Afanasyev, A., Kempka, T., Kühn, M., Melnik, O. (2016): Validation of the MUFITS Reservoir Simulator Against Standard CO2 Storage Benchmarks and History-matched Models of the Ketzin Pilot Site. - *Energy Procedia*, *97*, pp. 395–402.

DOI: http://doi.org/10.1016/j.egypro.2016.10.032

Available online at www.sciencedirect.com

ScienceDirect

Energy Procedia 97 (2016) 395 – 402

Energy Procedia

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

Validation of the MUFITS reservoir simulator against standard CO_2 storage benchmarks and history-matched models of the Ketzin pilot site

Andrey Afanasyev[a,*], Thomas Kempka[b], Michael Kühn[b], Oleg Melnik[a]

[a]*Institute of Mechanics, Moscow State University, Moscow 119192, Russian Federation*
[b]*GFZ German Research Centre for Geosciences, Fluid Systems Modelling, Telegrafenberg, 14473 Potsdam, Germany*

Abstract

We give an overview of the MUFITS reservoir simulator capabilities for modelling subsurface carbon dioxide storage using the EOS-modules GASSTORE and BLACKOIL. The GASSTORE module covers solid-liquid-gas flows of water, carbon dioxide and salt components, and includes an option for automatic generation of the BLACKOIL PVT tables. We test the simulator against several benchmarking studies and then consider an application case of CO_2 storage at the Ketzin pilot site, Germany. The modelling results are in excellent agreement with those produced with common scientific and standard industrial simulators.

Peer-review under responsibility of the organizing committee of the General Assembly of the European Geosciences Union (EGU)

Keywords: MUFITS; Reservoir simulator; CO_2 storage; Black-oil simulation; Model benchmark; Ketzin pilot site

1. Introduction

Understanding and quantifying processes in subsurface porous medium systems require application of robust reservoir simulators that include flexible modelling capabilities. A practical simulator should include advanced options for gridding, predicting fluid properties, accelerated simulations, etc. However, many free scientific simulators provide only a pale imitation of capabilities of commercial simulators commonly used in oil and gas industry.

* Corresponding author. Tel.: +7-495-939-57-67
E-mail address: afanasyev@imec.msu.ru

Peer-review under responsibility of the organizing committee of the General Assembly of the European Geosciences Union (EGU)
doi:10.1016/j.egypro.2016.10.032

We present several new options available now with the MUFITS reservoir simulator – a free software for hydrodynamic reservoir simulations [1–3]. MUFITS is a scientific software, but designed as a standard industrial simulator making advanced engineering-like techniques, similar to those provided with commercial software, available to the scientific community. This particular work aims at demonstrating and validating the capabilities of MUFITS for modelling subsurface CO_2 storage in simplified benchmark problems and a complex 3D scenario based on CO_2 storage at the Ketzin pilot site.

1.1. MUFITS architecture

The architecture of MUFITS includes the simulator kernel and several fluid property modules, i.e. EOS-modules (Fig. 1). Every EOS-module contains a mathematical description of the fluid properties, e.g. number of phases, number of components, equation of state, density, viscosity, etc. The simulator kernel contains all program procedures not depending on fluid properties, e.g. grids, petrophysical properties of rocks, wells, linear solver, etc. The kernel can be linked with various EOS-modules extending the application area of the software.

This work discusses the GASSTORE and BLACKOIL modules. The GASSTORE module, developed recently, covers three-component three-phase solid-liquid-gas flow of water, gas and salt components, including thermal processes, and salt precipitation and dissolution. Thermophysical properties of different gas components are tabulated in the simulator, e.g. the properties of CO_2, CH_4, N_2, etc. Thus, the GASSTORE module can be applied not only to subsurface CO_2 storage but also to gas storage in saline aquifers. The extended black-oil model is utilized in the BLACKOIL module [4], which can be applied in the CO_2 storage scenarios to two-phase flows of CO_2 and brine components, neglecting salinity variations and solid phase precipitation.

