Summary of
Princeton Workshop on Geological Storage of CO₂

November 1-3, 2005
Princeton University

Supported by:

The Carbon Mitigation Initiative
and
The Department of Civil and Environmental Engineering

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Summary of Workshop Activities and Outcomes

**Workshop Objectives**

The workshop had four general objectives:

1. Identification of the important physical and chemical processes that need to be included for practical estimation of leakage from subsurface CO$_2$ storage sites.
2. Identification of computational limitations for modeling CO$_2$ injection, migration, and leakage.
3. Identification of key data needs to predict CO$_2$ fate and estimate potential leakage.
4. Definition of a test problem, or series of test problems, that could serve as a common basis for model comparison, where the term 'model' is construed broadly. This common activity could then serve as a starting point for a community effort to develop shared, or common, components of CO$_2$ models.

**Motivation and Organization**

The workshop evolved from discussions among the organizers related to computational models for estimation of leakage from geological storage sites for CO$_2$. A significant number of organizations, including universities, national laboratories, government agencies, non-governmental organizations, and industries, are interested in this problem. In addition, a substantial number of organizations are involved in the development of computational tools to assess the risk of leakage from potential underground storage sites. While several recent international and national workshops sponsored by BP and IEA Greenhouse Gas Programme, and EPA, have focused on issues related to leakage and risk assessment, the idea of this workshop was to bring together the scientists who are actively developing the computational tools to discuss technical issues related to CO$_2$ injection and leakage. To this end, leading scientists and engineers were invited from Stanford University, The University of Texas, The University of Bergen, The University of Stuttgart, Los Alamos National Laboratory, Lawrence Berkeley National Laboratory, Lawrence Livermore National Laboratory, and Pacific Northwest National Laboratory. Each organization sent at least one of their leading researchers to the workshop. In addition, the U.S. Environmental Protection Agency was represented, as was BP. Scheduling conflicts made it impossible for participants from Cambridge University, and the International Energy Agency Greenhouse Gas Programme, to accept invitations to the workshop.

Prior to the workshop, the organizers sent out a questionnaire to each of the participating groups to solicit information about their modeling activities. Responses to the questionnaire were made available to all participants prior to the workshop; each response is also included as part of this workshop report. The workshop itself was structured to cover two full days, with each participating scientific organization given time to present their modeling work during the first day. The second day was spent entirely in discussions, using two break-out groups as well as discussions involving all workshop participants. It was during these discussions that the specific workshop objectives were discussed, and some general consensus emerged. Those specific ideas are presented in the next section. An extra half-day (the
morning of the third day) was added so that those interested could learn more about the
general activities being pursued under Princeton's Carbon Mitigation Initiative. While those
presentations and discussions were an important part of the overall experience of the
participants, they do not relate directly to the issue of leakage modeling and therefore are not
discussed further herein.

**Workshop Outcomes**

Workshop participants were in general agreement about several important points regarding
CO₂ storage and potential leakage. Three overall themes were considered: (1) physical and
chemical processes important to the leakage problem, (2) computational limitations in CO₂
modeling, and (3) data needs. Each of these will be discussed in turn. The group also
addressed the question of a common data set to define a test problem for modeling of
injection, migration, and leakage. This topic forms the fourth and last of the workshop
outcomes.

For almost all of these discussions, the participants found it both useful and necessary to
identify important length and time scales, in order for all the other issues to be framed
properly. Spatial scales were discussed in two different contexts. In one context, the relevant
spatial scale for an injection site was defined as the length scale associated with leakage into
an 'undesirable' location. Such undesirable locations include other hydrocarbon reservoirs or
mineral deposits (not including the target formation), shallow groundwater, soils, or the
atmosphere. This provided a site-specific length scales that defined important characteristics
for leakage. In the second context, more generic length scales were defined, across the
following range: pore scale (10-100 μm), cement interface/degradation scale (0.1-10 mm),
core scale (1-10 cm), well-bore scale (10-100 cm), near-well scale (1-50 m), field scale (1-100
km), and basin scale (>100 km). Processes, computational limitations, and data needs were
considered at these different scales.

There was general consensus that the important time scales for leakage are those less than a
few centuries (e.g., 500 years) after the start of injection, because this is the timeframe needed
to stabilize CO₂ levels in the atmosphere at the desired level. Processes that occur on time
scales longer than these, which usually lead to an increase of storage security by immobilizing
carbon, are considered to be of lesser importance in the context of assessing the potential for
CO₂ leakage.

**Processes**

Important processes considered in the discussions included the following: CO₂ migration, also
referred to as flow; geochemistry; geomechanics; CO₂ phase behavior, including thermal
effects; flow in and along leaky wells; and chemistry associated with material degradation
within and along leaky wells. Most discussion focused on injection into saline aquifers,
which is seen as the most likely large-scale, longer-term injection option. For the flow and
leakage problem, there was general agreement that the physics and phase behavior require a
model that includes three fluid phases (liquid brine, supercritical or gaseous CO₂, and liquid
CO₂), and three components (H₂O, CO₂, salt). In extreme cases where freezing could occur
(due to cooling associated with CO$_2$ expansion), solid (frozen) phases may also need to be included. Equations can be written across all identified length scales, but parametric information for these nonlinear equations are only known well at scales where measurements can be performed, which is usually the core scale. Identification of conditions under which the mathematical description of the system can be simplified remains an important research topic. The ubiquitous problem of parametric definitions across different length scales – the so-called upscaling problem – applies to this problem and remains as an additional important research topic.

Geochemistry was considered in several different ways: geochemical reactions within geological formations, geochemical reactions within engineered materials like well cements, and geochemical reactions at material interfaces. Reactions within formations are usually so slow that over the time scales that are important to leakage, these processes are not important. Reactions with engineered materials, which may play a central role in leakage along human-made features like abandoned wells, can happen over relatively short time scales, and therefore they are important to understand and model properly. However, the consensus of the group was that the proper focus for geochemical studies is at the interfaces between adjacent materials, which we refer to as material interfaces. Examples of these include the interface between rock and well cements, between casing and well cements, and between formation and caprock. These interfaces are the critical locations for chemical reactions that can have significant impacts on leakage potential. The length scales associated with interfacial geochemistry are small, on the order of micrometers to millimeters, and therefore geochemical processes need to be resolved at very fine scales.

Geomechanics can be treated effectively with standard descriptions when the system is viewed as a continuum. A continuum description usually implies a relatively large scale of resolution. The problem becomes more difficult when individual fractures are described. In that case the largest practical length scales is perhaps a few tens of meters. Coupling between geochemistry and geomechanics – for example precipitate infilling of fractures – may be important for some aspects of the CO$_2$ problem and research should continue in this area.

Overall, the complete description of the CO$_2$ system is mathematically complex, involving coupled nonlinear partial differential equations. Coupling of processes, especially those with large difference in their characteristic length or time scales, remains an extreme research challenge, whose solution will clearly require a community effort.

**Computational Limitations**

Models of multi-phase flow can be written and solved at essentially all of the length scales identified, from the pore scale to the field scale and beyond. Such solutions presume a set of well-defined governing equations, defined at a length scale of resolution commensurate with the scale of the problem. When solving the standard equations of multi-phase flow, including appropriate descriptions of phase behavior, the maximum problem size that can be solved using roughly a few days worth of computing on a desktop machine was estimated to correspond to a system with about $10^7$ grid blocks. This number of grid blocks, when distributed across the three dimensions of the physical problem, identifies a length scale (the size of the grid block) which is the minimum averaging scale at which the governing equations need to be written. This computational limitation inexorably ties the upscaling
problem directly to the computational limitations of current calculations. That is, if we wish to solve problems at the field or basin scale, we need to write equations over averaging volumes that have length scales of tens of meters or larger, meaning that functional relationships like relative permeabilities need to be written using variables (saturations, pressures, and other variables) averaged at that scale. This computational limitation also means that models that span multiple length scales – that is, resolve small scales like the core scale and cover large domains like the field or basin scale – are a practical impossibility. At most, two consecutive length scales may be able to be modeled, although even that is problematic under some conditions.

Geochemistry was seen as an even more difficult problem. Given that many of the important processes take place at material interfaces, the inherent length scale must be very small. Small grid spacing around these regions usually implies associated small time steps, so that the overall problem becomes extremely computationally demanding. Clearly some intelligent multi-scale modeling approaches need to be developed in order to effectively couple important geochemistry into the overall flow calculations. Feedbacks between geochemical reactions and changes in physical flow properties, like permeability and porosity, are critical links between flow and geochemical models.

Computational limitations on geomechanics depend on how the geomechanical system is described. When using continuum mechanics, problems at the field scale can and have been solved, on grids that are again on the order of $10^5$ to perhaps $10^6$ grid blocks, using the criterion of a few days of computing on a desktop machine. When individual fractures are considered, the scale of the problem is reduced substantially, to the tens of meter scale. If geochemistry is coupled with the geomechanics, further significant reductions occur in regard to length scales that can be captured.

Overall, even in systems with adequate data, computational limitations place significant restrictions on the problems that can be solved. If leakage along wells is to be considered, across a vertical scale that includes many layers, no single model exists that can capture all of the essential processes. Small-scale geochemical considerations may be equally as important as the field-scale response, and no model can capture both of these. Inclusion of other processes such as geomechanics makes the problem even more intractable.

**Data Needs**

Data needs for the carbon injection and leakage models are substantial. Basic core data to define porosity and intrinsic permeability may exist, but functional relationships for relative permeability are often absent, for two-phase case but certainly for three-phase systems such as liquid brine, liquid CO$_2$, and gaseous CO$_2$. These are fundamental properties and need to be measured. At the larger scale, measurements are difficult, so once again the upscaling issue becomes important, because it is the main tool to define parametric relationship at larger scales, based on data at smaller scales. Of course, for leakage considerations, these kinds of data necessary to perform multi-phase flow simulations need to be known from the deep subsurface where injection occurs to the land surface.

Other critical data needed for leakage analysis include appropriate geochemical rate parameters, across the wide range of possible systems and interfaces, and including conditions
where injected CO$_2$ has dried the porous medium so that aqueous chemistry no longer applies. Furthermore, basic data on the existence, location, history, and condition of wells need to be incorporated into any realistic models of leakage. These data may or may not exist, in useful form, at any particular location. More specific information like the vertical intervals along which the annulus was cemented, and the composition of the cement, are also important to know. For a complete analysis of the leakage problem, information about wells should include both deep wells (oil and gas wells) and shallow wells (drinking water wells). Collection of these data requires historical data mining rather than performance of specific laboratory tests. Of course, the current state of these materials, in situ, would also be extremely valuable information, but such determinations are very difficult at present.

