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Editorial

Special issue on computational methods in geologic CO_2 sequestration

1. Introduction

Human activity now impacts Earth's biogeochemical cycles at a global scale [1]. An example is the anthropogenic carbon footprint, which has led to an ever-increasing atmospheric concentration of greenhouse gases like carbon dioxide (CO_2) and methane (CH_4). This, in turn is responsible for global warming and possibly runaway positive-feedback effects on climate [2,3]. Much of the atmospheric emission of greenhouse gases originates from burning fossil fuels, which currently supply more than 80% of the primary power for the planet [4,5]. This link between energy production and climate change embodies one of the grand challenges of the 21st century: continuing to provide power for human activity while stabilizing and eventually reducing greenhouse gas emissions [6].

One promising technology to mitigate CO_2 emissions is carbon capture and storage (CCS), which involves capturing CO_2 from large stationary sources like coal-fired and gas-fired power plants, compressing it into a supercritical fluid, and then injecting it into deep geologic formations like saline aquifers for long-term storage [7–9]. CCS is attractive because it utilizes technology that is currently available [6] and because, if deployed at a sufficiently large scale, it would contribute to stabilizing greenhouse gas emissions while we continue to rely on fossil fuels to power our planet. In this sense, CCS would constitute a bridge technology for climate-change mitigation until our society transitions to a yet-to-be-determined low-carbon energy system [10].

However, many fundamental and practical aspects of migration and trapping of CO_2 underground are not well understood, and incorporating the relevant small-scale processes (the pore scale or the core scale) into the large-scale domains of interest (the geologic basin scale) is a pressing challenge. In addition to our partial knowledge of the physical–chemical mechanisms controlling CO_2 storage, uncertainty in the forecasts of CO_2 sequestration is exacerbated by the fact that the rock–fluid properties at depth (such as porosity, permeability, wettability, mineral and pore-fluid composition) are poorly constrained and often highly heterogeneous.

2. Scope of the special issue

Addressing the aspects outlined above require the development of modeling and computational approaches that guide the design and deployment of geological CO_2 storage. This is precisely the focus of the present Special Issue on *Computational Methods in Geological CO_2 Sequestration*: a series of contributions that improve our fundamental understanding of geological CO_2 storage, our ability to model it at different scales, and our ability to assess risk with scarce and imperfect data. These contributions provide a representative cross section of current research in the area of geological CO_2 sequestration and address, collectively, some of the outstanding challenges. We outline them below.

2.1. Pore-scale physics

Bandara et al. [11] present a Smooth Particle Hydrodynamics (SPH) method for the simulation of multiphase flow at the pore scale, which extends previous work to incorporate different contact angles of the fluid pair with the porous medium. They investigate the transition among the different regimes observed in micromodel experiments: capillary fingering, viscous fingering, and stable displacement.

2.2. Geochemical processes

Smith et al. [12] and Hao et al. [13] conduct experiments of carbonate rock dissolution as a result of core-flooding with CO_2-rich brine at reservoir pressure and temperature, and compare the results with a 3D continuum-scale reactive-transport model. They show that initial permeability and porosity variations control the development of the dissolution fronts in these highly reactive systems, and that these are captured by the continuum-scale model.

Leal et al. [14] revisit the problem of calculating chemical equilibria of general multiphase systems. They propose a new method based on a stoichiometric approach that employs Newton iteration to solve the system of mass-action equations coupled with a system of equilibrium constraints. They illustrate the use of the methodology to solve relevant geochemical equilibrium problems for modeling carbon storage in highly saline aquifers.

Saaltink et al. [15] present a methodology for reactive multiphase flow tailored to geochemical reactions in carbonate systems. The proposed method exploits linear combinations of the mass-balance equations for reactive transport to decouple the multiphase flow balance equations from the chemistry.

2.3. Multiphase flow in fractured rock

Oh et al. [16] present experiments and numerical simulation of multiphase flow in fractured rock, and reveal the potential importance of salt precipitation on the fracture–matrix interaction.

Fumagalli and Scotti [17] develop a new computational method for the simulation of two-phase flow in fractured porous media. The new method relies on representing the fractures as immersed interfaces, which does not require matching grids at the fracture-matrix interface, and therefore is more flexible with respect to the spatial discretization.

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2.4. Upscaling to the basin scale

Doster et al. [18] study the impact of the capillary transition region—in particular, capillary pressure hysteresis—on vertically-integrated models of CO_2 migration. They show that a proper treatment of capillary hysteresis can be important in redistribution of the CO_2 plume under buoyancy and capillary forces.