1.2. Converting GASSTORE to BLACKOIL

When using CO_2 component, the GASSTORE module utilizes the method proposed by Spycher et al. [5], and Spycher and Pruess [6] for predicting the properties of the H_2O–CO_2–NaCl mixture. Thus, there are three components, namely salt, water and CO_2, and there are three phases, namely solid, brine and the gas phase (Fig. 2). The simulator can optionally treat the salt and gas components as dissolving in brine, and it is capable to represent water vapor in the gas phase. The solid phase comprises only the salt component. Depending on pressure and temperature conditions as well as dissolved salt concentration, salt can precipitate or dissolve in brine. Each of the three components and the respective phases can be enabled or disabled in the simulation run. For instance, to speed up the simulation only two components can be enabled, e.g. gas and water, or water and salt.

The BLACKOIL model is capable to simulate three-phase three-component flows of water, oil and gas [4]. In this particular work, we assume that water is disabled when using BLACKOIL (Fig. 2). Thus, we assume that there are only two components and two phases with identical names, oil and gas. The gas component can optionally dissolve in the oil phase, and the oil component can vaporize in the gas phase. The BLACKOIL module is isothermal, so that flow in the porous medium is assumed to occur at constant reservoir temperature.

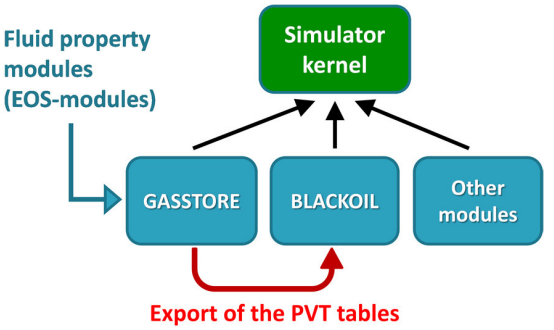

Fig. 1. Architecture of the MUFITS simulator. Black-oil PVT tables can be generated using the GASSTORE module.

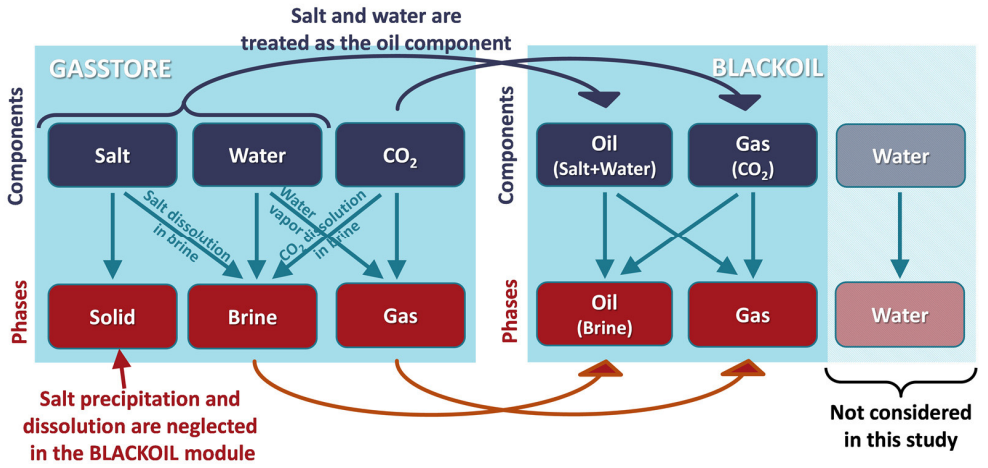

Fig. 2. GASSTORE models (left) can be automatically converted to BLACKOIL models (right).

The GASSTORE module can be further used for generating of the black-oil PVT tables for a given reservoir temperature and brine salinity. These tables can be used in the conventional black-oil modelling approach that may be significantly faster. When converting GASTORE to BLACKOIL models, the salt and water components are treated as the oil component, whereas CO_2 is represented as the gas component [7]. Gas dissolution in brine as well as water vapor in the gas phase can be optionally taken into account in the black-oil PVT tables. Salt precipitation and dissolution as well as thermal processes are neglected in the BLACKOIL module.

