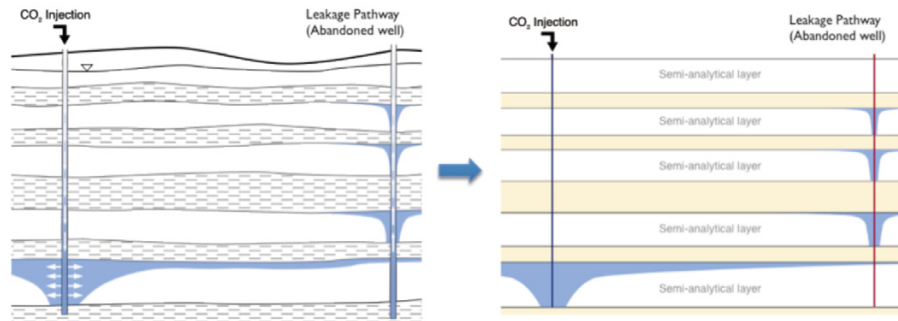


Figure 2: Semi-analytical model schematic.

While extensive work has been done to ensure the efficiency of the numerical module, the algorithm is inherently slower than the semi-analytical option. In many cases, while the semi-analytical approximations are not appropriate in the injection layer, and perhaps a few other formations in the system, it can be used in the majority of formations in the stack. Thus, a hybrid model has been developed that allows the user to specify the appropriate algorithm for each layer individually (Figure 4). The hybrid system is made practical due to the connectivity between layers (the leakage and upconing model) being the same for both the numerical and analytical modules. One challenge encountered in the implementation of the hybrid model is the difference in iterative solvers used for the pressure solution in a numerical and semi-analytical algorithm (Incomplete Cholesky preconditioned Conjugate Gradient and Jacobi preconditioned Generalized Minimum Residual solvers respectively). In order to continue using the appropriate solver for each layer type, an Additive Schwarz preconditioning was used. This hybrid system allows one to focus computational resources where needed, making it an ideal modeling algorithm for risk assessment purposes.

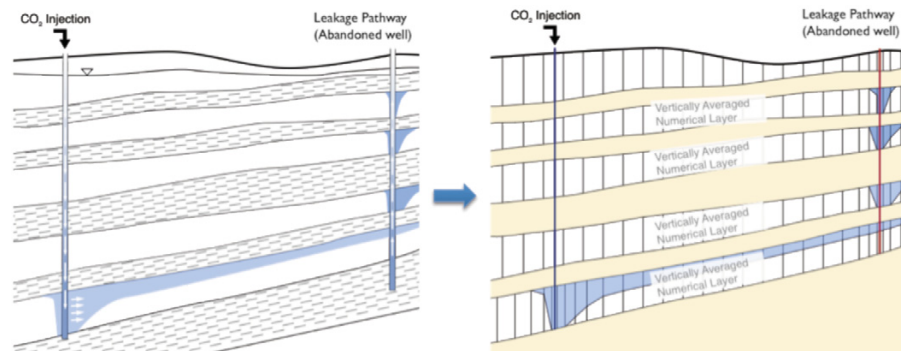


Figure 3: Vertically averaged numerical model schematic.

### *Model flexibility*

Another trait that a software package representing a wide array of uses must possess is flexibility. Alongside the algorithmic options described above, the framework has been designed to allow for a range of user interfaces and platforms. Additionally the code has been written in a modular and expandable way so that new algorithms and concepts may be included at a future date.

