Available online at www.sciencedirect.com

ScienceDirect

Energy Procedia 40 (2013) 365 – 374

Energy Procedia

European Geosciences Union General Assembly 2013, EGU

Division Energy, Resources & the Environment, ERE

Application of the reservoir simulator MUFITS for 3D modelling of CO_2 storage in geological formations

Andrey A. Afanasyev*

Institute of Mechanics Moscow State University, 1 Mitchurinskiy prospekt, Moscow 119192, Russia

Abstract

We propose a new reservoir simulator MUFITS for thermal compositional simulations of underground CO_2 storage. We test MUFITS against a benchmarking problem of CO_2 storage which is consistent with reservoir conditions in the Johansen formation. We also conduct a series of simulations of CO_2 injection using a real-scale geological model of the Johansen formation. We evaluate an optimized location of the injection well for a more complete structural trapping and reduction of potential CO_2 leakage out of the formation. The input data for MUFITS, related to the simulations presented in this work, can be downloaded at the simulator website.

Selection and peer-review under responsibility of the GFZ German Research Centre for Geosciences

Keywords: CO_2 sequestration; Geological storage; Reservoir simulator; Johansen formation; MUFITS

1. Introduction

The modelling of multiphase flows in geological formations remains a challenging issue. The flows are described by a strongly nonlinear system of partial differential equations. The nonlinearity is subject to complicated properties of fluids under reservoir conditions, e.g. phase transitions or critical conditions [1], as well as multiphase behaviour of the flows, e.g. nonlinear relative permeabilities. In engineering research the flows must be modelled in a complex geometry and topology of heterogeneous geologic

* Corresponding author. Tel.: +7-495-939-52-86 ; fax: +7-495-939-01-65 .
E-mail address: afanasyev@imec.msu.ru .

1876-6102
Selection and peer-review under responsibility of the GFZ German Research Centre for Geosciences
doi:10.1016/j.egypro.2013.08.042

medium [2]. All this requires application of robust numerical techniques, which are often developed within a reservoir simulator framework.

The simulation of flows related to underground CO_2 storage in saline aquifers represents an example of complicated reservoir simulation. The thermophysical properties of CO_2 significantly vary for a small alteration of pressure and temperature because CO_2 can be near critical for some reservoir settings. The mass of CO_2 dissolved in brine as well as the mass of water vapour in CO_2-rich phases also strongly depends on thermobaric conditions [1, 3]. Phase transitions between gaseous and liquid CO_2 are possible under subcritical thermodynamic conditions. Non-isothermal compositional reservoir simulations are required to account for this phase behaviour and compositional changes. The method for prediction the fluid properties plays a major role for the accuracy of simulations.

For modelling CO_2 storage, the simulators TOUGH2 and ECLIPSE are often used among others [4]. Discarding details, both codes use the same technique for prediction the fluid properties, which is based on a cubic equation of state [1, 3]. In this work, we propose a new code MUFITS (Multiphase Filtration Transport Simulator) for modelling the CO_2 storage processes [5]. MUFITS is a non-commercial compositional reservoir simulator for analysis of non-isothermal multiphase flows of binary mixtures in a porous media. The main feature of the code, which distinguishes it from the existing simulators, is the approach for prediction of the fluids properties under reservoir conditions [6, 7]. The properties are specified by the thermodynamic potential of the mixture, which is calculated before hydrodynamic simulations. The potential is used in conditional extremum problem, which corresponds to the entropy maximum condition in the thermodynamic equilibrium. Subject to this formulation, MUFITS can model the flows related to both sub- and supercritical thermodynamic reservoir conditions with two different CO_2-rich phases (liquid and gaseous CO_2), which cannot be simulated by the majority of the existing codes, e.g. TOUGH2 with ECO2N properties module [8] or ECLIPSE.