Tecklenburg et al. [19] introduce a model to upscale two-phase flow in strongly heterogeneous porous media like fractured rock. It consists of a flow equation for the saturation of the displacing fluid in a fracture, and a capillary flow equation for the saturation in the matrix. Both are coupled via a source term. By linearizing capillary counter current flow in the matrix, this system of equations is combined into a non-local single-equation model for the fracture saturation, which can be interpreted as a multi-rate mass-transfer model for immiscible displacement.

Li et al. [20] analyze, by means of high-resolution simulations using a continuum-scale model, the influence of the capillary-pressure model on CO_2 solubility trapping. They find that the average CO_2-dissolution flux is quite sensitive to the choice of the capillary pressure curve, and observe that the van-Genuchten model predicts accelerated CO_2 solubility trapping compared with the Brooks–Corey model.

Elenius and Gasda [21] present numerical simulations of convective dissolution at a horizontal CO_2/brine interface under the presence of horizontal barriers. They inspect the influence of the geometrical parameters that determine the barrier pattern on the diffusive CO_2 flux and the finger tip propagation velocity. They also test the possibility of using an upscaled anisotropic permeability as a means to capture the influence of unresolved horizontal barriers on the diffusive CO_2 flux.

Hidalgo et al. [22] analyze, by means of high-resolution simulation, the dynamics of convective dissolution during the upslope migration of a CO_2 gravity current. They show that the dynamics of the dissolution flux and the macroscopic features of the migrating current can be captured with an upscaled sharp-interface model.

Gasda et al. [23] study the impact of topography of the caprock on vertically-integrated models of CO_2 migration, including its effect on the different modes of storage (structural, residual, and solubility trapping).

Pool et al. [24] describe a new concept for carbon sequestration, based on injecting dissolved CO_2 instead of CO_2 in supercritical phase. In particular, they propose extracting brine from the geologic formation and mixing brine and CO_2 at depth in the injection borehole, which is more economical than surface dissolution. They evaluate the energy requirements for the system, and determine conditions under which the proposed method is viable.

Walter et al. [25] address the issue of models that are overly conservative and therefore produce risk assessments that far over-predict reality. This concept is illustrated by means of synthetic examples to study brine migration and saltwater intrusion into freshwater aquifers.

2.5. Modeling and monitoring of coupled flow and geomechanics

Jung et al. [26] propose a methodology for inversion of hydrogeological parameters and early detection of potential CO_2 leakage using pressure and surface-deformation anomalies. By applying their methodology to synthetic examples, they establish conditions under which surface-deformation measurements can contribute significantly to the fidelity of the forecasts.

Castelletto et al. [27] perform large-scale three-dimensional numerical modeling of CO_2 sequestration in an actual, offshore, multi-compartment reservoir. The study elucidates important aspects of the problem, including the role of flow–geomechanics coupling in the potential for shear failure of faults as a result of CO_2 injection.

This topic—coupled behavior of flow and geomechanics in the presence of fractures and faults—is a key emerging theme for CCS. Subsurface technologies (including others like geothermal energy or hydrocarbon recovery from shales) have come under increased scrutiny due to their potential to affect fresh groundwater bodies due to leakage of injected fluids [28–31], and to induce seismic activity as a result of overpressurization of geologic layers [32–35].

3. Outlook

Currently, CCS is at a crossroads. On the one hand, much progress has been made in the past decade in all aspects of the technology, including critical advances in our understanding of long-term geological storage. On the other hand, the high cost of implementation of CCS, together with the lack of an effective (and enforceable) international policy that internalizes the cost of carbon emissions, has led to the sobering experience that many large-scale CCS projects have been delayed or abandoned. This is, in our view, a case of "a problem dropped, not a problem solved", as the need for near-term climate-change mitigation technologies will inevitably be even more pressing in the future than it is now.

These challenges, in turn, should provide an incentive to the scientific community to provide the physical basis and the mathematical and computational tools required to implement CCS at scale. We believe that the contributions in this special issue constitute a step in this direction.

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Ruben Juanes
Department of Civil and Environmental Engineering,
Massachusetts Institute of Technology,
77 Massachusetts Ave,
Cambridge, MA 02139, USA
E-mail address: juanes@mit.edu

Holger Class
Department of Hydromechanics and Modelling of Hydrosystems,
Universität Stuttgart, Pfaffenwaldring 61, 70569 Stuttgart, Germany

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