A final consideration in data for modeling is the need to specify initial and boundary conditions for the problem. While initial conditions can often be estimated reasonably, boundary conditions are sometimes much more challenging. This is because the domains chosen for simulations often have boundaries that do not coincide with any physical features with which natural boundary conditions are associated. Rather, boundary locations are often dictated by computational limitations on the size of the domain, or by a general lack of information about the subsurface. Any data that can assist in the assignment of boundary conditions for computational models would be of great benefit.

**A Common Test Problem for Modelling CO$_2$ Injection and Possible Leakage**

One of the major objectives of this workshop was to put in place a mechanism that could serve as a starting point for a possible community activity that could eventually result in sharing of software, and modeling approaches, across the different groups. The workshop organizers decided that a common test problem, defined broadly and with significant flexibility in terms of modeling objectives, might serve as such a vehicle. To this end, a site for modeling studies was proposed and described at the workshop. The site is in the Alberta Basin, west-southwest of Edmonton. Its location places it close to several large point sources of CO$_2$ emissions. A group discussion produced a list of data that the different groups felt were essential to model the problem. The main data included: rock properties, stratigraphy (geometry of layers), mineralogy, fluid composition, formation pressures, location and depth of existing wells (both deep and shallow wells), information about well cements and casing, information about any leakage reported in any of the existing wells, and well logs. The workshop organizers will work over the next two months to put together the appropriate data sets and make them available, in suitable formats, to the workshop participants.

Rather than define a highly constrained problem for the purpose of code comparison, the participants decided to work from a common data base, but to leave the specific focus of each modeling effort flexible. To get a sense of the range of activities that might take place, each participating group stated the kinds of topics that they planned to explore using this data set. Topics ranged from specific processes (for example, well cement degradation) to implementation of specific kinds of numerical methods (for example, streamline methods) to an overall systems model to describe all of the important features and processes in the example problem. While almost all of the groups will have some common items, such as modeling of the injection plume, the variety of different topics was seen as especially important, because such variety serves at least three important functions. First, because each
group will (presumably) work on aspects of the problem that are of most interest to that group, there is a stronger likelihood that they will actually work on the test problem. Second, because the activity is flexible, and different groups will work on different aspects of the problem, there is less of a feeling of competition and more of a feeling of a group effort. Third, the aspects of the problem chosen by each group will, de facto, define that group’s interests and expertise. When the participants convene in one year to see what has been accomplished, the particular expertise exhibited by the groups will inherently define which parts of the problem are best addressed by which group. This can then form a basis for a community effort, where specific groups might contribute analysis tools, based on their identified expertise, for specific parts of the problem. If all of this happens, then when the groups reconvene in one year, the next steps in the process can begin to be addressed. These include a better assessment of relevant physico-chemical processes, further identification of data needs, coordination of the different pieces that can be contributed by each group, and an overall software tool to integrate the pieces.

**Conclusion**

This workshop on modeling of CO$_2$ injection, transport, and leakage, resulted in several important conclusions about the importance of different physical and chemical processes, about our abilities to model those processes, and about the need for specific kinds of data. Explicit consideration of both length and time scales formed the framework for much of the discussion in each of the three categories. A list of the processes important to leakage modeling was developed. Among many items identified, an important observation was that geochemical processes are most important when the focus is on behavior at material interfaces. Computational limitations are significant for models that include multi-phase and multi-component aspects of the problem in a general numerical modeling framework. An important observation was that flow processes can be modeled at almost all scales, but multi-scale models can span, at most, two consecutive length scales, and that these models are often constrained by lack of adequate upscaling procedures. Finally, a variety of data needs were identified, from standard core-scale measurements to data associated with existing wells.

All of these conclusions were reached through extensive discussions and highly collegial interactions involving a group of researchers who are directly involved in CO$_2$ modeling. Computational and data limitations make CO$_2$ modeling an evolving challenge, and require a coordinated effort to integrate the manifold aspects of the problem into a coherent framework. This workshop raised the possibility of a community modeling effort, whose initial step will be based on a common test problem that was outlined at this workshop. The next steps in this processes are to compile the data for the test problem and make it available to all workshop participants, to allow each group to work on aspects of the modeling problem that are of their own choosing, and to reconvene the group in about one year to see what has been done, and how those efforts can then be used to define a community activity.
Participants List

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Elizabeth Scheehle (EPA)

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Dmitri Kavetski (Princeton University)
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Mohammad Piri (Princeton University)
Jean Prevost (Princeton University)
George Scherer (Princeton University)
## Models at a Glance

<table>
<thead>
<tr>
<th>Name</th>
<th>Affiliation</th>
<th>Developers(^1)</th>
<th>Status(^2)</th>
<th>Phase transition</th>
<th>Geo-chemistry</th>
<th>Thermal</th>
<th>Solid matrix Deformation</th>
<th>Discretization method (space)</th>
<th>Discretization method (time)</th>
<th>Wells &amp; fractures</th>
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<tbody>
<tr>
<td>Athena</td>
<td>U. of Bergen</td>
<td>Heimsund</td>
<td></td>
<td>◐</td>
<td>◐</td>
<td>◐</td>
<td>×</td>
<td>MPFA (FV)</td>
<td>Implicit</td>
<td>No special treatment</td>
</tr>
<tr>
<td>CSLS</td>
<td>Stanford U.</td>
<td>Gerritsen Jessen</td>
<td></td>
<td>◐</td>
<td>✓</td>
<td>×</td>
<td>×</td>
<td>Pressure: MPFA</td>
<td>MMOC along streamlines</td>
<td>No special treatment</td>
</tr>
<tr>
<td>Spectral</td>
<td>Stanford U.</td>
<td>(Gerritsen)</td>
<td>✓</td>
<td>✓</td>
<td>×</td>
<td>×</td>
<td>×</td>
<td>Spectral Galerkin</td>
<td>Explicit 4(^{th}) order</td>
<td>Homogeneous medium</td>
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<tr>
<td>EOS7C</td>
<td>LBNL</td>
<td></td>
<td>✓</td>
<td>✓</td>
<td>×</td>
<td>×</td>
<td>×</td>
<td>FD</td>
<td>Implicit</td>
<td>No special treatment</td>
</tr>
<tr>
<td>Dynaflow</td>
<td>Princeton U.</td>
<td>Prevost</td>
<td>✓</td>
<td>✓</td>
<td>×</td>
<td>✓</td>
<td>×</td>
<td>MFEM, VCFV, CCFV</td>
<td>Implicit</td>
<td>No special treatment</td>
</tr>
<tr>
<td>Elsa</td>
<td>Princeton U.</td>
<td>Nordbotten</td>
<td></td>
<td>◐</td>
<td>◐</td>
<td>◐</td>
<td>×</td>
<td>Semi-Analytical</td>
<td>IMPES and fully implicit</td>
<td>1D wells with Darcy flow</td>
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<tr>
<td>FEHM</td>
<td>LANL</td>
<td>Pawar</td>
<td></td>
<td>◐</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>Integrated FV</td>
<td>Implicit</td>
<td>Coupled wellbore flow; Dual porosity</td>
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<td>GEM-GHG</td>
<td>Comp. Mod. Grp. U. of Texas</td>
<td>Viswanathan</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>×</td>
<td>Adaptive grid,</td>
<td>Implicit</td>
<td>Line source/sink wells</td>
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<td>MUFTE_UG</td>
<td>U. of Stuttgart U. of Heidelberg</td>
<td>Bielinski</td>
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<td>✓</td>
<td>◐</td>
<td>✓</td>
<td>×</td>
<td>Box method (FV)</td>
<td>Implicit or high order schemes</td>
<td>Lower dim. wells/fractures planned</td>
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<td>NUFT/LDEC/GEMBOCHS</td>
<td>LLNL</td>
<td>Johnson</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>FD, FE</td>
<td>Transport implicit</td>
<td>Dual porosity</td>
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<td>(Carey)</td>
<td>◐</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
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<td>Integrated FV</td>
<td>Implicit</td>
<td>No special modes</td>
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<tr>
<td>STOMP</td>
<td>PNNL Battelle</td>
<td>White</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>×</td>
<td>Integral FV</td>
<td>1(^{st}) or 2(^{nd}) order backward Euler</td>
<td>Separate subdomains</td>
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<tr>
<td>TOUGH2 ECO2N/EOSM</td>
<td>LBNL</td>
<td>Pruess</td>
<td>✓/☐</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>×</td>
<td>Integrated FD</td>
<td>Implicit</td>
<td>Multi-continua models</td>
</tr>
<tr>
<td>TOUGHEREACT</td>
<td>LBNL</td>
<td>(Pruess)</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>×</td>
<td>Integrated FD</td>
<td>Implicit</td>
<td>Multi-continua</td>
</tr>
<tr>
<td>CO2-PENS</td>
<td>LANL</td>
<td>Viswanathan</td>
<td>◐</td>
<td>◐</td>
<td>✓</td>
<td>✓</td>
<td>×</td>
<td>A systems level code used to integrate the process models into comprehensive systems model</td>
<td></td>
<td></td>
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<tr>
<td>T2CA</td>
<td>LBNL</td>
<td>Oldenburg</td>
<td>◐</td>
<td>◐</td>
<td>✓</td>
<td>✓</td>
<td>×</td>
<td>A TOUGH2 module for coupled subsurface-atmosphere transport of water, brine, CO2, 1 tracer, air</td>
<td></td>
<td></td>
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</tbody>
</table>

\(^1\) Developers present at workshop. For complete lists, see the questionnaires at the end of this document. Non-developer presenters are indicated with brackets.

\(^2\) Green checks (✓) indicate ‘yes’ (or ‘publicly accessible’ for the status column), grey circles (☐) ‘still in development’, and red crosses (☒) ‘no’.
Original Responses to Questionnaires
Athena

GENERAL

Code Name: Athena

Affiliation/Ownership:
Centre for Integrated Petroleum Research, University of Bergen

Status:
Under development. Our research code is under development. A rewrite of an older simulation code is the basis for making a tool which is flexible, has all main parts of a fully implicit multiphase flow simulator, and is easily extendable to new research activities at CIPR.

Availability:
Free, will be available on the web.

Current Developers:
Bjørn-Ove Heimsund and Erlend Øian

Presenter at Workshop:
Bjørn-Ove Heimsund and Geir Terje Eigestad.

Brief code summary/overview (max 100 words):
Currently a multi-phase simulator using general finite volume discretisations. Grids are allowed to be general, and incorporate faults and fractures. Discretisation uses general multi-point flux schemes, and allows integration with complex geometric/geological models. The simulator will be used for studies in the Fault Facies project at CIPR, where a key component is rigorous petrophysical modeling of fault zone properties.

