Available online at www.sciencedirect.com

ScienceDirect

Energy Procedia 97 (2016) 502 – 508

Energy Procedia

European Geosciences Union General Assembly 2016, EGU
Division Energy, Resources & Environment, ERE

Coupling of geochemical and multiphase flow processes for validation of the MUFITS reservoir simulator against TOUGH

M. De Lucia[a,*], T. Kempka[a], A. Afanasyev[b], O. Melnik[b], M. Kühn[a]

[a] *GFZ German Research for Geosciences, Section 3.4 Fluid System Modelling, Telegrafenberg, 14473 Potsdam, Germany*
[b] *Moscow State University, Institute of Mechanics, 1 Michurinsky Prospekt, Moscow 119192, Russian Federation*

Abstract

A benchmark study is presented comparing the outcome of two different simulators, the established TOUGH and the modern, more efficient MUFITS, with the purpose to evaluate the coupling of geochemical processes to multiphase flow in the context of subsurface CO_2 storage. The results of the two simulators are in excellent agreement. The implemented simplified one-way coupling is a computationally efficient alternative to fully coupled reactive transport simulations. Every coupled process simulation framework benefits from the inclusion of different tools, which is the only way to enable validation and control of numerical results.

Peer-review under responsibility of the organizing committee of the General Assembly of the European Geosciences Union (EGU)
Keywords: Reactive transport, CO_2 geological storage, benchmark, MUFITS, TOUGH

---

1. Introduction

Coupled reactive transport modelling at continuum or Darcy scale [1,2] finds increasing attention in the investigation of interacting hydrodynamical, physical, chemical and biochemical processes in natural or engineered systems. In particular, in recent years, it has been extensively employed to assess feasibility of subsurface CO_2 or gas storage in diverse geological settings [3–5]. From a geoscientific point of view, these models are characterized by a large computational demand (CPU-time) and by numerical instabilities and frequent non-convergence of the simulations. These issues limit in practice the applicability to relatively simple systems, usually at a much lower spatial resolution and for much shorter time scales than non-reactive multiphase flow simulations in the same geological settings. Published studies of reactive transport frequently consider only very simple geometries, 1D/2D or extremely coarse 3D grids [5–9]. It is obvious that in this way many geological features such as faults, discontinuities, spatial heterogeneity cannot be represented adequately.

Oversimplifications may concern the chemistry as well, including in the models only a subset of the potentially occurring reactions (or components) of a given system. This has two main reasons: (1) chemistry is usually the

---

[*] Corresponding author. Tel.: +49-331-288-2829 ; fax: +49-331-288-1529.
E-mail address: delucia@gfz-potsdam.de

Peer-review under responsibility of the organizing committee of the General Assembly of the European Geosciences Union (EGU)
doi:10.1016/j.egypro.2016.10.060

computational bottleneck for coupled reactive transport models, demanding up to 90 % of overall CPU time. (2) the geochemical models are affected by extremely large uncertainties concerning thermodynamic and kinetic parameters [10–12], as well as the mineralogical heterogeneity of the investigated porous media, which makes it difficult to define a representative medium.

In this context, coupled models can be used for qualitative process understanding rather than as reservoir-scale quantitative, predictive tools for subsurface utilization. It is important to stress that purely hydrodynamic (i.e. non-reactive) simulations, being much less demanding in terms of computational efforts, are routinely performed on multi-million element spatial discretizations, several orders of magnitude above what is currently achievable for coupled models.

A promising way to reduce the oversimplifications of the physical systems or the coarsening of simulation grids is represented by **simplifying the coupling** itself [13]. The typical characteristics of CO_2 storage systems in siliciclastic reservoirs are suited to be modelled employing a **one-way coupling** between hydrodynamical and chemical processes. Such a method has already been successfully applied to long-term, reservoir-scale assessment of mineral trapping at the Ketzin pilot site in Germany [14,15].

The complexity of the targeted physical and chemical processes under investigation can only be approached by numerical methods. It is, therefore, crucial to dispose of different tools to benchmark and verify simulation results, ideally using more than one numerical approach, which in practice means more than one simulator. These considerations led us to include in the original implementation of the one-way coupling presented in [13], which is based on the TOUGH family simulators [16,17], with one based on the more modern and efficient multiphase flow simulator MUFITS [18]. The aim of this paper is to benchmark the results of the two simulators with respect to the coupling approach defined in [13]. It is intended as validation of both the simulators and the coupling itself.

In the following sections, the simplified one-way coupling is first outlined, followed by the description of the actual case study. Finally, the predictions by the TOUGH and MUFITS simulators and their results when coupled with geochemistry are presented.

2. Simplified one-way coupling approach

The idea underlying the one-way coupling is to combine, in a post-processing approach, independently obtained batch geochemical simulations with non-reactive flow simulations. This means that the mutual feedback between chemistry and hydrodynamical processes is actually disregarded. It concerns both the mass balance of fluids or solutes (e.g., minerally trapped CO_2 which is not "available" for transport anymore) and the petrophysical properties of the porous medium (porosity, permeability). For the approach to be valid, however, only three necessary and sufficient conditions have been identified [13]:

1. the time scale of mineral reactions is much larger than that of hydrodynamical processes;
2. the main driving force for mineral alterations is the presence of a limited number of fluid components (e.g., the injected CO_2, either in a separate phase or in dissolved form);
3. the mineral reactions do not affect significantly the petrophysical properties of the medium (porosity, permeability) at least not until the system has reached substantial hydrodynamical equilibrium.

Even if they may appear quite strict, all these conditions are usually met with good approximation in the typical subsurface CO_2 storage system in siliciclastic reservoirs. In fact, chemical reactions capable of significantly altering porosity and permeability of the medium, such as precipitation of carbonates, are expected to be very slow (kinetically-limited), and thus to occur long after abandonment of a storage reservoir. Under these circumstances, the feedback of chemistry on petrophysical properties can be safely disregarded. Conversely, since the transport of solutes will be very slow when approaching hydrodynamical equilibrium, it will not affect chemistry when reactions start becoming significant. Therefore, also the feedback between transport and chemistry will be limited.

The simplified coupling itself proceeds as follows: First, one single batch geochemical simulation and the hydrodynamic simulation of CO_2 injection are run separately for the entire simulation time. From the hydrodynamic simulations, the exposure time to injected CO_2 of each grid element is computed, distinguishing whether CO_2 is dissolved or in a free phase. If only dissolved CO_2 reaches the element, its concentration must exceed a user-defined threshold to consider the element "chemically active". The single batch geochemical simulation is subsequently ap-