Carbon Dioxide Sequestration Research Directions

Farshad Malekzadeh, PhD, PEng[1] and Maurice Dusseault, PhD, PEng[2]

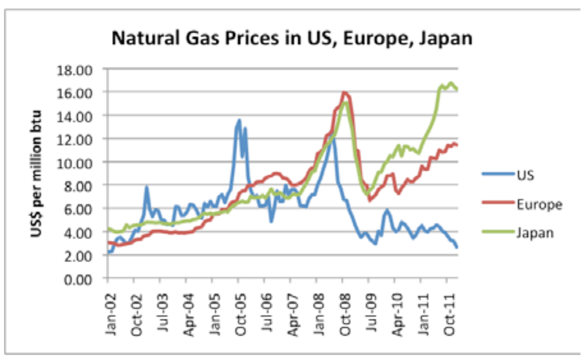
September 19. 2016

Background

Canada has aspirationally committed to reducing the carbon intensity of its energy industry, agreeing to the broad but non-binding strictures emerging from the Paris COP-21 meetings. Canada has not yet ratified the agreement, but at the G20 meeting in China, September 03, 2016, the USA and China formally announced their ratification of the COP-21 agreement. This means that, currently, about 18% of the initial signatory nations have ratified the agreement, but more important, these nations account for over 38% of the CO_2 global emissions. With the World's two largest emitting nations on board, COP-21 is starting to look inevitable, and Canada's ratification appears to be similarly inevitable. Ratification details may be found at:

https://treaties.un.org/Pages/ViewDetails.aspx?src=TREATY&mtdsg_no=XXVII-7-d&chapter=27&clang=_en

COP-21 will lead to a renewal in CO_2 sequestration, a subject that seemed highly relevant a few years ago which then fell off the media interest slate in the wake of the economic events of 2009 and the advent of cheap natural gas (NG) in the USA.



Cheap NG in the USA has changed the Energy Game, even in Canada

Indeed, the USA has rushed to replace aging coal-fired power trains that were being decommissioned at the end of their functional life. World-wide impacts on coal prices, the acceleration of a nascent fungible world market in LNG, the economic decline of the TransCanada NG Pipeline, the switching of Ontario from Western Canada NG to Pennsylvania NG from shale, even all of the concerns about hydraulic fracturing expressed in Quebec and the Atlantic Provinces can be traced, in substantial part, to the same set of events.

So, as COP-21 moves forward, several large trends will emerge including more renewable energy emphasis, slow decarbonization of transportation through NG inroads and electrification, a surging need

[1] Geomechanical Scientist, Computer Modelling Group, Calgary. Farshad.Malekzadeh@cmgl.ca
[2] Professor, University of Waterloo, Earth and Environmental Sciences. mauriced@uwaterloo.ca

for grid scale energy storage, renewed interest in CO_2 sequestration, and so on. Here, we focus on the upcoming CO_2 sequestration renewal in an attempt to identify important geological engineering research needs.

Research into CO_2 Sequestration

A few potentially interesting directions for research into CO_2 sequestration, with a definite bias toward geomechanics issues, are discussed below. An important aspect of such work is that the results are usually general and useful in other domains such as geothermal energy development (deep high-grade and intermediate-grade), multiphase fluid flow (CO_2 and brine in particular), deep waste disposal (water, slurried solids, acid gas…), petroleum engineering, and seismo-geophysics. Developing the analysis methods and monitoring methods for CO_2 sequestration will thus also have broad general benefit.

Analytical Analysis

The domain of analytic and semi-analytic solutions to clearly posed multi-phase fluid flow problems remains of great interest to all geoscience and geoengineering domains because such solutions have clarity (the physics and assumptions are clear), speed (especially for diffusion problems), and utility in risk analysis and probabilistic evaluations with uncertainty analysis.

