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EDITORIAL NOTES

Preface

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1 Carbon dioxide capture and storage (CCS)

Carbon dioxide capture and storage, a process where CO_2 is captured after combustion in power plants or from processing industries and then permanently stored in the deep subsurface, is considered an important option to contribute to a reduction of greenhouse gas emissions [3]. Since a shift in global energy production towards carbon-free sources is one ultimate goal, CCS will have to be an essential technology for the forthcoming decades until the use of fossil fuels is totally abandoned worldwide. However, there are, for example, still huge amounts of coal, a cheap fossil fuel, so that its combustion, especially in the USA, Australia, China and India, and, as a consequence, continuing CO_2 emissions into the atmosphere are highly likely - unless the CO_2 is captured and stored.

The implementation of CCS on a scale that can become relevant for climate protection requires public acceptance in the industrialised countries. In order to investigate the impact of an underground CO_2 injection on ecosystems and inhabited areas, mathematical and numerical modeling must play a vital role besides field explorations and laboratory investigations.

2 Processes during CO_2 storage in geological formations

The effective geological storage of CO_2 can occur by various interacting physical and geochemical processes and trapping mechanisms. When CO_2 is injected into a geological formation, for example into a deep saline aquifer, the CO_2 forms a discrete phase around the injection well. The ambient water (brine) is displaced and the CO_2 moves both laterally, due to the pressure gradient induced by the injection, and vertically, due to buoyancy. As long as the CO_2 phase is mobile, it requires hydraulic barriers such as caprock seals to prevent an escape from the target reservoir towards shallower depths or eventually back to the atmosphere. Faults in folded or fractured rocks can also serve as structural barriers although, depending on the circumstances, they can also represent preferential pathways, allowing CO_2 to escape. Potential pathways for CO_2 towards shallower regions can also be man-made, e.g. poorly completed or abandoned wells.

CO_2 migration will stop either upon the CO_2 reaching hydraulic barriers or when its mobility becomes zero, which occurs when the CO_2 saturation decreases to the residual saturation (residual trapping). The mobility of CO_2 in a CO_2-brine system is also affected by hysteresis. On the macroscopic scale, on which most model concepts are developed, this can be expressed by hysteretic relative permeability functions [2, 4]. In the long term, increasing quantities of CO_2 dissolve in the formation water and are then subject to the movement of the groundwater and the diffusion/dispersion processes in it (solubility trapping). Water that is rich in dissolved CO_2 is denser and tends to sink towards the bottom of the reservoir. In fact, this process is

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rather slow and occurs only on a larger time scale than the advection-dominated multiphase spreading. Dissolution of CO_2 in the water also forms ionic species. This causes changes in the pH and initiates geochemical reactions. If some fraction of the CO_2 can be converted to stable carbonate minerals, this mineral trapping is expected to be the most permanent form of geological storage. The geochemical processes themselves are comparatively slow, taking in the range of thousands of years.

3 Mathematical and numerical modeling

Mathematical and numerical flow and transport models allow a comprehensive investigation of complex physical systems. Such models have proven to be indispensable tools in many engineering problems, for example for improving process understanding and identification, optimization, pre-experimental predictions, planning of protection and remediation measures, interpretation of measurement data etc. A model can help explain situations, for example the origin/leakage path of CO_2 detected somewhere on the surface of the ground. Models can also simulate interventions into systems and predict their effects. Furthermore, analyses of risks and parameter sensitivities are an important purpose of model applications. Other aspects into which modeling can provide significant insights are, for example, the assessment of storage capacities, leakage rates, potential leakage pathways, or impacts on geo- and ecosystems, to name just a few.

In any of these cases, it is crucial to be able to have confidence in the results of a simulation. This includes confidence in the model concepts, which should be capable of representing the main physical (and chemical) processes, as well as confidence in the accuracy, and reliability of the models/codes, covering both the numerical algorithms and the mathematical descriptions of processes, fluid properties etc. Furthermore, it is necessary to estimate the potential uncertainties of model predictions which may arise from uncertainties in model input parameters, or from the choice of the model concepts or even the different codes.