The previous version of Athena has a black-oil fluid model, with various levels of implicit formulations. The code allows for coupling with an external geochemistry package, and has been used to model CO2-sequestration with reactive transport for the Utsira formation.

Ongoing research issues are related to near-well modeling, efficient compositional simulation, and efficient solving of large scale systems. Techniques being investigated include multi-scale finite volume, adaptive local grid refinements and domain decomposition.

Relevant publications (max 5, please attach if possible):
  Accepted for publication in Computing and Visualization in Science.

- "Implicit treatment of compositional flow", I. Garrido, E. Øian, M. Chaib, G. E. Fladmark and M. S. Espedal, Accepted for Publication in Computational Geosciences

- “Parallel Simulation of Multiphase/Multicomponent Flow Models”, Erlend Øian, Magne S. Espedal, Izaskun Garrido, Gunnar E. Fladmark, Accepted for publication in the proceedings
MAIN PHYSICAL PROCESSES MODELED

Physical/chemical processes currently modeled:
Immiscible fluids. An earlier version of the code was black-oil, and work is underway to add that capability. An old version modeled geochemical processes using a separate software package. These particles were modeled as tracers in the fluid model.

Main assumptions (list 5 most important):
Immiscible/incompressible fluids. Additional particles are tracers.

Additional processes in implementation stage:
Black-oil fluids and incorporation of the geochemical model.

Additional processes which will probably be included within 3 years:
CO2 sequestration using a geochemical model / reactive transport. A compositional formulation of the flow equations is also in the planning stages for implementation.

Additional comments:
The new code is steadily incorporating all major components of the physical models of the original code. Major code restructure is incorporated to enhance flexibility for future development.

NUMERICAL ISSUES

Numerical schemes applied to the governing equations:
General finite volume methods (Two-Point Flux Approximation, Multi-Point Flux Approximation) using different degrees of implicit formulations.

Handling of wells, fractures and/or other high risk leakage conduits:
Wells are handled as either boundary conditions or hydrostatic well pressures. The well operating conditions can be pressure, rate or total rate controlled. Fractures may be modeled as either equidimensional entities or as lower dimensional objects. When treated as lower dimensional objects embedded into the mesh, transmissibilities can be calculated both along the fracture and transverse to it. Equidimensional fractures are discretized using a multi-point flux approximation. Fractures are input from external fracture generators.

Largest problem simulated (include size, complexity, hardware, runtime etc.)
Fractured medium with about 10,000 grid cells, unstructured grid and sealing fractures. Synthetic cases of up to one million grid cells have also been tried.

Additional comments:
Ongoing work on streamlines on unstructured grids. Simulation of near-well flows.
CODE EXPERIENCE

Brief description of recent CO2 sequestration simulations:
Geochemistry studies on the Utsira formation.

Brief description of code comparison activities:
The previous code has been compared against Eclipse to verify the LGR implementation. It was also compared against a fracture flow simulator at Stanford. The new simulator has been verified on a highly fractured medium, in addition to analytical solutions.

Comments on robustness/stability:
Fully reliable for two-phase problems, using either a direct matrix solver (banded), or a preconditioned iterative scheme. An adaptive timestepping scheme is used, which selects new timestep sizes based on the convergence of the non-linear solvers.

Additional comments:
Further comparisons against Eclipse and RMS Flowsim will be made, with focus on unstructured grids. Test runs on SPE10 will also be performed using domain decomposition approaches. Such a code can then be used on full-field simulations on the Utsira formation.
CSLS – Spectral

GENERAL

Code Name:

For CO₂ injection (focused primarily on EOR):
- CSLS (Compositional Streamline Simulator) for multi-phase, multi-component gas injection processes

For CO₂ injection and sequestration research:
- CSLS with CO₂-brine property module.
- A separate highly accurate spectral code for investigation of instabilities (fingering) in CO₂ injection (buoyancy driven drainage process) in homogeneous media - purpose to investigate validity of Darcy and relative permeability models, look at onset of instabilities. Note that this code is stand alone and not coupled to CSLS.

Affiliation/Ownership:

CSLS:
CSLS is developed by SUPRI-C (Stanford University Petroleum Research Institute – C). SUPRI-Cs research focuses on simulation and physical understanding of compositional and thermal processes in heterogeneous reservoirs.

Spectral code:
The spectral code is developed by SUPRI-B (Stanford University Petroleum Research Institute – B). Research in SUPRI-B covers a wide range of topics in reservoir simulation and optimization.

Status:

CSLS:
Currently CSLS is primarily a research code (2D and 3D). It is complete for two phase flows, and has a preliminary extension to three phase flows. A parallel, extended and more user-friendly version is in development (generously funded by the Department of Energy). This version will include three-phase flows, improved GUIs and adaptive parallel flow and transport solvers.

Spectral code:
The spectral code has been completed.
Availability:

CSLS:
The code is made available to researchers on a “what you see is what you get” basis (limited user support). The new parallel version will be put in the public domain at the end of 2007.

Current Developers:

CSLS:
Margot Gerritsen and Kristian Jessen + SUPRI-C graduate students

Spectral code:
Amir Riaz and Hamdi Tchelepi

Presenter at Workshop:
Margot Gerritsen and Kristian Jessen

Brief code summary/overview (max 100 words):

CSLS:

Current research version:
- Sequential, portable to several platforms
- Uniform 2D/3D Cartesian grids
- Flow solver for heterogeneous media, nine-point stencil, solved with multigrid method
- Transport problem solved on a streamline grid (three-phase, compositional)
- Accurate streamline tracing algorithms
- Improved mappings between streamlines and flow grid
- Accurate higher order streamline solves (good representation of phase behavior), as well as analytical solutions for fast screening.
- Adaptive Mesh Refinement capability along streamlines
- Adaptive streamline grid (put streamlines where desired)
- Partial streamline tracing (do not have to trace streamlines from well to well)

Future version:
All of the above and:
- Adaptive flow solver (based on Cartesian, Cell-Based Refinement strategy) with integrated upscaling strategy. System solved using parallel AMG (BoomerAMG from Lawrence Livermore)
- Parallel streamline solver
- Robust refinement criteria
Relevant publications (max 5, please attach if possible):

- Riaz and Tchelepi (2005), J. Fluid Mech.

MAIN PHYSICAL PROCESSES MODELED

Physical/chemical processes currently modeled:

CSLS:
Two or three phases, any number of components, immiscible as well as miscible, gravity.

Spectral code:
Bouyancy driven drainage of CO$_2$ in homogeneous saline aquifers

Main assumptions (list 5 most important):

CSLS:
Advection dominated transport.
No fractures in reservoir (dual porosity models not available)

Spectral code:
Homogeneous rock
Small spatial scales
Small density differences between saturated water and brine

Additional processes in implementation stage:

N/A

Additional processes which will probably be included within 3 years:

Dual porosity and sorption for ECBM/ fractured systems.

Additional comments:
NUMERICAL ISSUES

Numerical schemes applied to the governing equations:

CSLS:
Cartesian adaptive method for flow on 3D grid with integrated upscaling. Nine-points stencil used for uniform Cartesian grids, 2-point flux with appropriate modifications for cell-based refined grids (special treatment of hanging nodes).
Streamline solves for transport problem use high-order upwind schemes on adaptive grids for improved accuracy.
High order mappings between streamlines and flow grid.

Handling of wells, fractures and/or other high risk leakage conduits:

CSLS:
Standard vertical wells.
Refinement capability to improve treatment of leakage conduits and near-well areas
No capability to handle fractures.

Largest problem simulated (include size, complexity, hardware, runtime etc.)

CSLS:
10 years of CO$_2$ injection in heterogeneous aquifer using numerical solvers along streamlines + gravity. 500K+ active cells. 2.8GHz CPU, 21 minutes.
No limit with use of MOC solutions along streamlines.

Additional comments:

CODE EXPERIENCE

Brief description of recent CO$_2$ sequestration simulations:

E100, E300, GEM (CMG), 3DSL (StreamSim)

Brief description of code comparison activities:

Investigate optimal simulation strategy for modeling of CO$_2$ sequestration during injection phase: Compositional vs. black oil formulation.

Comments on robustness/stability:

Compressibility and gas solubility cause 3DSL some problems.

Additional comments:
**Elsa**

**GENERAL**

**Code Name:** Elsa

**Affiliation:** Princeton University – Dept. of Civil and Environmental Engineering  
University of Bergen – Dept. of Mathematics

**Status:** Still in development.

**Current Developers:** Jan M. Nordbotten and Dmitri Kavetski

**Presenters at Workshop:** Jan M. Nordbotten and Dmitri Kavetski

**Brief code summary/overview** (max 100 words):

The code implements a semi-analytical methodology for solving the multiphase flow equations describing CO2 injection into aquifers, focusing on potential leakage through wells. The main advantage of the approach is its computationally efficiency, which enables statistical Monte Carlo analysis of the uncertainties associated with the characteristics of abandoned wells. The mathematical framework and several codes implementing it have been in development since 2002.

**Relevant publications** (max 5, please attach if possible):

MAIN PHYSICAL PROCESSES MODELED

**Physical/chemical processes currently modeled:**
Two-phase isothermal flow in vertically layered systems consisting of alternating permeable and impermeable formations. Vertical connection between the permeable formations is through abandoned wells. The code handles an arbitrary number of wells and aquifers, with pressure-dependent fluid properties.

**Additional processes in implementation stage:**
Phase transitions, multiple injection wells.

**Additional processes which will probably be included within 3 years:**
Fluid flow after injection ends (only partially included now), corrosion of well cement, mildly sloping aquifers.

**Main fundamental assumptions** (list 5 most important):
- Homogeneous aquifers: Each aquifer is taken to have uniform thickness, permeability, compressibility and porosity throughout. However these parameters may vary from aquifer to aquifer.
- Impermeable aquitards: The aquitards are assumed to be impermeable except for the abandoned wells. This implies that we cannot model slow seepage through shale, and that fractures and faults can only be modelled by approximating them as wells.
- No thermal effects: Energy transport is not included, although we do allow for an initial temperature gradient in the system.
- Local radial symmetry: To be able to use analytical solutions, we have frequently approximated distributions of pressure and plume thickness as locally symmetric around each well.
- Vertical equilibrium: In some of the analytical solutions, the vertical equilibrium assumption is employed.

NUMERICAL ISSUES

**Numerical schemes applied to the governing equations:**
The governing equations are solved analytically where possible, and the irresolvable non-linearities are handled through an IMPES-like time stepping algorithm. Space is not discretized, the state variables (pressure and saturations) are only evaluated at the wells, so that the number of unknowns in the system is proportional to the number of abandoned wells and the number of permeable formations.