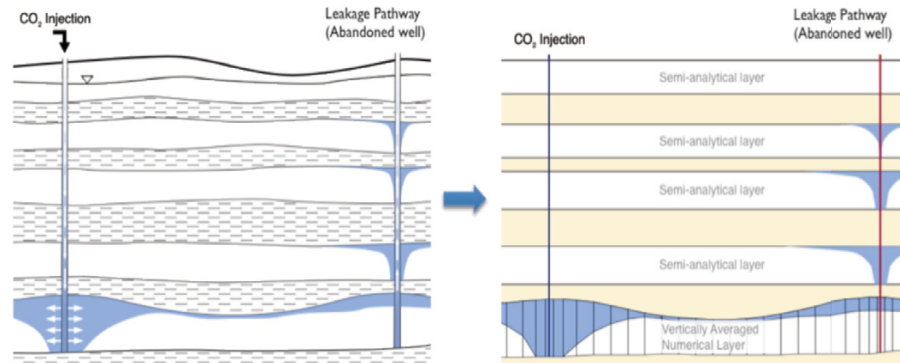


Figure 4: Hybrid model schematic

Often overlooked in scientific code, the process by which a user interfaces with software can play a key role in how effectively it is used. In the case of our target markets, these interfaces, primarily their complexity, will vary considerably. For example, a regulator needing to assess a simple area of review will utilize the software differently than an individual performing risk assessment using a super computer and thousands of runs. It is for this reason that our framework has been designed in such a way that the computational engine is independent of the user interface. To date, two separate user interfaces have been developed- a simple web interface that quickly facilitates simple calculations and visualizations for needs such as area of review assessment, and a TCL-based scripted front-end that allows for large-scale simulations and massively parallel Monte Carlo simulations. In the future, a graphical user interface-based workstation interface will be developed, appropriate to planning of a site. Such an interface will provide instant visual feedback as simulations are run, such that planners can quickly see the effect of changing model parameters.

Related to the user interface is platform-based flexibility. To date, the platform concept has been developed around parallelization. Two segments of the code have been targeted for parallelization due to the significant reduction in computation time provided: an obvious high level parallelization for distributing individual simulations of a Monte Carlo run, and a lower level parallelization within the iterative solver used to solve the pressure equations. The individual simulation runs are embarrassingly parallel, requiring no communication between processes. Thus, for this higher level of parallelization, a distributed memory/message-passing paradigm was used (MPI). Parallelization of the iterative solvers, however, requires significant sharing of information across tasks, which is better suited to a shared memory architecture (OpenMP). It should be noted that these two types of parallelization are not mutually independent. In the case of a MC simulation on a cluster with multiple CPUs per node, a user may specify the number of processes (simultaneous simulations) and threads per process (CPUs or cores per simulation to parallelize the solvers).

#### *Appropriate level of accuracy*

In a companion paper [16], the issue of model choice is discussed from the point of view of space and time scales, and the conditions under which simplified models are appropriate choices. In that paper, the important role played by the time scale associated with density segregation of the fluids is emphasized, and the nature of the simplification is discussed in detail. For practical models at what is referred to as the "macro" length and time scales, which involve lengths on the kilometer scale and larger, and time on the decadal time scale and larger, simplified models are often reasonable choices. We use these results to guide our modeling decisions in the framework described herein.

### 3. Case Study: The Alberta Basin [12,13]

As an example to illustrate how the software framework developed might be used as part of a risk assessment, previous modeling of a hypothetical injection site in the Alberta Basin near Edmonton, Canada is reviewed here. The site of the case study, shown in Figure 5, is a 50km by 50km region. The underlying stratigraphy modeled consists of 10 permeable formations and 10 impermeable caprock formations. The area is over a sedimentary basin attractive for CO<sub>2</sub> storage, and has several significant point sources of CO<sub>2</sub> nearby. The Alberta Basin, as with many mature sedimentary basins, has proven hydrocarbon reserves, and therefore has an extensive history of oil and gas exploration. Borehole exploration has resulted in over 1100 abandoned and active wells (Figure 5b), which pose a risk of unintended CO<sub>2</sub> leakage and brine displacement. Additionally, the extensive history of exploration and production has resulted in extensive data describing the geology of the area [13]. All of these factors make the Alberta Basin an excellent case study for analyzing the risk of leakage of stored CO<sub>2</sub>, and displacement of resident brine through existing wells.