In this work, we provide the results of MUFITS testing using a benchmarking problem of CO_2 storage in a deep saline aquifer [4]. We also simulate CO_2 injection in the Johansen formation of the cost of Norway, which is considered as a target reservoir for large-scale injection. As a lot of work was done before with respect to the storage in this formation [2, 4, 9], the main purpose of the present work is to demonstrate the MUFITS capability of real-scale reservoir simulations in complicated geological settings. Nevertheless, despite the demonstrational purposes, we also conduct an optimization of the injection. We show that, using an optimized location of the injection well, one can reduce potential CO_2 leakage out of the formation.

2. About MUFITS

2.1. Mathematical model

MUFITS is designed for simulations of non-isothermal flows of binary mixtures in a porous media [5]. The code can accommodate single-, two- and three-phase states of the mixture under sub- and supercritical thermodynamic conditions [6, 7]. The properties of the mixture are specified by the thermodynamic potential:

$$\sigma(P,h,\mathbf{x}) \tag{1}$$

Here, P is the pressure, h is the molar enthalpy, $\mathbf{x}$ is the mixture molar composition, σ is the molar entropy. The potential (1) is represented using a polynomial spline in the $(P,h,\mathbf{x})$ space, which coefficients are calculated before hydrodynamic simulations.

The total entropy of the mixture σ_t reaches a maximum if thermodynamic system is under P, h_t, $\mathbf{x}_t$ = const equilibrium conditions. We denote by the subscript t the total parameters of the mixture. Therefore, the thermodynamic equilibrium of the mixture is defined by the conditional extremum problem:

$$\sum_{i=1}^{3}\sigma_i V_i = \sigma_t \to \max, \quad \sigma_i = \sigma(P, h_i, \mathbf{x}_i) \tag{2}$$

$$\sum_{i=1}^{3} h_i V_i = h_t, \qquad \sum_{i=1}^{3}\mathbf{x}_i V_i = \mathbf{x}_t, \qquad \sum_{i=1}^{3} V_i = 1 \tag{3}$$

$$0 \le V_i \le 1 \tag{4}$$

Here, V is the phase molar fraction, the subscript $i = 1,\ldots,3$ refers to the i-th phase of binary mixture. The conditional extremum problem, that is, the relations (2) – (4), is applicable for a single-, two- and three-phase states of the binary mixture calculation. A single-phase state ensues if the entropy reaches the maximum at $V_1 = 1$, $V_2 = 0$, $V_3 = 0$ conditions. In this case the phases $i = 2,3$ are absent in the thermodynamic equilibrium. A two-phase state ensues if the entropy reaches the maximum at $0 < V_{1,2} < 1$, $V_3 = 0$ conditions, which imply that only phase $i = 3$ is absent. A three-phase state ensues if the entropy reaches the maximum at $0 < V_i < 1$, $i = 1,\ldots,3$ conditions. According to the problem formulation, namely, relations (2) – (4), P, h_t, $\mathbf{x}_t$ are the known parameters, whereas h_i, $\mathbf{x}_i$, V_i are the unknown parameters that need to be determined by the problem solution. A detailed description of problem, as formulated by the relations (2) – (4), and the corresponding solution method can be found in [6].

We use a system of mass (5) and energy (6) conservation equations and Darcy law (7) for modelling of the flows in a porous media [7]:

$$\frac{\partial}{\partial t}\left(m\sum_{i=1}^{3}\rho_i c_{ij} s_i \right) + div\left(\sum_{i=1}^{3}\rho_i c_{ij}\mathbf{w}_i \right) = Q_j, \qquad j = 1,2 \tag{5}$$

$$\frac{\partial}{\partial t}\left(m\sum_{i=1}^{3}\rho_i e_i s_i + (1-m)\rho_r e_r \right) + div\left(\sum_{i=1}^{3}\rho_i \tilde{h}_i \mathbf{w}_i - \lambda \mathbf{grad} T \right) = Q_e \tag{6}$$

$$\mathbf{w}_i = -K\frac{f_i}{\mu_i}\left(\mathbf{grad} P - \rho_i \mathbf{g}\right), \quad i = 1,\ldots,3 \tag{7}$$