**Handling of wells, fractures and/or other high risk leakage conduits:**
The wells themselves are included as 1-D flow paths between aquifers. The influence of the wells on the flow fields in permeable units is handled analytically.

**Largest problem simulated** (include size, complexity, hardware, runtime etc.):
We ran 1200 realizations of a system with 500 wells over a circular area of 15 km radius with 7 aquifers (more than 2 km deep) subjected to 100 years of CO2 injection. The whole set of computations took around one week of runtime on 8 desktop processors.
CODE EXPERIENCE

**Brief description of recent CO2 sequestration simulations:**
- Case study from Alberta, Canada, with 500 wells within a 15km radius of a hypothetical injection site. The site was chosen based on proximity to emission sources, as well as data availability. 1200 runs were completed investigating different distributions of the permeabilities of the abandoned wells.

**Brief description of code comparison activities:**
- Three versions of the code have been developed and compared to each other.
- Extensive comparison to Eclipse.
- Comparison to other in-house codes.

**Comments on robustness/stability:**
No known stability problems.

**Additional comments:**
**EOS7C**

**GENERAL**

**Code Name:** EOS7C (a TOUGH2 module)

**Affiliation/Ownership:** LBNL, Earth Sciences Division

**Status:** Research module

**Availability:** Could be made available to collaborators who hold TOUGH2 licenses.

**Current Developers:** Curt Oldenburg

**Presenter at Workshop:** Curt Oldenburg

**Brief code summary/overview** (max 100 words): EOS7C is a TOUGH2 module for modeling CO2 (or N2) injection into natural gas reservoirs. EOS7C models flow and transport of water, brine, CO2 (or N2), a gas tracer, and CH4 under isothermal or non-isothermal conditions. EOS7C uses a set of LBNL routines collectively called GasEOS for calculating mixture properties, e.g., using the Peng-Robinson equation of state, and solubility of the gas species in water.

**Relevant publications** (max 5, please attach if possible):


**MAIN PHYSICAL PROCESSES MODELED**

**Physical/chemical processes currently modeled:** EOS7C models 3-D flow and transport of five components (water, brine, CO2 (or N2), gas tracer, CH4) in porous media.

**Main assumptions** (list 5 most important): EOS7C assumes a single gas phase in which CO2, CH4, H2O, and the gas tracer are all fully miscible. EOS7C cannot model transition of CO2-rich gas to liquid conditions.
Additional processes in implementation stage: Improved solubility model to account for salinity in the aqueous phase for CH4 solubility.

Additional processes which will probably be included within 3 years: see above.

Additional comments:

The most important aspect of EOS7C from the leakage point of view is the accurate calculation of pressure increase due solely to the mixing of supercritical CO2 with small amounts of CH4. Pressure increases due to mixing could be the driving force for leakage long after cessation of CO2 injection.

NUMERICAL ISSUES

Numerical schemes applied to the governing equations: Linear equations are developed by standard integral finite difference scheme and solved by iterative solvers, with Newton-Raphson iteration using a Jacobian matrix of residuals to handle the non-linearity.

Handling of wells, fractures and/or other high risk leakage conduits: These are not handled in any special way in EOS7C, although such features can be discretized in the standard way.

Largest problem simulated (include size, complexity, hardware, runtime etc.). We have run 2-D and 3-D problems in simple geometries. Runs on a workstation.

CODE EXPERIENCE

Brief description of recent CO2 sequestration simulations: We have shown that repressurization with limited mixing is possible in gas reservoirs, especially when CO2 is injected low in the reservoir and CH4 is produced from high in the reservoir. We have also shown that CO2 could be an effective cushion gas for natural gas storage by virtue of its density change as it passes through the critical pressure.

Brief description of code comparison activities: We defined the first two problems for the GEOSEQ code intercomparison study. EOS7C compared well against other codes.

Comments on robustness/stability: Stable and robust.

Additional comments: Cannot be used for leakage scenarios in which transition to CO2 liquid may occur.
FEHM – PFLOTRAN – CO2-PENS

GENERAL

Code Name:
Pore scale code, FEHM, PFLOTRAN, CO2-PENS

Affiliation/Ownership:
Los Alamos National Laboratory

Availability:
Porescale code: contact Qinjun Kang (qkang@lanl.gov)
FEHM: Rajesh Pawar (rajesh@lanl.gov)
PFLOTRAN: Peter Lichtner (lichtner@lanl.gov)
CO2-PENS: Hari Viswanathan (viswana@lanl.gov)

Current Developers:
Porescale code: Qinjun Kang, Peter Lichtner
FEHM: Rajesh Pawar, Bruce Robinson, Phillip Stauffer, Hari Viswanathan, George Zyvoloski
PFLOTRAN: Peter Lichtner, Chuan Lu,
CO2-PENS: Phillip Stauffer, Hari Viswanathan

Presenter at Workshop:
Bill Carey, Rajesh Pawar, and Hari Viswanathan

Brief code summary/overview (max 100 words):
Los Alamos National Laboratory works with a suite of codes to study geologic CO2 sequestration. At the porescale, a lattice boltzmann code with multicomponent reactive transport capability is being used to study processes such as wormhole formation as well as homogeneous and heterogeneous reactions. At the continuum scale, FEHM and PFLOTRAN are used to study CO2 fate in the subsurface with a focus on flow, reactive transport and stress effects. At the systems level, CO2-PENS is being used to abstract the process level models into comprehensive systems model that will eventually be used to access the performance of various sites.
**Relevant publications** (max 5, please attach if possible):

**Pore scale code**

Kang, QJ; Tsimpanogiannis, Numerical modeling of pore-scale phenomena during CO2 sequestration, IN; Zhang, DX; Lichtner, PC, Fuel Processing Technology; October 2005; v.86, no.14-15, p.1647-1665, Conference: Symposium on Carbon Dioxide Capture and Sequestration held at 227th National Meeting of the American-Chemical-Society; March 2004; Anaheim, CA

**FEHM (Finite Element Heat and Mass Transfer Code)**


**PFLOTRAN**


**CO2-PENS**


**MAIN PHYSICAL PROCESSES MODELED**

**Physical/chemical processes currently modeled:**

Porescale Code: Lattice Boltzmann code with Multicomponent Reactive Transport

FEHM: Coupled Multiphase Flow, Heat and Multicomponent Reactive Transport, Coupled Flow and Stress (implicit coupling)

Parallel FLOTRAN: Coupled Multiphase Flow, Heat and Multicomponent Reactive Transport with Massively Parallel Capability

CO2-PENS: CO2 Sequestration Systems Model with coupled process models for multiphase flow and transport
NUMERICAL ISSUES

Numerical schemes applied to the governing equations:

Pore scale code: lattice boltzmann technique
FEHM: nonlinear equations formulated using integrated finite volume method and solved using LANL developed multiple degrees of freedom Krylov space solver
PFLOTRAN: integrated finite volume
CO2-PENS: links together several process models with differing numerical techniques

Handling of wells, fractures and/or other high risk leakage conduits:

FEHM: Capability to simulate coupled wellbore flow-reservoir flow, Generalized dual porosity approach to simulate fracture/fault heat and mass flow
Interested in incorporating Celia, Nordbotten, et al. semi-analytical solutions into CO2-PENS systems model.

CODE EXPERIENCE

Brief description of recent CO2 sequestration simulations:

Recent CO2 sequestration simulations cover topics such as: viscous and density driven CO2 fingering, wormhole formation in limestone, CO2 flow in a wellbore with phase changes, and co2-brine-cement-host rock interactions to evaluate cement stability.

Brief description of code comparison activities:

Porescale simulation results have been compared to the continuum model PFLOTRAN in order to determine macro-scale properties of the medium such as tortuosity, permeability, and reactive surface area. In addition, the LB simulations also enable the most appropriate continuum formulation.

TOUGH, PFLOTRAN and FEHM have been compared against one another to confirm they are giving similar results for various reservoir simulations scenarios.

Simple test problems have been constructed to verify individual pieces of the systems model CO2-PENS.

Comments on robustness/stability:

FEHM: nonlinear equations are formed using upwinded fluid properties. Control volumes are formed with positive volumes and connections (finite elements can not guarantee positive connections). Newton-Raphson iterations are performed with a robust Krylov space solver scheme.
Dynaflow

GENERAL

Code Name: Dynaflow (http://www.princeton.edu/~dynaflow/)

Affiliation/Ownership: Princeton University

Availability: License agreement with Princeton University

Current Developers: Jean H. Prevost

Presenter at Workshop: Jean H. Prevost

Brief code summary/overview (max 100 words):

**DYNAFLOW™** is a finite element analysis program for the static and transient response of linear and nonlinear two- and three-dimensional systems. In particular, it offers transient analysis capabilities for both parabolic and hyperbolic initial value problems in solid, structural and fluid mechanics. There are no restrictions on the number of elements, the number of load cases, the number of load-time functions, and the number or bandwidth of the equations. Despite large system capacity, no loss of efficiency is encountered in solving small problems. In both static and transient analyses, an implicit-explicit predictor-(multi)corrector scheme is used. The nonlinear implicit solution algorithms available include: successive substitutions, Newton-Raphson, modified Newton and quasi-Newton (BFGS and Broyden updates) iterations, with selective line search options. Some features which are available in the program include:

- Multi-field/physics analysis capabilities via selective specification of multiple solution staggers.
- Multi-staggered coupled solution analysis options.
- MPI implementation options to fully exploit the architecture of parallel computers.
- Domain decomposition options to partition equations for efficient processing on parallel computers.
- Selective element reordering options applicable to unstructured as well as structured meshes in order to allow parallel and/or vector processing of elemental arrays in blocks.
- Selective specification of high- and low-speed storage allocations options.
- Direct symmetric and non-symmetric matrix column equation solvers (in-core and out-of-core Crout profile solvers). Symmetric frontal solver (in-core and/or out-of-core).
- Iterative matrix equation solvers: preconditioned conjugate gradients and GMRES with diagonal and/or element-by-element Crout/LU or Gauss-Seidel preconditioning.
- Iterative matrix-free conjugate gradient and GMRES solution procedures.
- Eigenvalue/vector solution solvers including determinant search, subspace iterations and various Lanczos algorithms.
- Equation numbering optimization option to reduce bandwidth and column heights of stiffness matrix.
- Slave nodes, equivalence nodes and multi-node constraints capabilities.
Selective specification of element-by-element implicit, explicit or implicit-explicit options.
Selective specification of element-by-element reduced/selective integration options.
Coupled field equation capabilities for treatment of thermosolids, porous media, multi-phase flows, and piezoelectric solids.
Arbitrary Euler-Lagrange description options for fluid and/or fluid-structure(-soil) interaction problems.
Xfem procedures to model discontinuities, joints, shear bands and cracks growth without need for remeshing.
Prescribed nodal and/or surface forces options.
Prescribed nodal displacement, velocity or acceleration options.
Prescribed arbitrary load-time functions.
Earthquake acceleration time history generation capability, for earthquake motions compatible with prescribed acceleration response spectra.
Prescribed consistent free-field motion capability.
Wave transmitting boundaries.
Isoparametric data generation schemes (Cartesian, Cylindrical/Polar and Spherical).
Element birth/death options to model addition (birth) or removal (death) of elements (material) in the physical system.
Layout optimization analysis capabilities.
Capability to perform constitutive experiments along prescribed stress and/or strain paths on selected material elements within the finite element mesh.
Complete restart capabilities with options to selectively change input data.
Fully integrated interface with the graphical pre- and post-processing program FEMGV for both workstation and PC platforms.
Free input format mode organized into data blocks by means of corresponding macro commands.
Fully documented: http://www.princeton.edu/~dynaflow/

Relevant publications (max 5, please attach if possible):
See: http://www.princeton.edu/~dynaflow/vitae/Prevost.htm

MAIN PHYSICAL PROCESSES MODELED

Physical/chemical processes currently modeled: restricted to super-critical CO2 with brine (H2O + NaCl); three phase flash.