1.3. Initial vertical equilibrium

Both the BLACKOIL and GASSTORE modules include an advanced option for initializing a reservoir study. The option allows a fast calculation of the hydrostatic pressure distribution honoring given temperature and brine salinity distributions as well as capillary pressures [8]. This equilibration option saves a lot of time when applied instead of an iterative calculation of the initial conditions by time-stepping.

To initialize the vertical equilibrium with both gas and water components enabled in the GASSTORE module, the user must provide a pressure at a given depth as well as the depth of the gas-water contact, which divides the reservoir into the gas and water zones (Fig. 3). The reservoir is mainly saturated with gas above the contact depth, possibly with a residual brine saturation, and mainly with brine below that depth. The user can optionally provide the distribution of the gas fraction dissolved in brine versus depth for the water zone as well as the distribution of water vapor in the gas for the gas zone. If non-isothermal processes are enabled in the simulation run, the user must provide temperature dependence versus depth data, corresponding to the local geothermal gradient. If the salt component is enabled, then the user must provide the distribution of salinity or solid phase saturation versus depth. The dependence of all parameters on depth is specified in a tabulated form. The output of the equilibration option is the hydrostatic distribution of pressure, whereas all other parameters are distributed as previously specified by user.

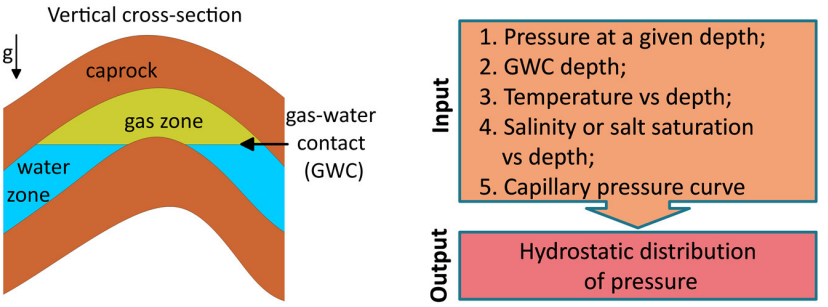

Fig. 3. Schematic view of the vertical equilibration option.

2. Modelling benchmark problems

2.1. CO_2 injection into a 2D layered brine formation

In order to validate MUFITS, we consider three benchmark problems. The first 2D isothermal problem concerns CO_2 injection into a 2D layered brine formation [9,10]. The reservoir model comprises high-permeable sandstone layers and thin low-permeable shale layers (Fig. 4). The injection of CO_2 occurs in the grid block denoted by '*Inj*' at the bottom of the domain (Fig. 4(a)). A complete formulation of the benchmark study is given in [9,10]. This problem was simulated using MUFITS with both the GASSTORE and BLACKOIL modules. The distributions of the gas saturation, s_g, and pressure, P, at $t = 2$ years as well as the vertical permeability, K_z, are shown in Fig. 4(a). The injection results in CO_2 accumulation beneath the shale layers. The results obtained using the GASSTORE module are in a very good agreement with those of other codes, shown by grey curves in the background figures. In particular, the saturations of gas, s_g, brine, s_l, and solid phase, s_s, in the well grid block denoted with '*Inj*' (Fig. 4(b)) and the gas flow rate from that grid block in the $x+$, $z-$ and $z+$ directions (Fig. 4(c)) are very close to the results of other codes. The gas saturations, in that well grid block and in the grid blocks immediately above, $z-$, below, $z+$, and to the right, $x+$, of *Inj*, and at $x = 0$ m, $z = 958.5$ m (Fig. 4(d)) as well as the distribution of s_g at x=500 m (Fig. 4(e)) are also in a good agreement.