Here, m is the porosity, ρ is the density, c_{ij} is the j-th component mass fraction in the i-th phase, s is the saturation, $\mathbf{w}_i$ is the Darcy velocity, Q_j (Q_e) is the j-th component (energy) influx out of the wells, point sources, etc., e is the internal energy, $\tilde{h}$ is the mass enthalpy, λ is the effective heat conduction coefficient, T is the temperature, K is the absolute permeability, f is the relative permeability, μ is the viscosity. We denote the parameters of the host rock by the subscript r.

3. Numerical methods

The primary variables used in MUFITS hydrodynamic simulations are the pressure P, the total molar enthalpy h_t and the total composition $\mathbf{x}_t$ of binary mixture. The system (5) – (7) singularities in the vicinity of critical thermodynamic conditions are eliminated if these variables are used. Therefore, the simulator can avoid dramatic time step cuts for the simulations under critical thermodynamic conditions. Another positive side is that the parameters P, h_t, $\mathbf{x}_t$ are also the primary variables for the calculation of the mixture properties using the relations (2) – (4). Thus, we avoid loss of CPU-time on the recalculations between different variables sets.

MUFITS is designed for parallel simulations using MPI interface. Therefore, the simulations can be performed both using laptops, which have MPICH installation, and in parallel using supercomputers. We link the simulator to the computational library Aztec [10] for the parallel solution of sparse linear systems. We also use the library METIS [11] for the computational grid decomposition.

The following approximations and numerical methods are used in the simulator:

- Finite volume discretization method. This is the control-volume formulation of the governing equations, which is often applied in reservoir simulations [8];
- Fully implicit method. The approximation of the governing equations is fully implicit. Therefore, we can provide stable calculations over large time steps;
- Upwind approximation of the fluxes. We use a traditional two-point upwind approximation of the fluxes, which also improves calculation stability [8];
- Potential ordering technique [12]. This procedure is used for accelerated convergence of numerical solutions. The parameters in the grid blocks are updated in the direction of the mixture flow. MUFITS determines adaptively at which time step and to which regions of the computational domain apply this technique.
- Restarted GMRES linear solver as well as ILUT subdomain preconditioning. These methods are provided using the library Aztec [10]. The alternative linear solvers can also be used.

3.1. Input data

MUFITS takes a free formatted input data file, which contains the simulation schedule description [5]. The description is formulated using keywords syntax. Both the numerical model parameters and computational options can be specified in the input data file. The properties in the form of functions are specified by tables. The simulator can accommodate the corner point grids commonly used in the reservoir simulation industry. The local grid refinement or geological faults can also be specified within the input data file.

The thermophysical properties of the mixture a supplied by a binary file (the EOS-file) [5]. This file contains:

- The polynomial spline coefficients for the thermodynamic potential (1);
- The initial guesses for the iterative numerical solution of the problem (2) – (4);
- The polynomial spline for the binary mixture viscosity in the form $\mu(P,h,\mathbf{x})$.

4. The code verification

We consider the benchmarking problem 3.1, given in the work [4], to verify the correctness of MUFITS simulations. The problem is based on a geological model of the Johansen formation [2, 13]. The computational domain is an extracted part of the model. The lateral extension of the domain is

approximately 9600×8900 m. The formation thickness varies between 90 and 140 m. The domain comprises 9 layers of grid blocks all representing the high-permeablity sandstones in the Johansen formation. The geological model contains a fault zone and the CO_2 injection well is located near the fault.