Main assumptions (list 5 most important): neglect thermal effects

Additional processes in implementation stage: four phase flash; thermal effects; geochemistry and reactive transports

Additional processes which will probably be included within 3 years: thermal effects for CO2 migrating to surface
NUMERICAL ISSUES

Numerical schemes applied to the governing equations: (mixed and/or stabilized) finite elements; vertex centered finite volumes; cell centered finite volumes (limited); finite difference time stepping

Handling of wells, fractures and/or other high risk leakage conduits:

Largest problem simulated (include size, complexity, hardware, runtime etc.): 1 million equations per solution stagger; restriction imposed by currently available 32 bits LINUX OS (2Gb per CPU node) (see: http://denali.princeton.edu/)

Additional comments:

CODE EXPERIENCE


Brief description of code comparison activities:

Comments on robustness/stability:

Additional comments:
GEM-GHG

GENERAL

Code Name: GEM-GHG

Affiliation/Ownership: Computer Modeling Group

Status: Commercial

Availability: Pre-release version available

Current Developers: Long Nghiem (CMG), Peter Sammon (CMG), Jim Grabenstetter (CMG)

Presenter at Workshop: Steven Bryant (UT-Austin)

Brief code summary/overview (max 100 words):
GEM-GHG is an equation of state geochemical compositional simulator for modeling CO$_2$ and acid gas enhanced oil recovery (EOR) and storage processes. The simulator uses an adaptive implicit discretization technique to model the component transport in porous media. The oil and gas phases are modeled with an equation of state, the gas solubility in the aqueous phase is modeled with Henry’s law. Geochemistry reactions, i.e. chemical equilibrium reactions between aqueous components and mineral dissolution and precipitation are available. Vaporization of H$_2$O into the gas phase, solid (asphaltene) precipitation, thermal effects and leakage through cap rock and sealing faults are also modeled.

Relevant publications (max 5, please attach if possible):


MAIN PHYSICAL PROCESSES MODELED

Physical/chemical processes currently modeled:
   Aqueous speciation; mineral precipitation/dissolution; mass transfer between fluid phases (water into gas, and gas components into water); capillary pressure; hysteretic two-phase relative permeabilities; spatial heterogeneity of rock properties; compositional PVT (Peng-Robinson EOS); gravity; arbitrary well inclinations; pore volume compressibility.
   The simulator also models the sequestration of CO$_2$ in coalbeds (modeling of muticomponent adsorption and coal swelling and shrinkage).

Main assumptions (list 5 most important):
   · Distance-from-equilibrium type of rate expression for mineral precipitation/dissolution
   · Aquifer capillary pressure and relative permeability properties can be characterized in terms of rock types
   · Gas solubility in the aqueous phase is modeled with Henry’s law. Correlations of Henry’s law constants for CO$_2$, N$_2$, H$_2$S, CH$_4$ as functions of pressure, temperature and salinity are available.
   · Darcy’s law for flow
   · Land’s model for hysteresis of relative permeability

Additional processes in implementation stage:
   · Leverett $j$-function scaling for assigning capillary pressure curves to geostatistical realizations of porosity-permeability
   · Coupling to a surface facility module.

Additional processes which will probably be included within 3 years:
   Coupling to a finite-element module for geomechanics.

Additional comments:
   Code keeps track of maximum CO2 saturation attained in each grid block so that the residual saturation to imbibition for that block can be determined during post-processing. This is useful in determining the extent of capillary trapping.

NUMERICAL ISSUES

Numerical schemes applied to the governing equations:
   · Adaptive implicit method for solving the discretized finite difference component transport and energy transport equation.
   · Simultaneous solution of transport equations, phase equilibrium equations and geochemistry equations.
   · Parallel techniques for multiple CPU computers
   · Static and dynamic grid refinement.

Handling of wells, fractures and/or other high risk leakage conduits:
   · Wells handled as line source/sinks within grid blocks
   · Leakage conduits including fractures modeled by assigning large permeabilities to grid blocks corresponding to the conduit
Largest problem simulated (include size, complexity, hardware, runtime etc.)

Field case: 135,000 grid blocks for a CO2/brine/rock system, with relatively complex structure geologically (the Frio pilot). This run did not include mineral precipitation/dissolution. Local grid refinement led to memory constraints on a 3GB machine (Win2000, 2GHz, dual processor) at about 150,000 grid blocks.

Model aquifer: Fine-scale 3D simulation of the flow of CO2 in brine under aquifer conditions including geochemistry; cartesian grid with 200,000 grid-blocks (100 x 5 x 400), stochastic porosity and permeability

Time step: Min = 10^{-5} days, Max = varied from 1 to 5 days
Simulation time = 30 years, run time = about 18 to 20 hours
Hardware: Intel Pentium IV 2.4 GHz processor, 2 GB RAM

Additional comments:
Increasing the number of grid blocks significantly increased the number of steps required to converge, especially during early times when there were large variations in CO2 saturation. Thus, the computation time increased with the number of grid blocks for two reasons: (1) increase in the number of calculations per iteration, and (2) increase in the number of iterations per time step.

CODE EXPERIENCE

Brief description of recent CO2 sequestration simulations:
- Simulations of the Frio pilot successfully predicted the arrival of CO2 at the monitoring well.
- Simulations of scenarios for Frio 2 indicated the scope for testing the concept of residual phase trapping by buoyancy driven flow.
- Simulations of CO2 injection in a generic reservoir for the dual purpose of EOR and sequestration.
- Very fine-grid simulations to evaluate (in)stability of a buoyancy-driven displacement front in the presence of realistic heterogeneity of rock properties (permeability, relative permeability, capillary pressure, anisotropy, correlation length) and the influence of dip angle, injection well characteristics and number of injectors.

Brief description of code comparison activities:
As part of the evaluation of buoyant instability, 1D and 2D flow of CO2 in brine aquifer were simulated using UTCOMP, a research code developed and validated for several processes (including fingering) over the last twenty years at The University of Texas, and GEM-GHG. The CO2 was placed at the bottom of brine-filled aquifer up to a certain height at a certain initial saturation and the resulting flows were simulated. While 1D simulation employed homogeneous domain, the 2D simulations were performed with homogeneous as well as heterogeneous domain.

The gas saturation profiles obtained from the two simulators for 1D simulation matched well at early and long times. The gas saturation profiles for 2D simulation obtained from the two simulators showed comparable heights of high concentration layers. Both the simulators
showed the occurrence of fingers. While the profiles from GEM showed fingers at all times, the results from UTCOMP showed fingers only at intermediate times. While the terminal gas saturation profile obtained from the two simulators were comparable, the average rise velocity of the gas phase obtained from UTCOMP lagged behind that from GEM. This could be due to the difference in the procedures by which the two simulators calculate the densities of the two phases.

**Comments on robustness/stability:**

GEM is commercial software and thus is quite robust. The visualization and graphical modules are powerful.

**Additional comments:**

CMG continues to be actively engaged with UT-Austin in identifying and implementing capabilities useful for CO2 sequestration research.
MUFTE_UG

GENERAL

**Code Name:** MUFTE_UG: Multiphase Flow, Transport and Energy Model on Unstructured Grids

**Affiliation/Ownership:**
University of Stuttgart, Institute of Hydraulic Engineering, Department of Hydromechanics and Modeling of Hydrosystems
University of Heidelberg, Interdisciplinary Center for Scientific Computing

**Status:**

**Availability:** open source

**Current Developers:**
University of Stuttgart, Institute of Hydraulic Engineering, Department of Hydromechanics and Modeling of Hydrosystems
University of Heidelberg, Interdisciplinary Center for Scientific Computing

**Presenter at Workshop:**
Andreas Bielinski, University of Stuttgart
Anozie Ebigbo, University of Stuttgart

**Brief code summary/overview (max 100 words):**

MUFTE-UG is a Multiphase Flow, Transport and Energy model which mainly contains the physical model concepts and discretization methods for isothermal and non-isothermal multiphase multicomponent flow and transport processes in porous and fractured porous media. It also includes the Unstructured Grid toolbox, which provides the data structures and fast solvers for the discretization of partial differential equations based on parallel, adaptive Multigrid Methods.

**Relevant publications (max 5, please attach if possible):**


MAIN PHYSICAL PROCESSES MODELED

Physical/chemical processes currently modeled:
- advective transport caused by pressure gradients and density differences considering sub- and supercritical fluid properties of the CO2
- diffusive transport of CO2 in brine
- dissolution of CO2 in brine with changing brine fluid properties
- dissolution of water in CO2 without changing CO2 fluid properties
- non-isothermal processes

Main assumptions (list 5 most important):
- chemical equilibrium
- local thermal equilibrium
- rigid porous medium
- no chemical reactions

Additional processes in implementation stage:

Additional processes which will probably be included within 3 years:
- change of CO2 fluid properties due to impurities (e.g. dissolved water, H2S)
- coupling with a simulation program taking into account chemical reactions
- if necessary: miscibility model

Additional comments:

The above information only refers to our work on CO2 sequestration. We pursue research in several other fields of multi-phase multi-component systems in porous media.

