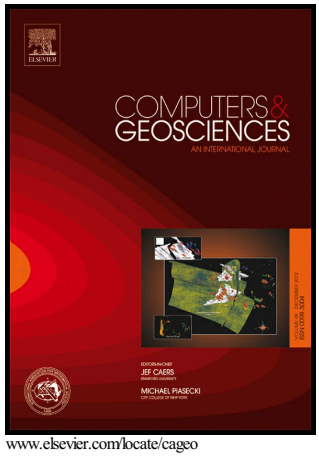
Impact of mineralogical heterogeneity on reactive transport modelling

Min Liu, Mehdi Shabaninejad, Peyman Mostaghimi



www.elsevier.com/locate/cageo

PII: S0098-3004(16)30456-3
DOI: http://dx.doi.org/10.1016/j.cageo.2017.03.020
Reference: CAGEO3936

To appear in: *Computers and Geosciences*

Received date: 27 September 2016
Revised date: 28 February 2017
Accepted date: 31 March 2017

Cite this article as: Min Liu, Mehdi Shabaninejad and Peyman Mostaghimi Impact of mineralogical heterogeneity on reactive transport modelling *Computers and Geosciences,* http://dx.doi.org/10.1016/j.cageo.2017.03.020

Impact of mineralogical heterogeneity on reactive transport modelling

Min Liu[1], Mehdi Shabaninejad[2], Peyman Mostaghimi[1*]

[1]School of Petroleum Engineering, The University of New South Wales, NSW 2052, Australia
[2]Department of Applied Mathematics, The Australian National University, ACT 2601, Australia
[*]Corresponding author: *peyman@unsw.edu.au*

Highlights
Effect of mineralogical heterogeneity on reactive transport was investigated.
Mineral map of sandstones was acquired using QEMSCAN SEM-EDS.
Lattice Boltzmann and Finite Volume Methods were applied to model reactive transport.
Pore-scale simulations of multi-mineral reaction were performed directly on rock images.

Abstract

Impact of mineralogical heterogeneity of rocks in reactive modelling is investigated by applying a pore scale model based on Lattice Boltzmann and Finite Volume Methods. Mass transport, chemical reaction and solid structure modification are included in the model. A two-dimensional mineral map of a sandstone rock is acquired using the imaging technique of QEMSCAN SEM with Energy-Dispersive X-ray Spectroscopy (EDS). The mineralogical heterogeneity is explored by performing multi-mineral reaction simulation on images containing various minerals. The results are then compared with the predictions of single mineral dissolution modelling. Dissolution patterns and permeability variations of multi-mineral and single mineral reactions are presented. The errors of single mineral reaction modelling are also estimated. Numerical results show that mineralogical heterogeneity can cause significant errors in permeability predictions, if a uniform mineral distribution is assumed which are related with flow regimes. The errors are smaller in high Péclet regimes than in low Péclet regimes in this sample.
Keywords: Reactive transport · Pore scale heterogeneity · Lattice Boltzmann · Rock minerals · Porous Media

1. Introduction

Reactive transport in porous media is of importance in several applications in subsurface transport processes, chemical sciences and engineering. For example, chemical reactions between pollutants and soil release toxic products resulting in serious environmental concerns. During sequestration of carbon dioxide in subsurface aquifers, the CO_2 dissolves