There is a variety of research projects that could be undertaken in the context of CO_2 sequestration, and depending on the way the subject is approached, new possibilities and directions emerge. Although highly general (abstract) mathematical approaches have profound value, it is also necessary to deal with specific sites and specific distributions of properties. Abstract mathematical modelling of multiphase systems in a simple geometry with some robust regulization is usually based on writing the system conservation equation and neglecting the diffusive term. The governing equation then becomes a hyperbolic partial differential equation similar to the compressible gas problem (also known as the Euler problem). There exists a large literature in Computational Fluid Dynamics in the applied mathematics and physics domains that addresses these types of equations. However, this approach is complicated and scientifically demanding and may not automatically nor easily result in a suitable stream of publications (for research scientists and students). Nevertheless, it appears to be a useful and ambitious direction for a computationally sophisticated group. Here are some ideas:

- The class of problems where there are two competing forces (gravity-capillarity; Δp-gravity…) are of interest mathematically because in many important circumstances robust simplifications can be made, allowing mathematical solutions to be developed for the set of conditions stipulated. Identification of the dominant force in the flow-displacement regime has a significant advantage and makes the behavior of the rock-mass more predictable.
- Introduction of thermal aspects into mathematical solutions to allow THM coupled problems to be addressed (geophysics, volcanic processes, geothermal, cold water disposal…). In some cases and at some scales, either diffusion, conduction or reaction can be ignored, and solutions are simpler in such cases. In time-dependent problems, knowing when one or the other assumption is valid is important, and this gives useful early-time or long-time solutions. It is widely

acknowledged that long-term solutions are of great interest to environmental issues such as CO_2 sequestration, and THM numerical modeling is a time-intensive process. Hence, long-term mathematical solutions have particular value, even if the problems are simplified.

- Developing full poroelastically coupled solutions or approximations for diffusion-mechanics problems remains of profound interest especially in cases where it is clear that geomechanics issues are paramount (fault reactivation, reservoir deformation, interpreting deformation monitoring data, microseismic emissions and analysis; risk assessment…).
- For cases where simple geometries can be used (e.g. the circular tunnel in an isotropic stress boundary condition is the same as the perforated cased borehole of CO_2 injection and fluid production wells), increasing the level of geomechanics, HM and THM coupling in solutions is interesting, and linearized elasto-plastic behavior can be included in some cases. For example, including heat flux (cooling) into a stability analysis of a deep injection borehole is of interest.

Numerical Solutions

Once the value of analysis of simple geometries, mildly non-linear problems, and homogeneous cases is exhausted, it becomes necessary to use numerical solutions. More and more, large problems with multiple coupled physical processes and strong non-linearities are being modeled. Increasingly, discrete element models (for fractured systems) are of interest, and these present interesting up-scaling possibilities and challenges. Some needs are discussed below.

Considering geomechanical interactions in CO_2 sequestration, fault reactivation due to pressuring the subsurface by CO_2 (or any fluid) injection is a highly visible, widely discussed, yet complicated problem for current commercial software packages. This is a more general problem; induced seismicity arises in many contexts including deep mining, hydroelectric reservoir impoundment, coproduced water disposal, geothermal energy extraction, acid gas disposal, and even conventional oil and gas production involving large magnitude and large volume pressure depletion. These issues can also be studied in the context of CCS research, based in development and use of multi-physics simulators which can be calibrated to real data and which can predictively assess injection scenarios that might trigger fault slip or, more generally, induced seismicity. Faults or other discontinuities can be addressed in a conventional DEM context, but can be introduced in novel ways into other types of continuum solutions. For example, in Finite Element Models, a fault can be modeled as a 2D manifold with constraints across the fault based on either continuity of normal traction or zero inter-penetration of the sides. Numerical techniques to enforce this set of constraints are not straightforward, they probably likely involve penalty functions and a Lagrange multiplier.

Reactive flow of CO_2, such as water stripping from shale which leads to shrinkage or dilation, or dissolution of carbonate cements which alters permeability or wettability of the reservoir, is another potential research area. In a manner similar to the previous issue of fault reactivation, developments in this area will be valuable in different applications. It is reasonable to develop a coupled THMC model, and also including the thermo-geochemical-chemical coupling into the transport equations. One interesting possibility is to upscale the geochemical micro-scale process to a macro-scale multi physics constitutive model, and use such a constitutive model in a mathematical simulator. This might be feasible using the methods of molecular dynamics simulation. Also, this type of research is usually coupled with experimental studies and field observations in order to constrain and confirm the up-scaling process.

Considering the size of the numerical models, their underlying computational load is extremely large for multi-physics diffusion-reaction processes. Giga cell models for compositional analysis of conventional oil reservoirs are considered the biggest in the reservoir simulation field. However, the number of cells in the static models can easily be more than billions. Simulation with a model of this size requires streamlined and massively parallel algorithms, which makes a case for usage of HPC - High Performance Computation. Aggregating of computing power in a way that delivers much higher performance than one could get out of an ordinary computer or workstation in order to solve large problems is not a trivial task and requires a great deal of mathematical, programming and computer science knowledge. Additionally, to reduce the number of cells in the numerical models, up-scaling of the models is a viable and valuable method. However, up-scaling requires a solution transfer between two spatial discretizations, which is a challenging research subject of its own. In multi-physics problems, optimal discretization for each conservation equation (i.e. physical process) could be different and may change during the simulation time (i.e. grid adaptively). One should add the geometrical complexities and non-trivial boundary conditions to the challenges of the numerical models. Consequently, development of HPC in the form of massively parallel adaptive numerical simulators is a demanding research subject for geo-modeling problems like CCS.

The most common type of "non-standard" information available for a project is microseismic information – the spatiotemporally distributed stick-slip events that accompany any change in pressure, temperature, mass (dissolution or swelling), or other state parameter (mass or porosity must be treated as a thermodynamic state parameter in porous media). To gain further insight into system evolution in THMC problems such as CO_2 sequestration, it is necessary to couple geomechanics stress-strain analysis with microseismic emissions data in a rigorous manner, such that stress changes can be deduced (to first-order only) from the temporal evolution of induced seismicity during long-term projects. Great improvements in risk assessment and predictive capabilities would come from such coupling.

Other subjects in the mathematical modeling domain could be discussed here, such as multi-scale modeling, incorporation of semi-analytical solutions as kernel functions into large-scale analyses, methodologies to address the predictive impacts arising from heterogeneity (e.g. Kalman filter approaches), and so on. As always, these developments have far broader implications than merely CO_2 sequestration.

Dissolution Reactors

Dissolution of CO_2 in the saline pore fluid of a porous, permeable geological formation has been considered to be the most secure disposal and trapping mechanism. However, the small surface contact area between injected CO_2 and the host fluid makes the dissolution process extremely slow and impractical for the targeted time-scale of CCS. To overcome this obstacle, scientists and researchers have suggested different ideas. One potential way to accelerate the dissolution of CO_2 in host fluid is to have a separate artificial formation (at surface or at depth) which is designed for fast dissolution of gas in the host liquid under high pressure, and disposal of the consequent CO_2-rich aqueous solution into a natural deep geological formation. Having a dedicated dissolution reactor that is designed to accelerate the dissolution could be a game changer for sequestration technology, since a prominent concern about the existing CCS technologies is unsecure trapping of CO_2 in the geological formations. It may even be possible to exploit the different solubilities of N_2 and CO_2 and use waste water streams (produced fluids in the oil industry, aqueous streams from industry before treatment…) to develop pressurized CO_2-saturated streams for direct injection. Such an approach could eliminate the need for N_2 separation using amine technologies, which current account for over 60% of the cost of CO_2 sequestration. These are crude ideas yet, and require careful investigation, however, they are interesting and appealing potential research topics and may result in a reasonable improvement of CCS technologies.

Metrics and Calibration

Ultimately, measurements are vital to the design and implementation processes associated with CCS. The standard approaches to measuring temperature, pressure and rate that accompany any injection system are insufficient to allow a rigorous approach to tracking and interpreting the evolution of a CCS system over time and space.

Installation of distributed strain measurements in fiber optics mode and the deployment of large arrays of sensitive tiltmeters are two methods that can be used to measure the deformation field as CCS goes forward. Given a sufficient spatial density of deformation measurements, calibration of a geomechanically coupled process becomes possible. New optimization approaches have been developed for other coupled systems, and can be further developed for a THM coupled system (temperature, pressure, deformation).

Conclusions

The world energy picture is changing in many interesting ways, and these changes, combined with the geological engineering aspects of many of the emergent technologies, will place new demands on industry and the knowledge sources (university training, research…), that are needed to support new technical developments and large-scale implementation. The research and development community is well-advised to understand these changes, and plan to accommodate the new personnel and knowledge needs they will bring. We conclude that a renewing of interest in sequestration of CO_2 will soon take place, and there are valuable directions in the area of CO_2 sequestration research that will have impact in other geo-applications.