NUMERICAL ISSUES

Numerical schemes applied to the governing equations:
- time discretization: fully implicit or higher order schemes
- space discretization: box method (vertex centered finite volume method), fully upwind technique

Handling of wells, fractures and/or other high risk leakage conduits:
- at the moment: full 3d discretization of fracture or wells
- planned: lower dimensional consideration of fractures and wells
**Largest problem simulated** (include size, complexity, hardware, runtime etc.)

ca. 10000 nodes, 30000 unknowns  
complexity: low, radial symmetric domain  
hardware: Linux-Cluster, 8 processors (1.5 Ghz each)  
runtime: 20 days for 100 years simulation time


**CODE EXPERIENCE**

**Brief description of recent CO2 sequestration simulations:**
- principle studies: CO2 plume evolution, long-term dissolution and diffusive transport, non-isothermal processes  
- applied studies: computation of near-wellbore scenarios in a CO2 sequestration project (CO2SINK)  
- first steps to setting up large-scale problems for comparison with analytical solutions (J. Nordbotten)

**Brief description of code comparison activities:**
- participation in the code intercomparison study conducted by K. Pruess (LBNL) in 2001  
- ongoing project on benchmarks/intercomparison of different model approaches for problem-oriented applications, start in April 2005

**Comments on robustness/stability:**
Primary variable substitution works for this application quite well.  
Time stepping scheme needs improvement. Currently we use a convergence criterion concerning the global defect.  
Regularizations of non-linear constitutive relationships have to be taken care of.

**Additional comments:**
**NUFT**

**GENERAL**

**Code Names:**
NUFT: multiphase/multicomponent flow and reactive transport simulator
GEMBOCHS/SUPCRT92: thermodynamic/kinetic database and software library
LDEC: distinct element geomechanical model

**Affiliation/Ownership:**
Lawrence Livermore National Laboratory (LLNL)

**Status:**
Although NUFT, GEMBOCHS/SUPCRT92, and LDEC are relatively mature software packages, development activities continue for each.

**Availability:**
NUFT: flow/transport-only version (no reactive chemistry) is available
GEMBOCHS: not distributed off-site at this time (requires Oracle installation)
SUPCRT92: original software with updated thermodynamic database is available
LDEC: not distributed off-site at this time, although ultimate availability is planned

**Current Developers:**
NUFT: John J. Nitao & Yue Hao (LLNL)
GEMBOCHS: James W. Johnson (LLNL)
LDEC: Joseph P. Morris (LLNL)

**Presenter at Workshop:**
James W. Johnson
**Brief code summary/overview:**

NUFT (Nitao, 1998) is a C++ software package that facilitates numerical simulation of non-isothermal multiphase/multicomponent flow and reactive transport within a wide range of subsurface environments characterized by multi-scale physical and compositional heterogeneity. The package implements an integrated finite-difference, spatial discretization to solve the flow and reactive-transport equations, using the Newton-Raphson method to solve the resulting nonlinear systems at each time step. Explicit account is taken of multiphase advection, diffusion, and dispersion; of relative permeability and capillary pressure, using an extended Van Genuchten formulation; and of kinetically controlled fluid-mineral reactions, using rate laws from transition state theory. Moreover, explicit account is also taken of *coupling between* these transport and geochemical processes through the dependence of permeability on porosity changes due to mineral precipitation/dissolution, using a normalized Kozeny equation, and through the dependence of fluid-phase volumetric saturations on gas (e.g., CO$_2$(g)) generated or consumed by fluid-mineral reactions.

The GEMBOCHS system (Johnson and Lundeen, 1994) integrates a comprehensive relational thermodynamic/kinetic database and dedicated software library (C++/SQL and FORTRAN/SQL components) that together facilitate generation of application-specific thermodynamic/kinetic datafiles for use with a variety of geochemical modeling codes (e.g., EQ3/6, GWB) and reactive transport simulators (e.g., NUFT, CRUNCH). The thermodynamic database covers about 3200 distinct chemical species, spanning 86 elements of the periodic table; its core component is the current version of the SUPCRT92 database (Shock, 1998), which covers about 1550 species, spanning 82 elements. Custom datafiles are generated using Jewel, a GUI-driven software package that extrapolates reference-state properties to elevated P-T conditions using a number of standard algorithms, the core set of which are those encoded with the SUPCRT92 software package (Johnson et al., 1992). These include global- and critical-region equations of state and a dielectric formulation for H$_2$O (Johnson and Norton, 1991) that are explicitly integrated with equations of state for both aqueous solutes (Tanger and Helgeson, 1988; Shock et al., 1992) and minerals/gases (Helgeson et al., 1978).

LDEC (Morris et al., 2004) is a C++ geomechanical code that implements the distinct element method, which facilitates representation of fractured rock mass using arbitrary polyhedra, detection of new contacts between blocks resulting from relative block motion using the “Common-Plane” approach, exact conservation of linear and angular momentum, and simplified tracking of material properties as blocks move. Use of an explicit integration scheme allows extreme flexibility with respect to joint constitutive models, which here include effects such as cohesion, joint dilation, and friction angle. Both rigid and deformable approximations to block response are implemented. The rigid block approximation assumes that the compliance of fractured rock mass is closely approximated by lumping all compliance at the joints alone; however, this formulation also includes an optional second joint stiffness term that approximates deformation of the rock matrix.
Relevant publications:


MAIN PHYSICAL PROCESSES MODELED

Physical/chemical processes currently modeled:

Outlined above in code summary/overview section.
Main assumptions (list 5 most important):

NUFT:

The drying (drainage) capillary pressure curve is used to represent both drying and wetting (imbibition) processes; i.e., capillary hysteresis is not represented.

Intra-fluid mass transfer processes assume instantaneous kinetics.

Aqueous-phase density is approximated by that of pure H\textsubscript{2}O; i.e., its dependence on evolving solute concentrations as a function of intra-fluid and fluid-mineral mass transfer processes is not represented.

NUFT/LDEC interface:

This interface facilitates mapping pressure evolution into the corresponding effective stress, fracture aperture, and permeability history; however, at present, this geomechanical-dependent evolution (LDEC) is not back-coupled into the multiphase flow and reactive transport model (NUFT). As a result, the dependence of permeability, fluid flow, and pressure (including capillary pressure) evolution on concomitant geomechanical aperture history is not represented.

The dependence of geomechanical properties (e.g., fracture stiffness [LDEC]) on mineralogical evolution (NUFT) is not represented.

Additional processes in implementation stage:

NUFT:

A finite-element version is nearing completion.

Additional processes which will probably be included within 3 years:

NUFT:

Hydrocarbon EOS and viscosity formulations

EOS and viscosity formulations for key CO\textsubscript{2} impurities (e.g., SO\textsubscript{X}, NO\textsubscript{X}, H\textsubscript{2}S)

Capillary hysteresis

Dependence of aqueous-phase density on solute concentrations

Aqueous-phase solubility in “immiscible” CO\textsubscript{2}

Bi-directional coupling with LDEC
NUMERICAL ISSUES

Numerical schemes applied to the governing equations:

Outlined above in code summary/overview section.

Handling of wells, fractures and/or other high risk leakage conduits:

NUFT implements a dual-permeability option, which permits explicit representation of porous media as interacting matrix and fracture continua, the latter of which can be used to represent a variety of potential leakage conduits.

Largest problem simulated (include size, complexity, hardware, runtime etc.)

NUFT: Most of our simulation studies to date (Johnson et al., 2004, 2005, and references therein) have been conducted on a local 9-node Linux cluster, which features 800 MHz processors and 1 GB memory/node. In these investigations, 2D production runs carried out over 2000-4000 cell spatial domains and involving 10-component chemistry (100-150 aqueous, gas, and mineral species) required 25-40 hours CPU time. While current simulations of laboratory-scale batch reactor experiments (Johnson et al., 2006) have computational requirements similar to these, our 2D/3D models of long-term CO$_2$ influx at the McElmo Dome (Johnson et al., 2006), represented by spatial domains of order $10^4$ cells, have significantly steeper requirements, and for this work we are using the local 67-node ILX (Intel Linux Capacity) cluster, which features 2.4-2.8 GHz processors, 2 CPU/node, and 4 GB memory/node. Although to date our modeling of geologic CO$_2$ storage has not required exploiting parallel versions of NUFT, such versions have already been developed and deployed for simulation work that supports the Yucca Mountain Project, and future exploitation of these versions for geologic CO$_2$ storage modeling is planned.

LDEC: Modeling studies (unrelated to CO$_2$ storage) conducted by Dr. Morris that involve order $10^6$ elements have been carried out using parallel versions of this code on a variety of local advanced architectures (e.g., Thunder, a highly integrated 1024-node Digital Linux Cluster, which features 1.4 GHz processors, 4 CPU/node, and 8 GB memory/node).

CODE EXPERIENCE

Brief description of recent CO2 sequestration simulations:

Our initial reactive transport modeling work on geologic CO$_2$ storage focused on identifying the fundamental migration and storage processes during saline aquifer disposal as well as on
quantifying near-field sequestration partitioning among hydrodynamic, solubility, and distinct mineral trapping mechanisms (Johnson et al., 2004, and references therein). Subsequent recent efforts have targeted simulating long-term cap-rock integrity—the single most important constraint on long-term isolation performance—for both engineered and natural storage sites as a function of influx-triggered geomechanical deformation and geochemical alteration processes (Johnson et al., 2005, and references therein). Current work is focused on experimental and field assessment of key predictions from our earlier modeling studies; in particular, enhanced hydrodynamic seal capacity of typical shale cap rocks through mineral trapping (Johnson et al., 2006).

**Brief description of code comparison activities:**

NUFT: LLNL participated in the GEOSEQ-sponsored code comparison study (Pruess et al., 2004, “Code intercomparison builds confidence in numerical simulation models for geologic disposal of CO$_2$”: *Energy*, v. 29, p. 1431-1444.).

LDEC: LLNL is a current participant in the ACTD (Advanced Concept Technical Demonstration) verification & validation exercise (together with LANL, Sandia, Titan, and Weidling & Assoc.).
**STOMP**

**GENERAL**

**Code Name:**

STOMP (Subsurface Transport Over Multiple Phases)

**Affiliation/Ownership:**

Pacific Northwest National Laboratory (PNNL):
- configuration management
- development
- verification
- documentation
- website

Battelle Memorial Institute (BMI):
- copyright
- proprietary modules

**Status:**

STOMP is currently being applied to a variety of multifluid subsurface flow and transport problems by national laboratories, national and international universities, national and international governmental agencies and national government contractors. In addition to these applications, the simulator currently has development support for numerically simulating the geological sequestration of carbon dioxide in saline aquifers, natural gas and petroleum reservoirs and coal beds, the production of methane hydrates, the performance of sparsely vegetated and bare surface barriers, high resolution simulation of carbon tetrachloride migration through the deep vadose zone, and multicomponent volatile and nonvolatile organics. The simulator is documented through guide documents that are periodically updated (i.e., User’s Guide, Theory Guide, Short Course Guide), published laboratory reports, and journal articles. Instruction in the use and application of the simulator is offered through periodic short courses (e.g., Hyderabad STOMP Short Course, Hyderabad University, January 2-5, 2006). Information on example applications, references, scientific staff, code acquisition, documentation, and the short course are additionally available on the STOMP website (http://stomp.pnl.gov).