In the present work, we simulate the injection in terms of CO_2-H_2O binary mixture flows in porous media and we do not account for NaCl solution in the formation water. We suppose that the formation is initially saturated by pure water. The initial pressure is 31.31 MPa whereas the initial temperature is 100 °C at the reference depth 3100 m [13]. The geothermal gradient is 3 °C per 100 m. The fault plane is impermeable. The top and the bottom boundaries of the reservoir are impermeable and fully insulated. The pressure and the temperature at the lateral boundaries of the domain and at the fault plane are constant and are equal to the initial parameters before injection (the open boundary condition).

CO_2 is injected in the formation over the bottom 50 m of an injection well located at $x = 5440$ m and $y = 3300$ m. The injection rate is 15 kg/s [4]. At the present time MUFITS doesn't support the well option for coupled simulations of flows both in the reservoir interior and in the wellbore. Therefore, we replace the injection well by four point sources located at $x = 5440$ m and $y = 3300$ m in layers 6 – 9 of the domain (a source in every layer). The injection rate for each source is 3.75 kg/s giving the overall injection rate of 15 kg/s. The point sources approximate the influence of the injection well, perforated in layers 6 – 9, if the injection rates are equal for all perforations. The injection occurs over 25 years period, after which the well is (the point sources are) shut down. The total simulation time is 50 years. The parameters of the problem, which are not specified in this work, can be found in [4].

The results of MUFITS simulation for the benchmarking problem are in a good agreement with the results of the other simulations (Fig 1). The CO_2 plume shape in the top layer [4], the total mass of CO_2 in gas phase and the mass dissolved in water are similar to values obtained by other codes. The percentage of CO_2 in gas phase is 81.5% and in liquid phase is 18.5% at t=50 years. Thus, the mass of CO_2 dissolved in water (brine) is a bit overestimated in comparison with TOUGH2 (13.5%) and ECLIPSE (14.1%). This is related to the fact that MUFITS does not account for NaCl solution in water, which reduces the CO_2 solubility and, consequently, the mass of dissolved CO_2 [3]. Nevertheless, we have confidence that MUFITS simulations are reliable for thermobaric conditions related to the storage in the Johansen formation.

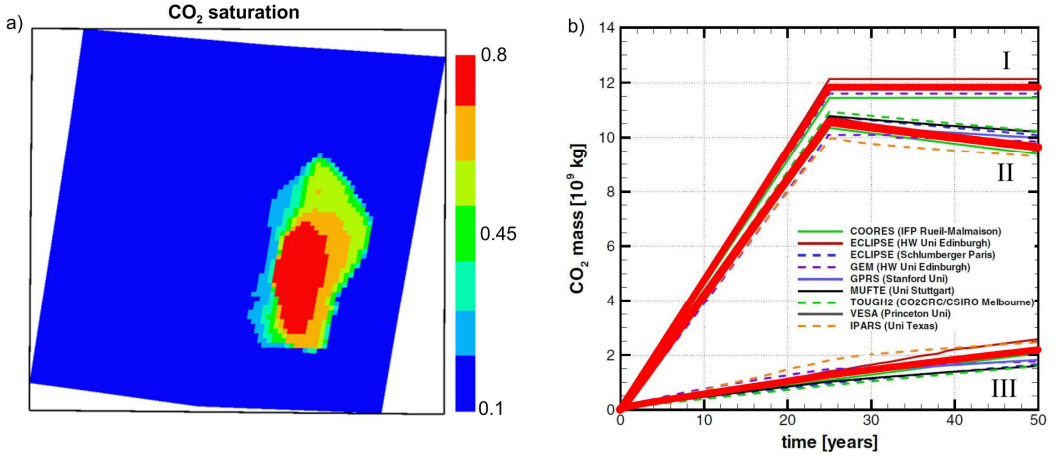

Fig. 1. (a) CO_2 saturation in the top layer after t=50 years; (b) I – total injected mass of CO_2, II – mass of CO_2 in gas phase, III – mass of CO_2 dissolved in water. The background figure is taken from [4]. The bold red lines are for the present simulations.

5. Simulation of CO_2 injection in the Johansen formation

5.1. The problem formulation

For modelling the CO_2 injection in the Johansen formation, we use the "sector model with heterogeneous rock properties", which can be downloaded at [13]. The computational grid is shown in Fig 2. The lateral extensions of the domain are up to 100 km. The model comprises 11 layers of grid blocks. The top 5 layers represent a shale (caprock) above the formation. The layers 6 – 10 are the high-permeablilty layers representing the sandstones of the Johansen formation. The layer 11 is the low-permeability shale. There are 5 vertical faults in the model. The initial and the boundary conditions are identical to that specified for the benchmarking problem except that the permeability across the fault is 10 times less than the permeability in the surrounding rocks (the transmissibility multiplier for all faults is 0.1). The open boundary condition is not imposed at the faults planes. A detailed description of the geological settings and relative permeabilities is given in [2].

In the present work, we consider two injection scenarios for two different coordinates of the injection well that are given in Table 1. The well INJ1 location is the same as in [2]. The well INJ2 is shifted with respect to the well INJ1 for approximately 3 km to the west (Fig 2). We suppose that both wells are perforated only in the layers 6, 7 and 10 because the layers 8, 9 around the well INJ2 represent a low-permeability wedge. The *i*- and *j*-indexes of the grid blocks, in which the well is perforated, are also provided in Table 1.

We simulate the injection of 400 Mt of CO_2 over 100 years. Therefore, the constant injection rate 4 Mt/year is consistent with [2]. As in the benchmarking problem, we approximate the injection wells INJ1 and INJ2 by three point sources. The *x* and *y* coordinates of the point sources are equal to the coordinates of the injection well. The sources are located in the layers 6, 7 and 10 of the domain (a source in every layer). The injection rate for every source is 1.333 Mt/year, thus the overall injection rate is 4 Mt/year. The point sources approximate the injection well if the injection rates are equal for all perforations. After the injection is shut down, we continue the simulation over 2500 years to evaluate the preferable directions of CO_2 migration. The total simulation time is 2600 years.

We apply local grid refinements for better resolution of the CO_2 plume spreading along the caprock as well as for the simulator capabilities demonstration. The regions of the domain, to which the refinement is applied, can be seen in Fig 2. In details, the grid refinement parameters are provided at the simulator website [5]. Following [2], we double the number of grid blocks in the *x* and *y* directions and quadruple the number of blocks in the vertical direction. The refinement is applied to the lowest layer of the caprock and to the upper three layers of the formation (layers 5 – 8). We use a nested refinement for demonstrational purposes.

Table 1. The injection well coordinates

Well #	*x* [m]	*y* [m]	*i*-index	*j*-index
INJ1	523737	6692500	58	48
INJ2	520873	6693333	64	47

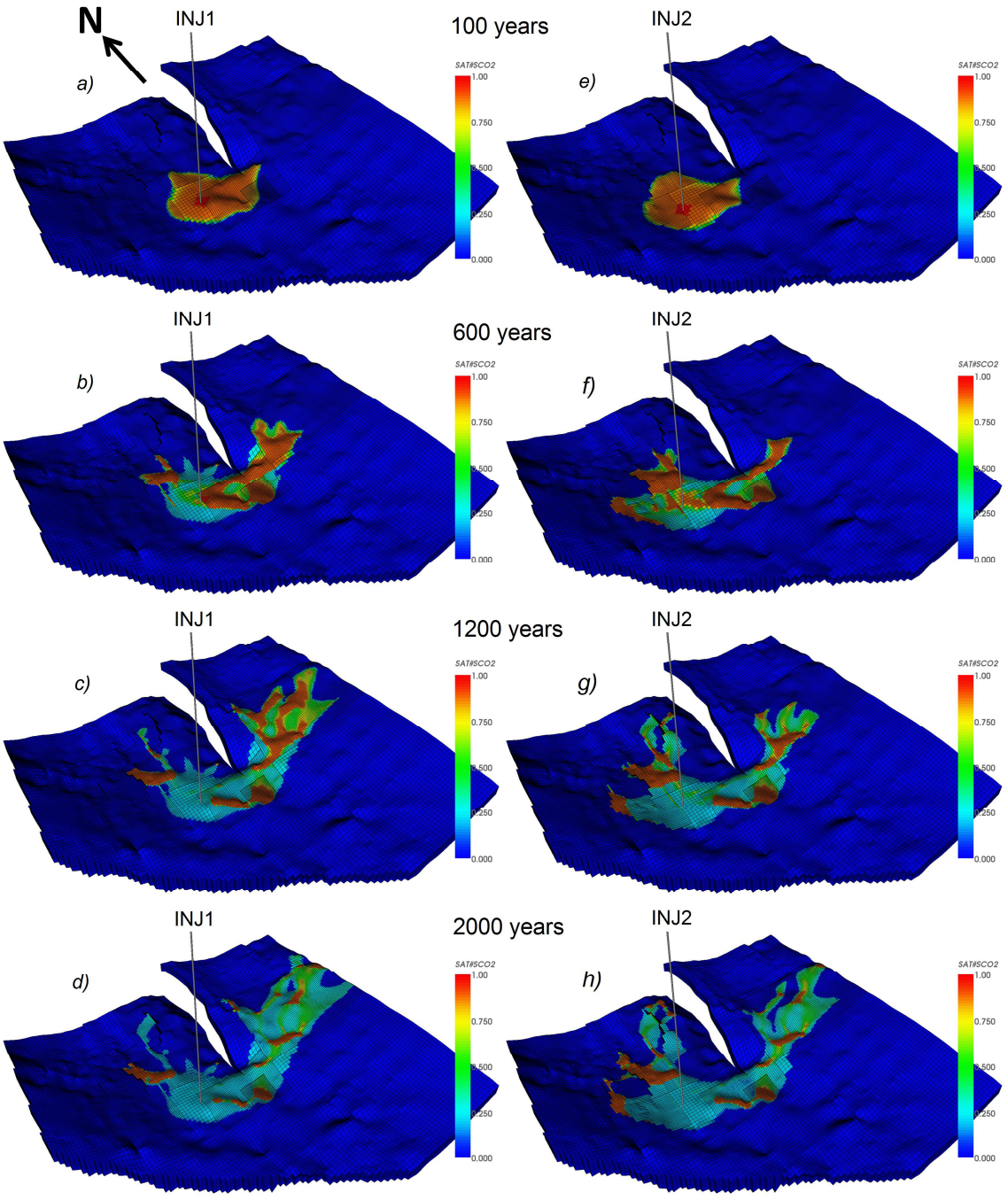

Fig. 2. CO_2 saturation in the top layer of the Johansen formation (layer 6). (*a–d*) – results for the well INJ1, (*e–h*) – results for the well INJ2; (*a, e*) – *t*=100 years (the injection is shut down); (*b, f*) – *t*=600 years; (*c, g*) – *t*=1200 years; (*d, h*) – *t*=2000 years.

5.2. Results

The distribution of supercritical CO_2 saturation in the top layer is shown in Fig 2. The injection occurs in the most deep-seated region of the computational domain (in the depression region). There is buoyancy-driven flow after the injection is shut down (t>100 years). The preferable direction of the CO_2 migration to the east is determined by the structural dip direction. The CO_2 distribution is controlled by the local topology of the caprock. At some point in time, the CO_2 plume reaches the eastern boundary of the domain and flows out (Fig 2(d,h), t=2000 years). In this work, we consider this situation as CO_2 leakage.

The mass of CO_2 in different states as a function of time is shown in Fig 3. The saturation of the mobile (movable) s_{mob} and the residual s_{res} mass of CO_2 in the gas phase is calculated by the relations:

$$s_{mob} = \max(s - s_{cr}, 0), \qquad s_{res} = \min(s, s_{cr})$$

Here, $s = s_{mob} + s_{res}$ is the saturation of the gas phase, $s_{cr} = 0.2$ is the critical saturation of the gas phase [2] that is the maximum saturation at which the gas remains immobile.

In the injection period ($t \le 100$ years), the total mass of CO_2 in the formation rises reaching 400 Mt. After the injection is shut down, the total mass is constant over a period of time. When the plume reaches the eastern boundary of the domain the leakage begins causing the decrease of the total mass of CO_2 (Fig 3, the black dashed line). Immediately after the injection is shut down, the CO_2, is mainly mobile rather than residual or dissolved in water (Fig 3). Later on, while CO_2 migrates upward along the caprock it partly remains in the residual form (light blue regions in Fig 2) and it dissolves in the formation water. Therefore, the mass of residual CO_2 as well as the mass of dissolved CO_2 rises. This is the typical situation, in which the role of the structural trapping decreases while the role of the residual and the solubility trapping increases with time [14].

There is a single migration path to the east for the well INJ1, which is determined by the local structural dip direction. In this injection scenario, the leakage through the eastern boundary begins approximately at t=1200 years reaching 15% of the injected CO_2 at t=2600 years. The region to the north of the injection well, and particularly the anticline structure along the main vertical fault, are not involved significantly in the storage.

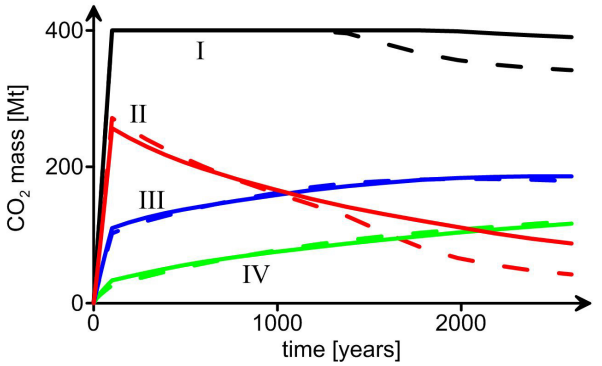

Fig. 3. I – total mass of CO_2, II – mass of mobile CO_2 in gas phase, III – mass of residual CO_2 in gas phase, IV – mass of CO_2 dissolved in water. The dashed lines are for the well INJ1, the solid lines are for the well INJ2.

We can control the direction of CO_2 migration by slightly changing the well location within the depression region. The CO_2 migration to the north is intensified in the second injection scenario INJ2. Using the shifted well, we partly redistribute the CO_2 migrating to the east to the second migration path, which is to the north. In this case, the eastern part of the plume is smaller while the northern part is larger than in the first injection scenario INJ1. Thus, we intensify stratigraphic and structural trapping. Indeed, to the north of the injection well, gaseous CO_2 is captured by the anticline structure along the main fault. To the west of the injection well, gaseous CO_2 is trapped because of the formation pinch out.

The more complete structural trapping can also be seen in Fig 3. At t=2600 years, the mass of mobile CO_2 in gas phase for the well INJ2 is twice as high as for the well INJ1. Therefore, the total mass of CO_2 is not decreasing so rapidly in the second injection scenario because the leakage through the eastern boundary is strongly reduced. For the well INJ2, the leakage begins at approximately t=1900 years reaching only 2.5% at t=2600 years in comparison with 15% for the well INJ1. Thus, we can conclude that the well INJ2 is more preferable than the well INJ1.

The fault zones can cause CO_2 leakage in the uppermost formations along the fault plane [2]. In the second injection scenario, more CO_2 is migrating north-east to the main fault but not reaching the fault plane. This is because CO_2 is captured by the anticline structure located along the fault.

6. Conclusions

We propose a new reservoir simulator MUFITS for modelling CO_2 storage in geological formations. The simulator can accommodate geologic, petrophysic and thermophysic data of the real-world complexity. The results of MUFITS testing against a benchmarking problem of CO_2 injection in a deep saline aquifer are in a good agreement with the results of the existing codes. We conduct several simulations of CO_2 injection in the Johansen formation, which demonstrate the MUFITS capabilities for real-scale reservoir simulations. We evaluate an optimized location of the injection well, which intensify structural and stratigraphic trapping. The CO_2 leakage can be significantly reduced if the well is located in the western regions of the formation.

Acknowledgements

The work was supported financially by a Grant from the President of the Russian Federation for the support of the Young Scientists and the Leading Scientific Schools (Project No. SP-2222.2012.5, NSh-1303.2012.1) and by the Russian Foundation for Basic Research (Project No. 12-01-31117)

The simulations were conducted at the Moscow University Supercomputing Center.

We would like to thank Min Jin from the Heriot Watt University for providing preprocessed computational grid and petrophysical data for the benchmarking problem.

Supplementary data

The input data for MUFITS, related to the problems considered in this work, can be downloaded at the simulator website [5]. The problems are reference to as the examples H3 and H4.

References

[1] Spycher N, Pruess K, Ennis-King J. CO_2-H_2O mixtures in geological sequestration of CO_2. I. Assessment and calculation of mutual solubilities from 12 to 100C and up to 600 bar. *Geochim Cosmochim Acta* 2003; **67**: 3015–31.

[2] Eigestad GT, Dahle HK, Hellevang B, Johansen WT, Riis F, Øian E. Geologic modeling and simulation of CO_2 injection in the Johansen formation. *Comput Geosci* 2009; **13**: 435–50.

[3] Spycher N, Pruess K. 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.

[4] Class H, Ebigbo A, Helmig R, Dahle H, Nordbotten J, Celia M, et al. A benchmark study on problems related to CO_2 storage in geologic formations. *Comput Geosci* 2009; **13**: 409–34.

[5] Afanasyev AA. MUFITS Multiphase filtration transport simulator website. 2013; http://www.mufits.imec.msu.ru.

[6] Afanasyev AA. Simulation of the properties of a binary carbon dioxide-water mixture under sub- and supercritical conditions. *High Temperature* 2012; **50**: 340-7.

[7] Afanasyev AA. Multiphase compositional modelling of CO_2 injection under subcritical conditions: The impact of dissolution and phase transitions between liquid and gaseous CO_2 on reservoir temperature. *Int J Greenhouse Gas Control* 2013; (in press) doi: 10.1016/j.ijggc.2013.01.042.

[8] Pruess K, Spycher N. ECO2N – A fluid property module for the TOUGH2 code for studies of CO_2 storage in saline aquifers. *Energy Convers and Manag* 2007; **48** (6): 1761–7.

[9] Wei L, Saaf F. Estimate CO_2 storage capacity of the Johansen formation: numerical investigations beyond the benchmarking exercise. *Comput Geosci* 2009; **13**: 409–34.

[10] Tuminaro RS, Heroux M, Hutchinson SA, Shadid JN. Official Aztec User's Guide. Version 2.1. Sandia National Laboratories report SAND99-8801J; 1999.

[11] Karypis G, Kumar V. A fast and highly quality multilevel scheme for partitioning irregular graphs. *SIAM J Sci Comput* 1999; **20** (1): 359—92.

[12] Kwok F, Tchelepi H. Potential-based reduced Newton algorithm for nonlinear multiphase flow in porous media. *J Comput Phys* 2007; **227**: 706–27.

[13] Eigestad GT, Dahle H, Hellevang B, Johansen WT, Lie K-A, Riis F, Øian E. Geological and fluid data for modelling CO_2-injection in the Johansen formation. 2008, http://org.uib.no/cipr/Project/MatMoRA/Johansen/index.htm.

[14] Special report on carbon dioxide capture and storage. Technical report, Intergovernmental Panel on Climate Change (IPCC). Cambridge: Cambridge Univ Press; 2005.