A problem that seems to be inherent in modeling processes during and following CO_2 injection into geological reservoirs is that model validation with well-controlled experiments is limited because of the very large time scales on which the processes occur.

4 Code/model intercomparison

A useful approach towards improving confidence in simulation results is a comprehensive intercomparison of models and codes applied to specific problems or benchmarks, e.g. [5].

Formulating benchmark problems and evaluating the results of the intercomparisons of models and/or codes is no trivial task. First of all, there is a basic difference between mere code intercomparison and model intercomparison although, in fact, there can be smooth transitions. The idea of comparing codes assumes that all codes are based on the same or similar physical (or also chemical) model concepts and the aim of the intercomparison is a matter of checking the implementations, numerics etc. Code intercomparison by means of benchmark problems can then be considered as the verification of a given code or mathematical/numerical method.

A model intercomparison can be seen as a more relevant approach where different models, i.e. different concepts, different assumptions etc., are applied to the same question, for example the leakage rate over time. A major aim of comparing model concepts is then to find the range of predictions for given questions. However, beyond the model concepts and the codes, there are further sources of uncertainties like the influence of different gridding, different interpretations of the problem by the modeler, and others.

Modelers will have to address a number of important questions concerning the role that modeling can play for practical CO_2 storage projects, for example:

- Can models be predictive, e.g. concerning leakage scenarios?
- Which are the really important processes that need to be implemented in the models?
- Given the many sources of uncertainties, in particular from geological input data: is numerics important at all?
- How can the true solutions to given problems be identified?

We believe that well-formulated benchmark problems are an important step for a systematic approach to answering these questions.

Previous benchmarks like the LBNL [5] and SPE (http://www.spe.org/web/csp/) studies have been very important in pointing out a path the modelling community can follow. For example, both these studies have highlighted the importance of geological heterogeneity and the need for computational speed. For one thing, the current benchmark demonstrates that different simulators give quantitatively similar results when the benchmark is sufficiently simple and well specified. On the other hand, when modelling choices become important, results start to diverge - even qualitatively. If anything, we believe the Stuttgart benchmark studies presented in this Special Issue of Computational Geosciences have shown the importance of understanding the uncertainty related to the modeller's choices. This also shows the importance of a continuous effort to establish sets of benchmarks to bring more insight into the uncertainty-related choices made by different modellers. As part of this ongoing effort, a new benchmark study has been initiated in conjunction with the Svalbard workshop [1].

5 Outline of this special issue

This Special Issue of Computational Geosciences comprises a collection of manuscripts related to the numerical modelling of processes during CO_2 storage in geological formations. The strong focus of this Special Issue is on the above-mentioned Stuttgart benchmark study.

The first article by *Class et al.* summarises the description of the benchmark problems. They are all based on 3D geometries, and one of the benchmark problems is related to geological input data of the Johansen formation off the coast of Norway, provided by the Norwegian Petroleum Directorate. The paper of *Eigestad et al.* gives more details on the geological modeling and simulated injection scenarios in this Johansen formation. In the third manuscript, the authors *Wei & Saaf* go beyond the time scale of 50 years given in the original description of the Johansen benchmark problem. They also present studies on parameter sensitivities for this benchmark. The next two papers by *Gasda et al.* and *MacMinn & Juanes* both address the integration of analytical mathematical solutions for simulating the multiphase flow during the injection of CO_2, while the manuscript of *Qi et al.* describes the application of a streamline approach including rather complex compositional effects like mutual dissolution and salt precipitation.

In summary, one might conclude that the mathematical and numerical models currently developed for simulating CO_2 storage in geological formations span a wide range of methods. Nevertheless, as long as they consider the same physics, their range of predictions appears to be rather small in comparison with uncertainties arising from sources other than the model concept and the numerics, for example from geological uncertainties and from all the choices a modeller has to make; these include the generation of a suitable grid, the assignment of initial and boundary conditions, the choice of accurate equations of state etc. Future work should address in particular the issue of a better quantification of the many different uncertainties that are inherent in the overall modelling procedure.

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