The black-oil tables were generated using MUFITS for a temperature of 37°C and a low brine salinity of 0.00045, neglecting water vapor in the gas phase [9,10]. These tables were loaded into a BLACKOIL simulation considering the same benchmark scenario. In general, the results of the black-oil simulation show a good agreement with the results obtained using the GASSTORE module, but there is a high deviation in the well grid block (Fig. 4(b)), because the BLACKOIL module is neglecting salt precipitation in the near-well area. The saturation of the solid phase, s_s, is identically zero, and therefore the gas and liquid saturations are also different from that provided in [9,10]. However, the results of the both modules coincide at any location in the model, where the salt precipitation does not occur (Fig. 4(e)).

2.2. A 3D benchmark study on CO_2 storage

The second problem concerns CO_2 injection in a realistic 3D reservoir with a geological fault [11]. There is a single injection well (Fig. 5). A constant injection rate is maintained over the time $0 \le t \le 25$ years, and further the injection is stopped over the time $t > 25$ years. Salt precipitation and dissolution are not taken into account. A complete formulation of the problem is given in Class et al. [11]. The spreading of CO_2 along the caprock results in a complex spatial distribution of gas saturation, s_g, in the top layer. This distribution as well as the total mass of CO_2 (summed over all grid blocks in the domain) in the gas phase and in brine are in good agreement with other codes, shown by grey lines (c.f. [11]). This benchmark problem was simulated using both MUFITS modules, whereby those produced by the BLACKOIL module are indistinguishable from the results predicted by the GASSTORE module. Earlier, the simulator was also tested against this benchmark using a different BINMIXT EOS-module [3].

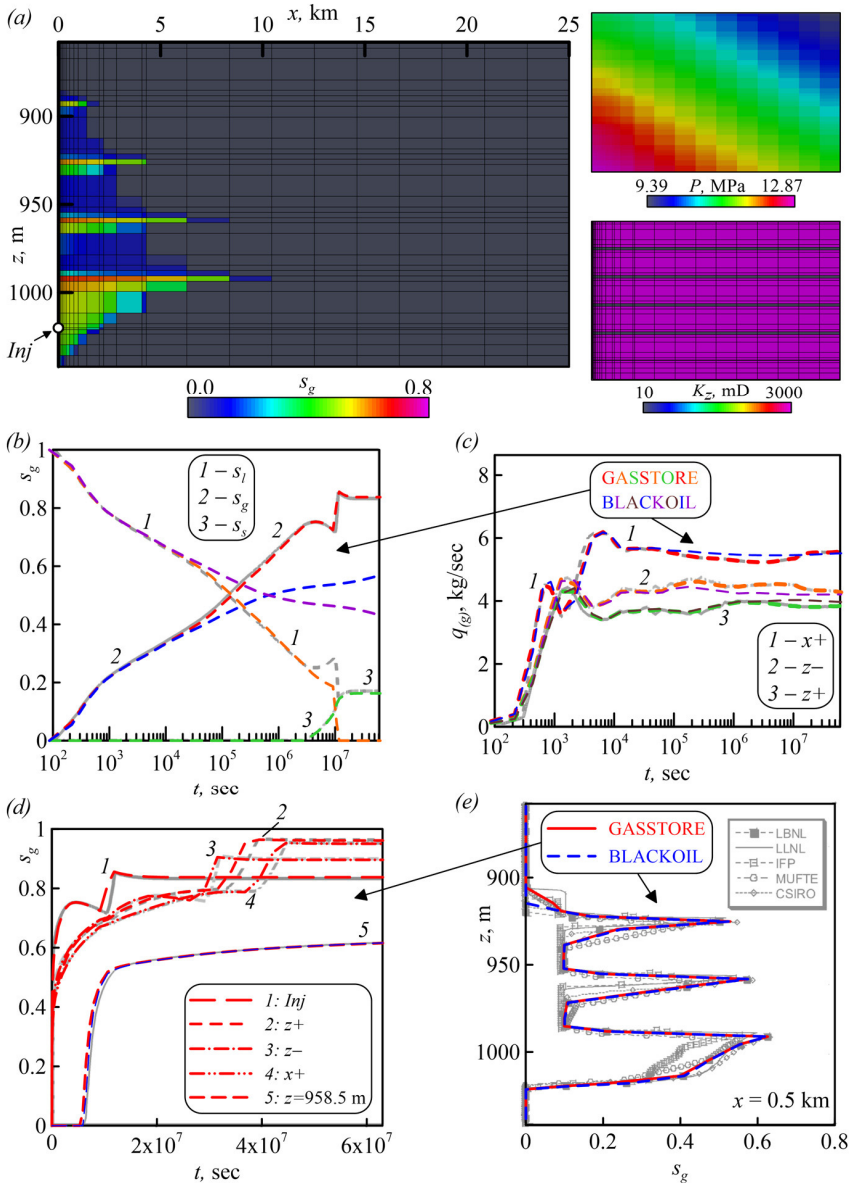

Fig. 4. Results of the simulation of CO_2 injection into a 2D layered brine formation. The background figures are modified after Pruess et al. [9] and Pan et al. [10].

2.3. Benchmark against history-matched 3D models for CO_2 storage at Ketzin pilot site

The third benchmark problem is dedicated to the Ketzin pilot site for CO_2 storage located close to the town of Ketzin, about 40 km west of Berlin, Germany [12]. About 67 kt of CO_2 were injected from June 2008 until August 2013 into the Triassic Stuttgart Formation of fluvial origin, consisting of sandstone channels embedded in a highly heterogeneous floodplain facies [13,14]. The high heterogeneity in porosity, and thus permeability, as well as the complex structure of the graben zone at the top of the Ketzin anticline result in high requirements to be fulfilled by the numerical simulator (Fig. 6). This is also emphasized by the high variations in the injection regime [15,16]. Further information on the model setup is given in Class et al. [17] and Kempka and Kühn [18].

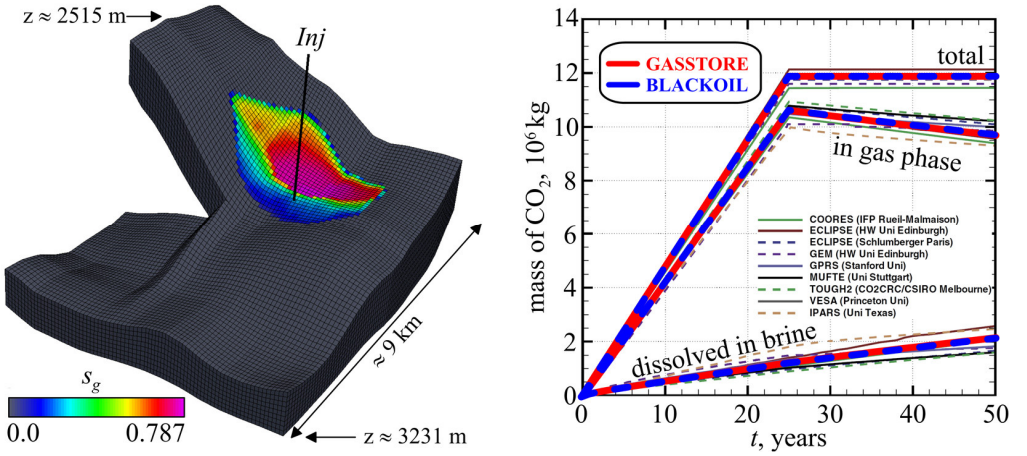

Fig. 5. Results of the simulation of CO_2 injection into a realistic reservoir. The background figure is modified after Class et al. [11].

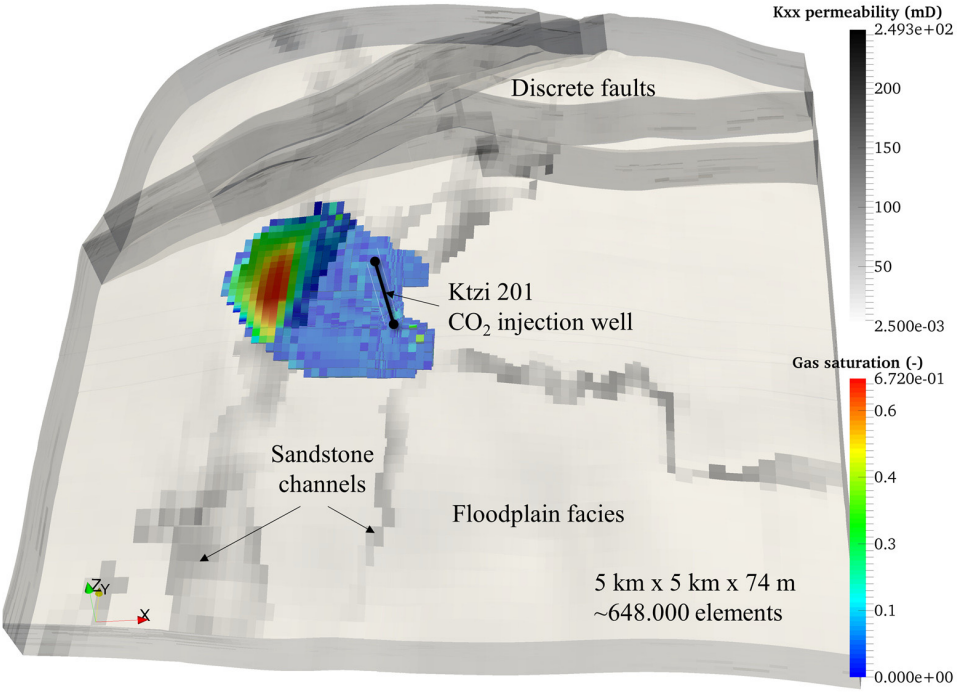

Fig. 6. Effective permeability and simulated gaseous CO_2 saturation at the Ketzin site in July 2014.

In the present benchmark comparison, we investigated the conformity of modelling results between the Schlumberger ECLIPSE 100 [17,18] and the MUFITS (BLACKOIL module) simulators [1]. The results show an excellent match between predictions of the two simulators (Fig. 7). In particular, the gas and liquid phase pressures, P_{gas} and P_{lig}, in the near-wellbore zone simulated with ECLIPSE 100 and MUFITS do not show any deviations for the period from June 2008 until July 2015 (Fig. 6(a)). Here, the P_{gas} and P_{liq} values are different due to consideration of capillary pressure. The volumes of CO_2 in different phase states (summed over all grid blocks) predicted by ECLIPSE

100 and MUFITS are also identical (Fig. 6(b)), whereby sm^3 denotes cubic meters at surface conditions. In view of other existing benchmarks using scientific simulators [19], we especially want to point out the excellent agreement achieved.

For the last benchmark, MUFITS requires roughly twice the computational time compared to ECLIPSE for the same simulation run, using identical hardware and number of CPU cores. However, it has to be noted that MUFITS shows a good linear scalability (up to 50–60 cores for a model comprising 250–300 thousand grid blocks) [20], while ECLIPSE does not show any relevant speed-up when using more than six cores [21]. Hence, assigning more cores to the MUFITS process will result in a lower computational time compared to ECLIPSE. It has also to be noted that TOUGH2 is significantly slower than ECLIPSE (by about factor 20) when modelling CO_2 injection at the Ketzin site [18]. Thus, MUFITS is significantly faster than TOUGH2 in parallel mode.

Consequently, MUFITS is perfectly suited to deal with highly complex reservoirs, including faults and highly varying production/injection data.

3. Conclusions

Our results show that MUFITS is a flexible and robust simulator capable of modelling subsurface carbon dioxide storage in complex 3D geological settings. The simulator includes different EOS-modules and comprehensive options to ease the modelling process. The results of the simulations of benchmark problems using MUFITS are in excellent agreement with those produced with other scientific and industrial standard simulators.

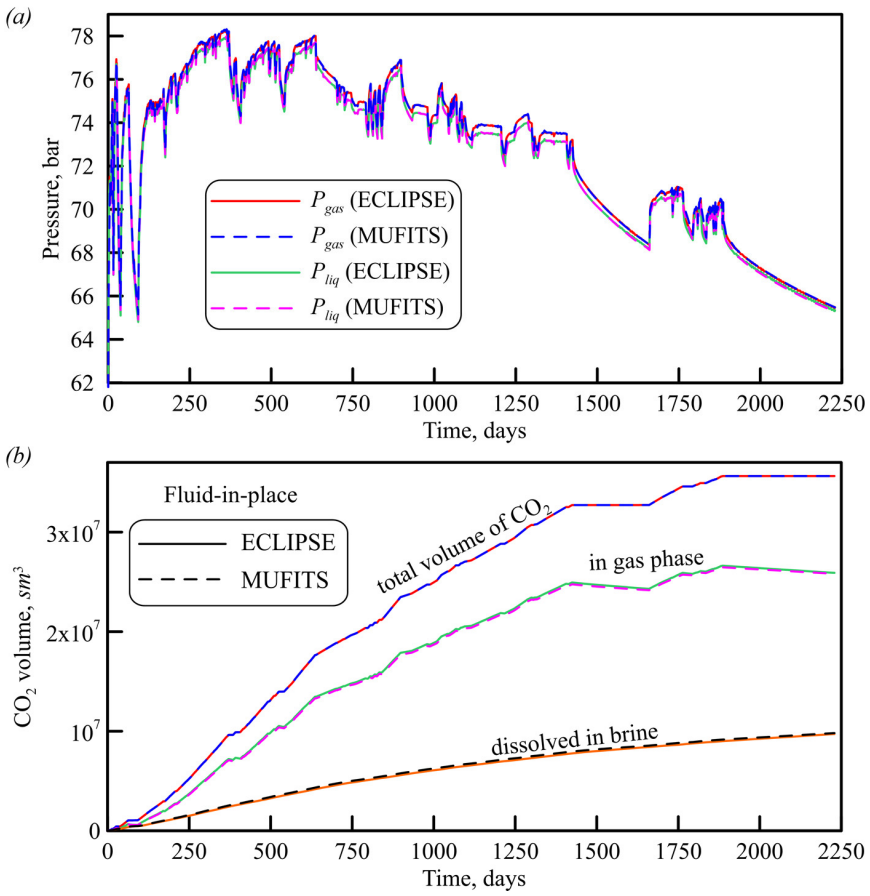

Fig. 7. Comparison of the simulated reservoir pressures and mass balances at the Ketzin pilot site, using MUFITS and ECLIPSE.

Acknowledgements

A. Afanasyev acknowledges financial support by the Russian Foundation for Basic Research (project No. RFBR 15-31-20585).

References

[1] Afanasyev AA. Website of the MUFITS reservoir simulation software; 2015. www.mufits.imec.msu.ru.
[2] Afanasyev AA. Hydrodynamic modelling of petroleum reservoirs using simulator MUFITS. *Energy Procedia* 2015;76:427–35.
[3] Afanasyev AA. Application of the reservoir simulator MUFITS for 3D modeling of CO_2 storage in geological formations. *Energy Procedia* 2013;40:365–74.
[4] Trangenstein JA, Bell JB. Mathematical structure of the black-oil model for petroleum reservoir simulation. *SIAM J Appl Math* 1989;49(2):749–83.
[5] Spycher N, Pruess K, Ennis-King J. CO_2–H_2O mixtures in the geological sequestration of CO_2. I. Assessment and calculation of mutual solubilities from 12 to 100°C and up to 600 bar. *Geochim Cosmochim Acta* 2003;67:3015–31.
[6] Spycher N., Pruess K. CO_2–H_2O mixtures in the geological sequestration of CO_2. II. Partitioning in chloride brines at 12–100°C and up to 600 bar. *Geochim Cosmochim Acta* 2005;69:3309–20.
[7] Hassanzadeh H, Poladi-Darvish M, Elsharkawy AM, Keith DW, Leonenko Y. Predicting PVT data for CO_2–brine mixtures for black-oil simulations of CO_2 geological storage. *Int J Greenhouse Gas Contr* 2008;2:65–77.
[8] Fanchi JR. Principles of applied reservoir simulation. Gulf Prof Publ, Elsevier; 2006.
[9] Pruess K, Garcia J, Kovscek T, Oldenburg C, Rutqvist J, Steefel C, Xu T. Code intercomparison builds confidence in numerical simulation models for geologic disposal of CO_2. *Energy* 2004;29:1431–44.
[10] Pan L, Spycher N, Doughty C, Pruess K. ECO2N V2.0: A TOUGH2 fluid property module for mixtures of water, NaCl, and CO_2. Scientific report LBNL-6930E; 2015.
[11] Class H, Ebigbo A, Helmig R, Dahle H, Nordbotten J, Celia M, Audigane P,·Darcis M,·Ennis-King J,·Fan Y,·Flemisch B,·Gasda SE,·Jin M, Krug S, Labregere D,·Beni AN,·Pawar RJ, Sbai A,·Thomas SG,·Trenty L, Wei L. A benchmark study on problems related to CO_2 storage in geologic formations. *Comput Geosci* 2009;13:409–34.
[12] Martens S, Liebscher A, Möller F, Henninges J, Kempka T, Lüth S, Norden B, Prevedel B, Szizybalski A, Zimmer M, Kühn M. CO_2 Storage at the Ketzin pilot site, Germany: Fourth year of injection, monitoring, modelling and verification. *Energy Procedia* 2013;37:6434–43.
[13] Norden B, Frykman P. Geological modelling of the Triassic Stuttgart Formation at the Ketzin CO_2 storage site, Germany. *Int J Greenhouse Gas Contr* 2013;19:756–74.
[14] Förster A, Schöner R, Förster HJ, Norden B, Blaschke AW, Luckert J, Beutler G, Gaupp R, Rhede D. Reservoir characterization of a CO_2 storage aquifer: the Upper Triassic Stuttgart Formation in the Northeast German Basin. *Marine Petr Geol* 2010;27(10):2156–72.
[15] Möller F, Liebscher A, Martens S, Schmidt-Hattenberger C, Kühn M. Yearly operational datasets of the CO_2 storage pilot site Ketzin, Germany, (Scientific Technical Report - Data ; 12/06), Potsdam : Deutsches GeoForschungsZentrum GFZ; 2012. 14 p. doi:10.5880/GFZ.6.3.2016.001
[16] Möller F, Liebscher A, Schmidt-Hattenberger C. Report on the dataset of the Brine Injection at the CO_2 Storage Pilot Site Ketzin, Germany, (Scientific Technical Report STR ; 16/05), Potsdam : GFZ German Research Centre for Geosciences; 2016. 12 p. doi:10.5880/GFZ.b103-12066.2012
[17] Class H, Mahl L, Ahmed W, Norden B, Kühn M, Kempka T. Matching Pressure Measurements and Observed CO_2 Arrival Times with Static and Dynamic Modelling at the Ketzin Storage site. *Energy Procedia* 2015;76:623–32.
[18] Kempka T, Kühn M. Numerical simulations of CO_2 arrival times and reservoir pressure coincide with observations from the Ketzin pilot site, Germany. *Environ Earth Sci* 2013;70(8):3675–85.
[19] Kempka T, Class H, Görke UJ, Norden B, Kolditz O, Kühn M, Walter L, Wang W, Zehner B. A Dynamic Flow Simulation Code Intercomparison based on the Revised Static Model of the Ketzin Pilot Site. *Energy Procedia* 2013;40:418–427.
[20] Afanasyev A. Compositional three-phase modelling in problems of subsurface CO_2 storage [In Russian]. Presentation, Workshop on High-performance computing in oil and gas industry, Moscow; 2012. Online:http://www.hpc-oilgas.ru/hpc-oilgas/reports12/Afanasyev.pdf
[21] Brazell O, Messenger S, Abusalbi N, Fjerstad P. Multi-core evaluation and performance analysis of the ECLIPSE and INTERSECT Reservoir simulation codes. Presentation, Schlumberger; 2010. Online:http://static.og-hpc.org/Rice2010/Slides/Brazell-Fjerstad-OG-HPC-2010-SLB-Chevron.pdf