SIMULATION OF MULTIPHASE WATER-CARBON DIOXIDE MIXTURE FLOWS IN POROUS MEDIA

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Abstract

Two-phase models are widely used for simulation of CO_2 storage in saline aquifers. These models support gaseous phase mainly saturated with CO_2 and liquid phase mainly saturated with H_2O (e.g. TOUGH2). For aquifers where CO_2 injection may result in a plume of supercritical CO_2 compositional simulation approach must be applied.

The goal of the present study lies in development of a new mathematical approach for compositional simulation of CO_2 sequestration processes. The approach is applicable both for single-phase and two-phase states of liquid-gas type as existing simulators and also for two-phase states of liquid-liquid type and three-phase states at high pressures. The liquid-liquid states are formed by two liquids. The first liquid is mainly saturated with H_2O while the second is mainly saturated with CO_2. These thermodynamic equilibriums with liquefied CO_2 phase were detected experimentally (Takenouchi et. Al. 1984). The three phases in the three-phase states are liquid H_2O and CO_2 in liquid and gaseous states. The proposed approach was implemented in MUFITS simulator that was used for 1D, 2D and 3D simulations of CO_2 injection in water saturated reservoirs subjected to CO_2 liquefaction effect.

Balance equations

$$\frac{\partial}{\partial t}\left(m\sum_{i=1}^{3}\frac{M_{(j)}x_{i(j)}}{v_i}s_i\right)+\operatorname{div}\left(\sum_{i=1}^{3}\frac{M_{(j)}x_{i(j)}}{v_i}\mathbf{w}_i\right)=0$$

- mass conservation equation for each component, $j=1,2$, $j=1$: CO_2, $j=2$: H_2O

$$\frac{\partial}{\partial t}\left(m\sum_{i=1}^{3}\frac{e_i}{v_i}s_i+(1-m)\frac{e_s}{v_s}\right)+\operatorname{div}\left(\sum_{i=1}^{3}\frac{h_i}{v_i}\mathbf{w}_i-\lambda\frac{\partial T}{\partial \mathbf{r}}\right)=A_g$$

- energy conservation equation, Ag – work done by the force of gravity

$$\mathbf{w}_i=-K\frac{f_i}{\mu_i}\left(\frac{\partial P}{\partial \mathbf{r}}-\frac{M_i}{v_i}\mathbf{g}\right)$$

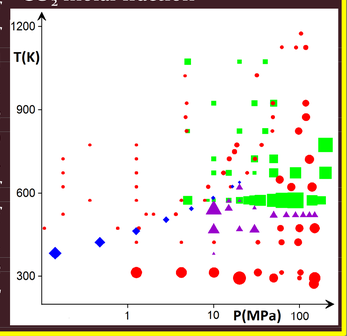
- multiphase Darcy correlation, $i=1\ldots3$ – phase number

Mixture properties design

A Peng-Robinson type equation of state was fitted to more than 150 CO_2-H_2O mixture properties measurements. The equation has an advantage for polar substances (e.g. H_2O) properties prediction. Both measurements of single-phase state and two-phase states of liquid-liquid and liquid-gas type were used for the equation coefficients determination. The figure shows parameters of the measurements of pure water or CO_2-H_2O mixture in single- (red or green) and two-phase (blue or violet) states. The sizes of the symbols correspond to the equation of state error under the measured conditions. The bigger the symbol is the larger the equation of state error. The maximum error does not exceed 20%.

$$P=\frac{RT}{v-b(x)}-\frac{a(T,x)}{\left(v-c(x)\right)\left(v-d(x)\right)}$$

- equation of state. P – pressure, T – temperature, v – volume, x – CO_2 molar fraction



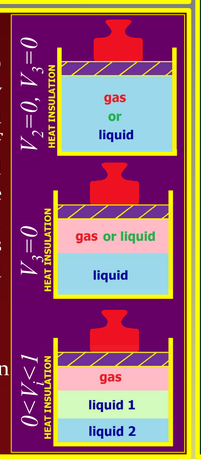
Multiphase equilibrium

The tuned cubic equation of state was used for CO_2-H_2O binary mixture thermodynamic potential calculation. Entropy $\sigma(P,h,x)$ depending on pressure P, enthalpy h and composition x is determined. This approach results in simplification of three-phase states calculation. The following conditional extremum problem is solved to determine the multiphase equilibrium. The entropy maximum is evaluated over 1-phase, 2-phase and 3-phase states. Pressure P and summed by phases enthalpy h_t and composition x_t are known. The problem solution defines parameters of phases h_i, x_i and V_i.

