Considering non-ideal gas mixtures in geochemical modeling of gas-water-salt-rock interactions: Application to impure CO\textsubscript{2} geological storage

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Abstract

When captured, CO\textsubscript{2} is often collected with a variety of impurities depending on the origin of CO\textsubscript{2}, the considered capture process and the concerned industrial sector [1]. Moreover, since it is quite costly to reach 99.999\% of CO\textsubscript{2}, the geological co-storage of CO\textsubscript{2} and of these co-captured impurities should be studied.

Therefore, if the underground storage of gaseous mixtures (i.e. impure CO\textsubscript{2} in deep saline aquifers or depleted reservoirs or other gases storage in salt caverns for the purpose of energy storage) is initiated, it is crucial to ensure the stability and safety of the storage itself at rather important space and time scales. This kind of operations induces complex and coupled fluid migrations, chemical reactions, porous media modifications… Reactive-transport numerical simulations are thus essential to handle these multi-phase multi-component flow, transport and geochemistry and to model the fate of the gas plume. They could also help to estimate the quantity of gas stored, and to manage the whole storage integrity anticipating potential leakage and defining site-monitoring plans.

Recent developments in reactive-transport codes CHESS/HYTEC [2-4], incorporating the analytical resolution of an equation of state for the gas phase (such as the classical cubic EOS Peng-Robinson), allow a better representation of gaseous mixtures, of their non-ideal thermodynamic behavior at high pressure and high temperature and of the coupling with 2-phase flow and transport. These codes are now able to simulate the co-injection of CO\textsubscript{2} and various impurities in order to determine the potential impacts on plume migration, taking into account density effects, chemical reactivity…

Coupled reactive-transport approach and associated numerical simulations will be exposed in another abstract [5]. The present paper will be focused on the geochemical part of the model and on its ability to accurately reproduce various experimental results from the literature.

In a first part, the whole modeling approach will be recalled.

Secondly, an overview of previously obtained results will be summed up. They exhibited the faculty of the code to model precisely the solubility of various pure gases in water and a comparison with other models [2,3,6]. Furthermore, since the same EOS is used for each gaseous compound combined with a classical mixing rule, the method was also successfully applied to various gaseous mixtures [2,3,6]. Coupling a robust activity correction model (such as the specific ion theory) for the electrolyte, the model described also really well the solubility in single and mixed brines [2,3].
Figure 1. pH vs pressure of CO$_2$-saturated water at 323 (diamonds and line), 368 (triangles and dashed line) and 423 K (squares and dotted line). Symbols corresponds to experimental data and lines to CHESS numerical simulations.

New results focused on reactivity will also be detailed in a third part. PH, which is an indicator of the speciation, has been measured for CO$_2$+water and CO$_2$+brine solutions [7] and these systems were satisfactorily modeled (fig. 1). Furthermore, other recent gas mixtures+water+rock experiments from the literature provided water composition and/or mineralogy evolution through time. Numerical simulations attempts to reproduce these last results will be presented.

Finally, some orders of magnitude for the influence of impurities on CO$_2$ solubility and mineralization will be discussed.

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References