**Availability:**

STOMP is available as source code through license or use agreements to those countries not identified by the U.S. Department of Energy as being sensitive.

- Academic-Use License: U.S. and International Universities
- Government-Use Agreement: U.S. Government and Contractors
- Foreign Government-Use License: Foreign Governments
- Commercial-Use License: Industry and Others
Current Developers:

Mark D. White, Ph.D., P.E., Hydrology Group, Pacific Northwest National Laboratory
Mart Oostrom, Ph.D., Hydrology Group, Pacific Northwest National Laboratory
Mark L. Rockhold, Ph.D., Hydrology Group, Pacific Northwest National Laboratory
Andy L. Ward, Ph.D., Hydrology Group, Pacific Northwest National Laboratory
Diana H. Bacon, Ph.D., P.G., Hydrology Group, Pacific Northwest National Laboratory

Presenter at Workshop:

Mark D. White, Ph.D., P.E., Hydrology Group, Pacific Northwest National Laboratory

Brief code summary/overview (max 100 words):

STOMP is a computer model, designed to be a general-purpose tool for simulating multifluid subsurface flow and transport, that complements other analytical capabilities developed by Pacific Northwest National Laboratory's Hydrology Group. The simulator was specifically designed to provide scientists and engineers from varied disciplines with multidimensional analysis capabilities for modeling multifluid subsurface flow and reactive transport phenomena. The simulator's modeling capabilities address a variety of subsurface environments, including nonisothermal conditions, fractured media, multiple-phase systems, nonwetting fluid entrapment, soil freezing conditions, supercritical carbon dioxide, nonaqueous phase liquids, chemical reactions, radioactive decay, solute transport, dense brines, gas hydrates, nonequilibrium dissolution, surfactants, and multifluid wells.

Relevant publications (max 5, please attach if possible):

CO$_2$ Geologic Sequestration


Multifluid Well Models

STOMP Guides


**MAIN PHYSICAL PROCESSES MODELED**

**Physical/chemical processes currently modeled:**

*Multifluid subsurface flow and transport:*
Flow and transport: advection, buoyancy, diffusion, hydraulic dispersion, conduction
Thermodynamics: equilibrium conditions, multicomponent phases, supercritical CO₂
Phases: aqueous, NAPL, gas, ice, precipitated salt, hydrate, liquid CO₂
Components: water, oil, air, CO₂, CH₄, surfactant, salt
Saturation: interfacial tension scaling, nonwetting fluid entrapment, residual NAPL
Phase permeability: anisotropic phase relative permeability
Boundary Conditions: Dirichlet, Neumann, mixed-type, surface barrier
Wells: multifluid, injection, withdrawal, monitoring, variable head, variable rate

*Nonreactive Transport:*
Solute: infinitely dilute, radioactive decay, first-order reactions
Transport: advection, diffusion, hydraulic dispersion
Transport schemes: Patankar, Roe-Superbee, TVD

*Reactive Transport:*
Species: aqueous, gas, nonaqueous phase liquid, solid
Reactions: equilibrium, kinetic
Equations: equilibrium, conservation, kinetic
Transport: advection, diffusion, hydraulic dispersion
Transport schemes: Patankar, Roe-Superbee, TVD

**Main assumptions** (list 5 most important):

1. Darcy’s law describes advective flow.
2. Grid cells are under thermodynamic equilibrium conditions.
3. Capillary pressure-saturation functions can be scaled using interfacial tensions.
4. Relative permeability-saturation functions describe phase permeability.
5. Properties for the grid-cell centroid describe the entire grid-cell volume.
Additional processes in implementation stage:

- Simulation of mixed CH₄ and CO₂ hydrate systems.
- Multifluid wells for CO₂-saline aqueous and CO₂-air-saline aqueous systems

Additional processes which will probably be included within 3 years:

- Compositional gas for simulating CO₂ injection into depleted or partially depleted natural gas and petroleum reservoirs and coal beds.
- Compositional gas for simulating contaminated CO₂ into saline aquifers
- Geomechanical simulation of caprocks.
- Conversion of all CO₂ operational modes to scalable form.

Additional comments:

The STOMP simulator is a scientific tool for modeling multifluid subsurface flow and reactive transport processes whose capabilities have been guided by client need. Funding support for development of the simulator continues, allowing

- applications of complex multifluid subsurface systems
- parallel implementations
- investigation and development of new multifluid constitutive theories
- simulation of innovative environmental remediation and hydrocarbon production technologies

NUMERICAL ISSUES

Numerical schemes applied to the governing equations:

- Governing equations converted to algebraic form via discretization on an structured orthogonal grid (e.g., Cartesian, cylindrical, boundary fitted), using the integral volume finite difference approach.
- Time discretization uses a first-order (or second-order) backward Euler time differencing scheme (i.e., implicit solution).
- Nonlinearities in the coupled flow and transport equations are solved using multivariable Newton-Raphson iteration scheme.
- Partial derivatives in the Jacobian matrix are computed numerically and regenerated every Newton-Raphson iteration.
- Phase transitions, appearances, and disappearances are handled through primary variable switching schemes; where, primary variable switching is allowed between Newton-Raphson iterations.
- Discretized algebraic forms of the solute transport equations are solved implicitly using a Patankar scheme to combine advective and diffusive-dispersive transport.
- For strongly advective (i.e., grid Peclet number > 2) systems, TVD or Roe Superbee scheme can be employed to reduce numerical dispersion.
- Reactive transport is solved using a sequentially to the coupled flow system, using operator splitting of the transport and chemistry.
Batch chemistry involves nonlinear equations of three types: equilibrium, conservation and kinetic (named ECKEChem) which are solved using Newton-Raphson iteration with mixed analytical and numerical derivatives.

Scaling on parallel computers is handled by distributing the computational domain over the processor domain.

Well modules in the scalable versions of the simulator are treated as sequential components that can cross processor boundaries.

Handling of wells, fractures and/or other high risk leakage conduits:

For field-scale applications wells are handled as subdomains within the computational domain, fully or loosely coupled to the governing subsurface conservation equations. This approach allows for the simulation of multiluid wells (e.g., aqueous-gas-oil wells) with well bore capacity. A principal assumption for field-scale simulations with wells is that the areal dimension of a well is small compared with the areal dimension of the computational grid. Multifluid wells are coupled to the subsurface domain via geometric factors, well skin resistance factors, and phase permeabilities. Well can comprise multiple sections of screened and solid casings.

Largest problem simulated (include size, complexity, hardware, runtime etc.)

The scalable version of the STOMP simulator has been used to solve a problem involving the migration and remediation, using soil vapor extraction, of the disposal of carbon tetrachloride into the deep vadose zone at the Hanford site, for a problem involving over 3 million unknowns (3 unknowns per grid cell – over 1 million grid cells) over a simulation period of 40 years. These simulations were executed on the MPP2 supercomputer at the Environmental Molecular Science Laboratory at the Pacific Northwest National Laboratory. The most efficient processor count for these simulations was roughly 100 processors. The sequential version of the simulator has been used to execute problems up to 0.5 million unknowns on a 3 GHz Linux workstation, with 4 GB of memory. A reasonable upper limit for sequential simulations, however, is 0.25 unknowns.

Additional comments:

Development of well modules for the STOMP simulator for simulating leakage of CO₂ from wells that penetrate deep aquifers, intermediate aquifers or the vadose is slated for this fiscal year. At present the simulator has no specialized well models for investigating the leakage of geologically sequestered CO₂.

CODE EXPERIENCE

Brief description of recent CO2 sequestration simulations:

STOMP-CO2 is currently being applied to predict the injectivity of RoseRun and Copper River saline aquifer formations at the American Electric Power’s (AEP’s) Mountaineer Power Plant in New Haven, West Virginia, considering both vertical and horizontal well configurations. STOMP-HYD is currently being applied to predict the production of CH₄ hydrates and sequestration of CO₂ for the Milne Point formations in Alaska.
Brief description of code comparison activities:

STOMP-CO2 participated in the GeoSeq code intercomparison study (Pruess et al. 2002). STOMP-HYD is currently participating in the gas hydrate simulation comparison study being conducted by the U.S. Department of Energy, National Energy and Technology Laboratory (NETL).


Comments on robustness/stability:

The kernel of the STOMP simulator is a nonlinear system solver, that includes under relaxation schemes and primary variable switching to handle difficult phase transitions. The simulator has an user-controlled automatic time-stepping scheme that allows the simulation time step to grow with each successfully converged time step. Initial guesses of the primary variables are those of the last converged time step. When convergence failures occur the time step is cut and the Newton-Raphson iteration procedure is restarted. Extreme divergence is generally trapped by identifying out of range primary variable values or changes. Convergence is determined by the maximum residuals across all active grid cells and governing equations. The simulator automatically stops and produces a restart file after four successive time cuts due to convergence failures. As with most classical Newton-Raphson schemes, quadratic convergence is observed. Phase transitions, associated primary variable switching, and constitutive function discontinuities yield slower convergence rates and under certain circumstances prevent convergence.

Additional comments:

The principal focus for STOMP applications and code development has been environmental remediation of contaminated sites; in particular, those site contaminated with NAPLs. Considerable effort (i.e., five-years of laboratory directed research and development funding) went toward making the simulator scalable to solve the complex field-scale problems associate with high resolution modeling of the carbon tetrachloride plume on the Hanford Site. The simulation of geologic sequestration of CO$_2$ is a relatively new technical application and code development area for STOMP, starting with the participation in GeoSeq code comparison study and now continuing with the Gas Hydrate code comparison study.
**T2CA**

**GENERAL**

**Code Name:** T2CA (stands for TOUGH2 for CO2 and Air)

**Affiliation/Ownership:** LBNL, Earth Sciences Division

**Status:** Research module

**Availability:** Could be made available to collaborators who hold TOUGH2 licenses.

**Current Developers:** Curt Oldenburg

**Presenter at Workshop:** Curt Oldenburg

**Brief code summary/overview** (max 100 words): T2CA is a TOUGH2 module for coupled subsurface-atmosphere transport of water, brine, CO2, a gas tracer, and air. T2CA retains all of the subsurface flow and transport capabilities of TOUGH2 and adds limited atmospheric dispersion capability by assuming constant winds with logarithmic velocity profile and variable-K theory for dispersion.