$$\sigma_t=\sum_{i=1}^{3}\sigma_i V_i\to\max,\quad \sigma_i=\sigma\left(P,h_i,x_i\right)$$

V – phase molar fraction

$$\sum_{i=1}^{3}V_i=1,\quad \sum_{i=1}^{3}h_iV_i=h_t,\quad \sum_{i=1}^{3}x_iV_i=x_t,\quad 0\le V_i\le 1$$



MUFITS simulator

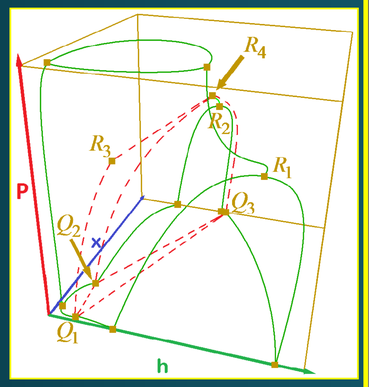
The proposed approach was implemented in MUFITS (MUltiphase FIltration Transport Simulator) code for three-phase compositional simulations of non-isothermal flows in porous media. The code is capable of real heterogeneous reservoir geology and support parallel computations and commonly used input data formats. Mixture thermodynamic properties can be specified within the code. The simulator was used for 1D, 2D and 3D simulations of carbon dioxide injection in water saturated reservoirs.

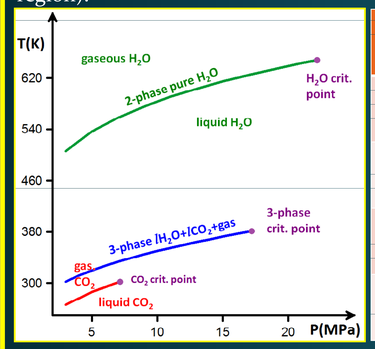
CO_2 injection (1D example)

The sample 1D simulation demonstrates a simple scenario when gaseous CO_2 injection through the left boundary of the layer results in underground CO_2 liquefaction and evolution of the three-phase flow zone with liquid CO_2 phase. The two-phase and three-phase flow zones are separated by a clearly visible phase discontinuities.

Phase diagram

The CO_2-H_2O phase diagram in pressure (P), enthalpy (h) and CO_2 molar fraction (x) space. R_1 (R_2) is H_2O (CO_2) critical point. Outside the surface bounded by the green lines the mixture is single-phase state while inside the region bounded by the surface the mixture is in two-phase state. The two-phase states at high pressure are of liquid-liquid type. The red lines bound the three-phase state parameters ($Q_1Q_2Q_3R_3R_4$ – region).





Parameters of three-phase state at P=10MPa

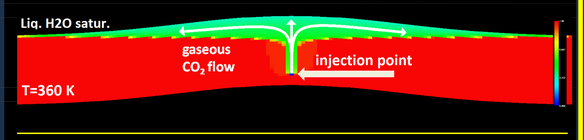
Phase	Density (kg/m³)	CO_2 mass fraction
Liquid H_2O	995	0.039
Liquid CO_2	1026	0.773
Gas	246	0.989

The negatively buoyant liquid CO_2 can result in non-classical hydrodynamic effects in the aquifer with CO_2 sinking and consequently in non-classical structural trapping scenarios. The possibility of the liquefaction strongly depends on the reservoir pressure, temperature and mixture composition.

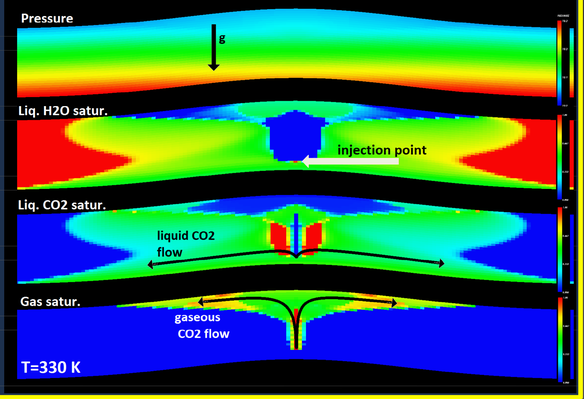
The CO_2 plume evolution

The gaseous CO_2 buoyancy is the principal effect used for conventional CO_2 structural trapping. The gas comes to the surface filling the upper regions of the folded reservoir. The sample simulation conducted for quite high reservoir temperature ($T=360$ K) demonstrates this effect. The reservoir is initially saturated with water. Hydrostatic conditions are hold on the left and right boundaries of the reservoir. The negatively buoyant liquid CO_2 sinks in the aquifer filling the lowest regions of the reservoir. The second sample simulation on the right conducted for $T=330K$ reservoir temperature demonstrates this effect. Liquid H_2O, liquid CO_2 and gas phase are present in the reservoir. As in the conventional scenario gas fills the upper layers of the reservoir. However, the CO_2 liquefaction process results in non-classical CO_2 distribution with liquid CO_2 sinking.

Conventional structural trapping scenario

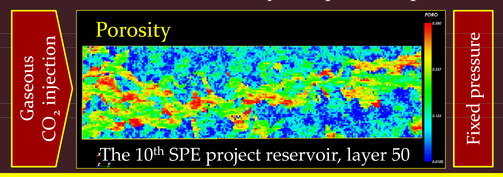


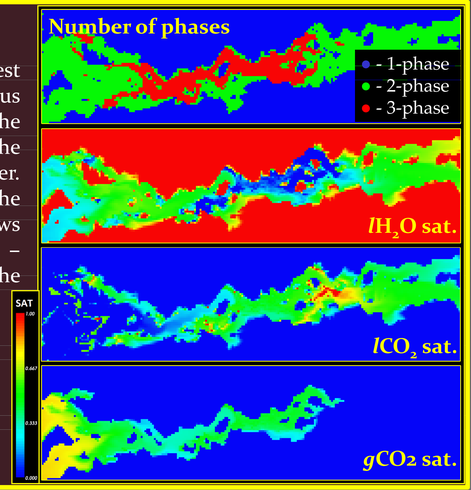
Liquid CO_2 evolution in the reservoir



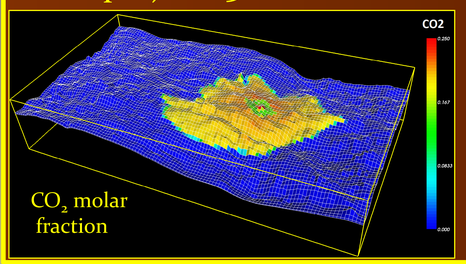
CO_2 injection in heterogeneous reservoir

The 10th SPE comparative solution project reservoir was used to test MUFITS robustness in simulation of flows in highly heterogeneous reservoir. The simulation was conducted in the 50th layer of the reservoir. The channels in the layer are clearly visible through the porosity distribution. The layer was initially saturated with water. Gaseous CO_2 is injected through the left boundary while at the right boundary pressure is fixed. Thus CO_2-H_2O mixture flows from the left to the right through highly permeable zones – channels in the porous media. Subject to phase transitions the saturations distribution in the layer is quite complicated.





SACS projects 3D simulations



MUFITS code was applied to simulations of CO_2 plume evolution at the Sleipner storage site. The CO_2 plume shape is in a good agreement with the existing hydrodynamic simulations results (Varunendra Singh et al 2010). However some details of the plume behavior determined by the seismic surveys still can't be predicted. Detailed simulation results can be demonstrated on the laptop. Discussions of the proposed model improvement for better calibration of the reservoir uncertainties are appreciated.

Acknowledgments: Statoil and the Sleipner License are acknowledged for provision of the Sleipner 2010 Reference dataset. Any conclusions in this paper concerning the Sleipner field are the authors' own opinions and do not necessarily represent the views of Statoil

Conclusions

A new approach for three-phase compositional hydrodynamic simulations is proposed. The approach is applicable for single-phase, two-phase and three-phase CO_2-H_2O mixture flows with liquefied CO_2 phase. The proposed model results in a more accurate prediction of supercritical CO_2 plume evolution because it accounts for possible three-phase thermodynamic equilibriums. The approach was implemented in MUFITS simulator applied to 1D, 2D and 3D sample simulations of CO_2 injection subjected to CO_2 liquefaction effect. The simulator can be applied to analysis of CO_2 injection in real storage sites taking into account the reservoir heterogeneity and complex multiphase character of the flow in gravity field.