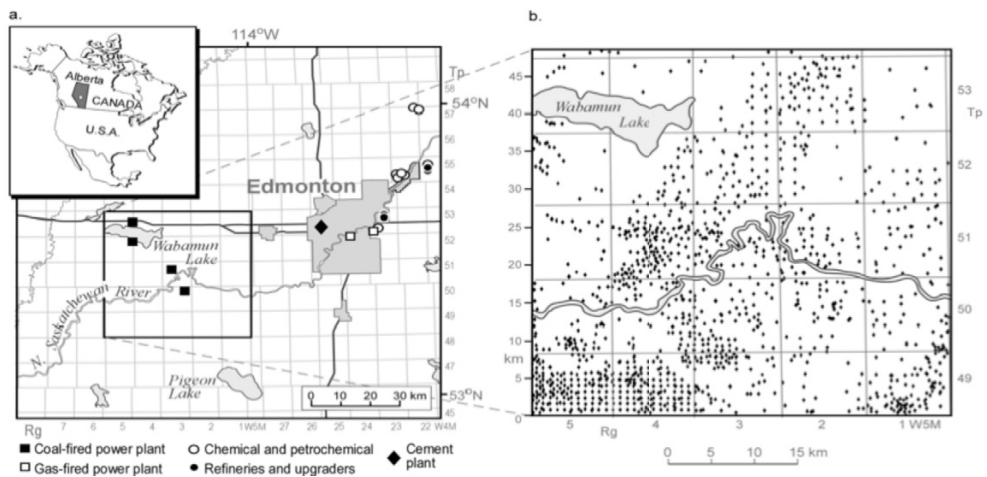


Figure 5: Alberta Basin Site (a.) and well distribution (b.) [12,13].

A model was assembled using the extensive data describing the rock properties within the geological stack. Due to the low dip of the formations in the area of study, the semi-analytical algorithm was deemed sufficient for this study [12]. Data regarding the location and depth of existing wells was used to assemble the well field. The depth of each well was correlated against the existing stratigraphic data to assign an end formation for each well. As expected, no data were available describing the bore permeability of any wells in the system. Thus well permeability became the random variate for the simulations. Two different sets of simulations were run, each using a different method to assign a distribution of permeability to each well. The first set used a bimodal lognormal distribution, where the two means in the distribution correspond to intact and degraded wells [12]. The ratio of intact to degraded wells was varied from 1:3 to 3:1. The second set utilized a study on the leakage potential for the wells in the region [13]. Each well was given a shallow and deep leakage potential depending on several factors including the age of the well, how it had been capped, and the materials used. These scores were

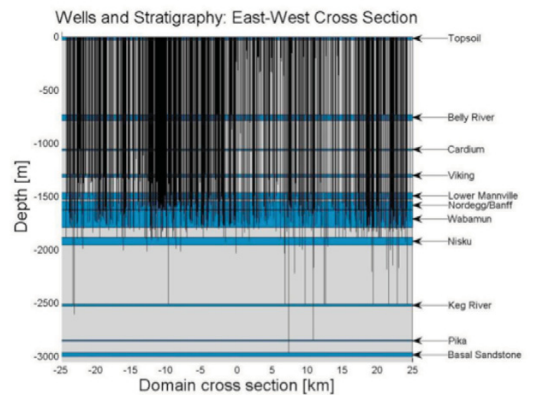


Figure 6: Alberta Basin stratigraphy and well distribution [13]

then mapped to a mean permeability for each well. A lognormal distribution with one order-of-magnitude variance was assumed around this mean. These two scenarios represent the two cases where (1) a planner knows nothing about the permeability of the wells (the lognormal case), and (2) some research has been done to reduce the uncertainty (the scoring system). Finally, cases were run assuming the permeability fully correlated or fully uncorrelated along the length of the well.

Scenarios were run with two injection formations- the Nisku and Basal Sandstone formations (Figure 6). An injection rate was calculated at 90% of fracture pressure, and the injection period was assumed to be 50-years. 1000 simulations were run for each combination of permeability distribution, vertical permeability correlation, and injection formation.

A sample of the results can be seen in Figures 7 and 8. While only CO<sub>2</sub> leakage to the “Topsoil” formation is presented here, similar results were obtained for all formations for both CO<sub>2</sub> leakage and brine displacement. These results would be beneficial to risk assessors and planners alike. First, the distributions of leakage to each formation can be used as a part of a cost assessment, to estimate the probability of cost liabilities over the course of the project. Second, one can assess the reduction in leakage by moving to a deeper formation. Finally, conclusions can be drawn as to the value additional information (i.e.- the scoring system) gives to the analysis.

Along with seeing the potential use of data from such a system, it is also important at this stage to mention the computational speed with which these simulations were run. With a 32-core 2.26ghz Xeon “Nehalem” cluster, each set of 1000 runs was completed in around an hour. Thus, risk assessment simulations for a domain of this size are quite practical to obtain, and with a reasonable computer, larger and more complex systems can be modeled.

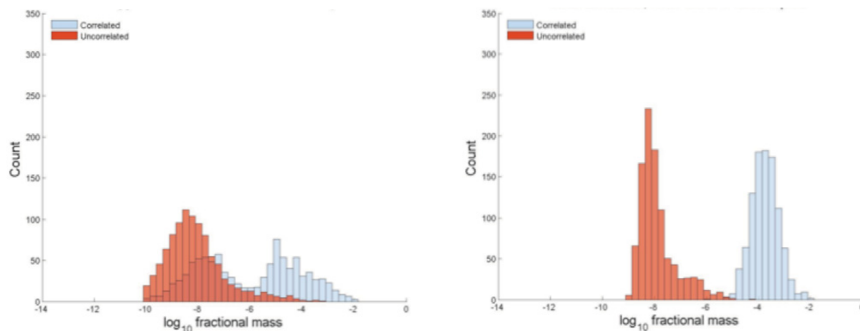


Figure 7: Fractional leakage of CO<sub>2</sub> to the shallow zone using the bimodal distribution, injection into the Basal Sandstone formation (left) and Nisku formation (right) [13].

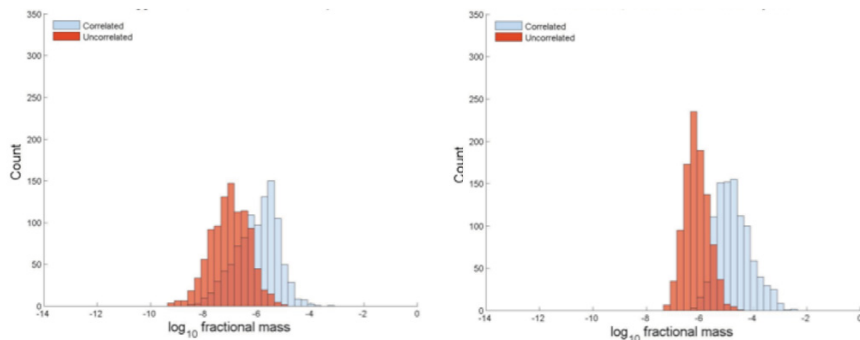


Figure 8: Fractional leakage of CO<sub>2</sub> to the shallow zone using the scoring system, injection into Basal Sandstone formation (left) and Nisku formation (right) [13].



#### 4. Conclusions

Modeling software capable of efficient risk assessment will be a key tool required by regulators, planners and risk assessors in order to make the widespread geological storage of CO<sub>2</sub> a safe, reliable, and practical option for reducing green house gas emissions. Due to the inherent natural (geology) and anthropomorphic (wells, modeling error) uncertainty found in geological CO<sub>2</sub> storage schemes, stochastic modeling will be necessary. Particularly, due to the overlap in attractive basins to store CO<sub>2</sub> and hydrocarbon reserves, leakage through abandoned wells is a risk that must be addressed by these tools.

The software framework described here, currently being brought to market by Geological Storage Consultants, LLC, targets these preceded needs of the CCS industry. Special care has been taken to develop the framework in a flexible and efficient manner, such that it fills these needs from different perspectives across the industry.

A case study to assess the leakage of CO<sub>2</sub> and displacement of brine for a hypothetical injection in the Alberta Basin shows the type of useful data that can be obtained through our software framework. The study illustrates the results one can expect to obtain, which gives insight into the scope of risk assessment that can be performed.

#### References

- [1] IPCC (Intergovernmental Panel on Climate Change). *IPCC Special Report on Carbon Dioxide Capture and Storage*, edited by B. Metz, O. Davidson, H.C. de Coninck, M. Loos and L.A. Mayer, Cambridge University Press, Cambridge, U.K., and New York, NY, U.S.A., 442 p., 2005.
- [2] U.S. EPA, Federal Register, 2008. *40 CFR Parts 144 and 146 Federal Requirements Under the Underground Injection Control (UIC) Program for Carbon Dioxide (CO<sub>2</sub>) Geologic Sequestration (GS) Wells; Proposed Rule*. Friday, July 25, 2008 Federal Register/vol. 73, no. 144, pp. 43492–43541.
- [3] OSPAR Commission, 2007. *OSPAR Guidelines for Risk Assessment and Management of Storage of CO<sub>2</sub> Streams in Geological Formations*. OSPAR Convention for the Protection of the Marine Environment of the Northeast Atlantic. Reference Number: 2007-12.
- [4] Trabucchi, C., M. Dolan, S. Wade, A multi-disciplinary framework to monetize financial consequences arising from CCS projects and motivate effective financial responsibility. *Int J Greenh Gas Con.* 2010, 4(2), 388-395.
- [5] Oldenburg, C.M., S.L. Bryant, J. Nicot, Certification framework based on effective trapping for geologic carbon sequestration, *Int J Greenh Gas Con.* 2009, 3(4), 444-457
- [6] Gasda, S.E., J.M. Nordbotten, M.A. Celia, Determining effective wellbore permeability from a field pressure test: a numerical analysis of detection limits. *Environ Geol.*, 2008, 54(6), 1207-1215.
- [7] Watson, T.L., S. Bachu. 2008. Identification of Wells with High CO<sub>2</sub>-Leakage Potential in Mature Oil Fields Developed for CO<sub>2</sub>-Enhanced Oil Recovery; Paper SPE 112924.
- [8] Nordbotten, J.M. and M.A. Celia, Similarity Solutions for Fluid Injection into Confined Aquifers, *Journal of Fluid Mechanics*, 2006, 561, 307-327.
- [9] Nordbotten, J.M., M.A. Celia, and S. Bachu, Injection and Storage of CO<sub>2</sub> in Deep Saline Aquifers: Analytical Solution for CO<sub>2</sub> Plume Evolution during Injection. *Transport in Porous Media.* 2005, 58(3), 339-360.
- [10] Nordbotten, J.M. and M.A. Celia, Interface Upconing around an Abandoned Well. *Water Resources Research.* 2006, 42, (doi:10.1029/2005WR004738).
- [11] Celia, M.A. and J.M. Nordbotten, Practical Modeling Approaches for Geological Storage of Carbon Dioxide. *Ground Water.* 2009, 47(5), 627-638.
- [12] Nordbotten, J.M., D. Kavetski, M.A. Celia, S. Bachu, Model for CO<sub>2</sub> Leakage including Multiple Geological Layers and Multiple Leaky Wells. *Environmental Science and Technology.* 2009, 43, 743-749.
- [13] Celia, M.A., J.M. Nordbotten, B. Court, M. Dobossy, and S. Bachu, Field-scale Application of a Semi-analytical Model for Estimation of Leakage Potential Along Old Wells. *Int J Greenh Gas Con.* Under Revision.
- [14] Gasda, S.E., J.M. Nordbotten, and M.A. Celia, Vertical Equilibrium with Sub-scale Analytical Methods for Geological CO<sub>2</sub> Sequestration. *Computational Geosciences.* 2009, 13, 469-481.
- [15] Nordbotten, J.M. and H.K. Dahle, Impact of the capillary fringe in vertically integrated models for CO<sub>2</sub> storage, submitted to *Water Resources Research.*
- [16] Celia, M.A., J.M. Nordbotten, How Simple Can We Make Models for CO<sub>2</sub> Injection, Migration, and Leakage? GHGT-10.