**Relevant publications** (max 5, please attach if possible):


**MAIN PHYSICAL PROCESSES MODELED**

**Physical/chemical processes currently modeled:** T2CA models 3-D flow and transport of five components (water, brine, CO2, gas tracer, air) in porous media coupled to a pseudo-atmospheric region.

**Main assumptions** (list 5 most important): T2CA assumes (1) steady-state and unidirectional wind, (2) logarithmic velocity profile over horizontal ground, (3) CO2 seepage flux low enough that CO2 in atmospheric region does not affect viscosity and/or density (i.e., no effect on flow field), (4) neutral atmospheric stability, and (5) solubility in aqueous phase is modeled by Henry’s Law.
Additional processes in implementation stage: Improved solubility model. Consideration of stable and unstable atmosphere conditions.

Additional processes which will probably be included within 3 years: see above.

Additional comments:

This approach has recently been implemented into T2VOC, the volatile organic compound simulator, to model attenuation of VOCs from the ground surface by volatilization into wind.

NUMERICAL ISSUES

Numerical schemes applied to the governing equations: Linear equations are developed by standard integral finite difference scheme and solved by iterative solvers, with Newton-Raphson iteration using a Jacobian matrix of residuals to handle the non-linearity.

Handling of wells, fractures and/or other high risk leakage conduits: These are not handled in any special way in T2CA, although such features can be discretized in the standard way.

Largest problem simulated (include size, complexity, hardware, runtime etc.). We have only done 2-D problems for CO2, but we did a 3-D problem for VOCs with 45,000 gridblocks. Runs on a workstation.

CODE EXPERIENCE

Brief description of recent CO2 sequestration simulations: We showed with this code the large degree of atmospheric dispersion that occurs due to wind. CO2 concentrations can be very high in the shallow subsurface due to leakage, but once CO2 seeps out of the ground into wind, dispersion is very effective at reducing CO2 concentrations.

Brief description of code comparison activities: We have not done any formal code comparison with T2CA, but we have verified the code against analytical solutions of Gaussian plume dispersion.

Comments on robustness/stability: Stable and robust.

Additional comments: Users must ensure that assumptions are not violated, particularly by keeping flux low enough that atmospheric transport is passive (CO2 does not affect flow field).
**TOUGH2_ECO2N**

**GENERAL**

**Code Name:** TOUGH2/ECO2N

**Affiliation/Ownership:** LBNL, Earth Sciences Division.

**Status:** Code completed with full documentation and sample problems.

**Availability:** Available to the public from DOE’s Energy Science and Technology Software Center (ESTSC; http://www.osti.gov/estsc/).

**Current Developers:** Karsten Pruess

**Presenter at Workshop:** Karsten Pruess

**Brief code summary/overview** (max 100 words): ECO2N is a fluid property module for the TOUGH2 simulator that includes a comprehensive description of the thermodynamics and thermophysical properties of H2O - NaCl - CO2 mixtures. Temperature, pressure and salinity conditions cover the range of 10 °C ≤ T ≤ 110 °C; P ≤ 600 bar; salinity up to full halite saturation. Flow processes can be modeled isothermally or non-isothermally, and phase conditions represented may include a single (aqueous or CO2-rich) phase, as well as two-phase mixtures. Fluid phases may appear or disappear in the course of a simulation, and solid salt may precipitate or dissolve.

**Relevant publications** (max 5, please attach if possible):


MAIN PHYSICAL PROCESSES MODELED

Physical/chemical processes currently modeled:
Multi-phase fluid and heat flow. Multi-phase diffusion. Phase partitioning between brine and CO2. Salt dissolution and precipitation, with associated porosity and permeability change. Appearance and disappearance of aqueous, CO2-rich, and solid salt phases.

Main assumptions (list 5 most important):
Local thermodynamic equilibrium. General PTX-conditions may be handled, but no provisions are made for phase change between liquid and gaseous CO2 at subcritical conditions.

Additional processes in implementation stage: Multiphase flow model for wells. Improved treatment of hysteresis.

Additional processes which will probably be included within 3 years: Gaseous tracers.

NUMERICAL ISSUES

Numerical schemes applied to the governing equations: Conservation equations are discretized in space by integral finite differences. Fully implicit time discretization. Discretized equations are solved by Newton-Raphson iteration. Linear equation solution is by preconditioned conjugate gradients or direct solvers.

Handling of wells, fractures and/or other high risk leakage conduits:
Options include interpolating flowing well pressures from tables, and multi-continua techniques for high-permeability features.

Largest problem simulated (include size, complexity, hardware, runtime etc.):
Heterogeneous Frio model for CO2 injection with approximately 46,500 grid blocks in 3-D. 10-day injection period takes approximately 22 hr of CPU-time on a dual 64bit Opteron CPU made by AMD that runs 64bit Suse Linux.

CODE EXPERIENCE

Brief description of recent CO2 sequestration simulations:
Simulations of the Frio test prior and post injection have been helpful for test design and interpretation.

Brief description of code comparison activities:
Code has been compared to simulations with earlier versions of TOUGH2/ECO2, including several of the test problems of the recent LBNL-organized code intercomparison study.

Comments on robustness/stability: Satisfactory.

Additional comments: Code cannot handle situations with phase change between liquid and gaseous CO2.
TOUGH2_EOSM

GENERAL

Code Name: TOUGH2/EOSM

Affiliation/Ownership: LBNL, Earth Sciences Division.

Status: Research code.

Availability: In the future.

Current Developers: Karsten Pruess

Presenter at Workshop: Karsten Pruess

Brief code summary/overview (max 100 words): EOSM is a module for the TOUGH2 simulator that represents mixtures of H2O - NaCl - CO2, using similar fluid property correlations as the ECO2N module. The main difference is that EOSM is capable of treating phase change between liquid and gaseous CO2, including associated heat effects, as well as transitions between super- and sub-critical CO2. EOSM treats four active phases: aqueous – liquid CO2 – gaseous CO2 – solid salt.

Relevant publications (max 5, please attach if possible):


MAIN PHYSICAL PROCESSES MODELED

Physical/chemical processes currently modeled:
Main assumptions (list 5 most important):
Local thermodynamic equilibrium. When three fluid phases are present (aqueous – liquid CO2 – gaseous CO2), aqueous phase is considered wetting, gaseous CO2 non-wetting, with liquid CO2 having intermediate wetting properties.

Additional processes in implementation stage:
Full accounting for salinity effects.

Additional processes which will probably be included within 3 years: Improved description of 3-phase relative permeability and capillary pressure relationships.

Additional comments:

NUMERICAL ISSUES

Numerical schemes applied to the governing equations: Conservation equations are discretized in space by integral finite differences. Fully implicit time discretization. Discretized equations are solved by Newton-Raphson iteration. Linear equation solution is by preconditioned conjugate gradients or direct solvers.

Handling of wells, fractures and/or other high risk leakage conduits:
Options include interpolating flowing well pressures from tables, and multi-continua techniques for high-permeability features.

Largest problem simulated (include size, complexity, hardware, runtime etc.)
Approximately 18,500 grid blocks in 3-D. Approximately 40 hr CPU-time on an IBM RS/6000 for a 6 yr simulation of leakage up a fault.

Additional comments:

CODE EXPERIENCE

Brief description of recent CO2 sequestration simulations:
Numerical simulation experiments have shown that leakage up faults or fracture zones may be accompanied by strong cooling effects, and by evolution of three-phase zones (aqueous – liquid CO2 – gaseous CO2). Interplay between multiphase flow and heat transfer effects can give rise to non-monotonic leakage behavior.

Brief description of code comparison activities:
Code was compared with earlier two-fluid-phase versions.

Comments on robustness/stability:
CO2 phase change and its impacts on fluid flow and heat transfer can be numerically difficult. Special techniques are needed to achieve simulations over meaningful time scales

Additional comments:
Code development is ongoing.
TOUGHREACT

GENERAL

Code Name: TOUGHREACT

Affiliation/Ownership: LBNL, Earth Sciences Division.

Status: Code completed with full documentation and sample problems.

Availability: Available to the public from DOE’s Energy Science and Technology Software Center (ESTSC; http://www.osti.gov/estsc/).

Current Developers: Tianfu Xu and collaborators.

Presenter at Workshop: Karsten Pruess

Brief code summary/overview (max 100 words): TOUGHREACT is based on TOUGH2, to which it adds capabilities for chemical reactions between aqueous, gaseous, and solid phases.

Relevant publications (max 5, please attach if possible):


MAIN PHYSICAL PROCESSES MODELED

Physical/chemical processes currently modeled:
Multiphase fluid and heat flow and mass transport as in TOUGH2. Homogeneous and heterogeneous chemical reactions between fluid and solid phases.

Main assumptions (list 5 most important):
Homogeneous reactions subject to local equilibrium. Heterogeneous reactions may be modeled by local equilibrium or kinetic rates.

Additional processes in implementation stage:
Kinetic treatment for homogeneous redox reactions.

Additional processes which will probably be included within 3 years:
Additional comments:

NUMERICAL ISSUES

Numerical schemes applied to the governing equations:
Flow and transport as in TOUGH2. Sequential iteration for chemical reactions. Capabilities for automatic time stepping and recognizing quasi-stationary states.

Handling of wells, fractures and/or other high risk leakage conduits:
Same as TOUGH2.

Largest problem simulated (include size, complexity, hardware, runtime etc.)
2-D dual permeability model of heater tests at Yucca Mountain with approximately 4,500 grid blocks. Approximately 3 months of real time simulated per hour of CPU-time on an IBM RS/6000.

Additional comments:

CODE EXPERIENCE

Brief description of recent CO2 sequestration simulations:
Simulated injection of CO2-H2S-SO2 mixtures into a sand-shale system representative of Texas Gulf Coast sediments. Chemical impacts of H2S are minor, while SO2 gives rise to strong acidification near the injection point. Impacts of shales are minor for simulation times of up to 10,000 years. CO2 sequestration capacity is on the order of 80 kg per m^3 medium.

Brief description of code comparison activities:
Performed a code intercomparison study on a batch reaction problem. Intercomparison studies are ongoing for geothermal reservoir problems.

Comments on robustness/stability:
Redox-sensitive reactions can be numerically difficult.

Additional comments: