Reactive flow of cold water injected into the thermal aquifer; 1-D numerical model

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ABSTRACT

To appreciate the changes in porosity in the carbonate rocks a simple, one dimensional model of fluid flow and dissolution reaction has been elaborated. The results indicate how porosity changes evolve during replacement of the original saturated solution by a cold undersaturated fluid injected into the carbonate aquifer. Such modeling, with hydraulic feedback via porosity - permeability relationship, could be potentially used to recognize the sites of unfavorable development of porosity.

KEYWORDS

Reactive flow, porosity change, numerical model

Introduction

Although there exists a large number of numerical codes able to simulate dissolution/precipitation reactions with advective diffusioddispersion transport, still, only few of them can deal with porosity changes due to coupled reaction and fluid flow. Porosity evolution with hydraulic feedback is not explicitly included in the current models of the karst evolution (DREYBRODT 1988), but it is studied in some detail elsewhere (ORTOLEVA et al. 1987; STEEFEL & LASAGA 1990). The present model was intended to predict porosity and concentration changes when cold waters supplied through a borehole penetrate carbonate aquifer filled with saturated, thermal solution. When the cold water starts dissolving the solid phase, the rock porosity is increasing and, in turn, influences the **true** velocity of fluid and the spatial extent of reaction. The goal of the present model applied to carbonate rocks. Temperature was considered to be in a steady-state, linearly increasing along the 1-D horizontal profile. Estimating porosity development in space and time could be one of the procedures necessary to predict a risk in **the** process

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of continuous cold water injection into the aquifer, in dams foundation and other engineering construction works.

Governing equations

The 1-D differential equations for advective transport, reaction and porosity changes due to dissolution reaction in steady-state temperature field could be written as :

$$\frac{\partial C}{\partial t} = \frac{\partial (D_c \partial C)}{\partial x^2} - \frac{q}{\phi^*} \frac{\partial C}{\partial x} - A_m^* k_r \exp[-E_{\phi}/R(1/T - 1/298.2)](C - C_{eq})$$
(1)
$$\frac{\partial \phi_m}{\partial t} = \phi_m^* v^* A_m^* k \exp[-E_{\phi}/R(1/T - 1/298.2)] (C - C_{eq})$$
(2)

with initial and boundary conditions as follows:

$$C = C_{eq} (x, t=t_0)$$
$$C = C_B (x=0, t)$$
$$\partial C/\partial x = 0 (x=L, t)$$

where D_c is the combined diffusion/dispersion coefficient [m²/s], q designates Darcy velocity [m/s], A_m denotes reactive surface per unit volume of rock [m²/m³], k_r is for kinetic rate constant of the first order [mol/m²/s], v indicates molar volume [m³/mol], ϕ_m , ϕ and C are mineral volume [], porosity [] and concentration [mol/m³], respectively. Darcy velocity is obtained from the relation:

$$q = -k_p \rho g / \mu \nabla H$$
 (3)

where k_p is the permeability $[m^2]$, ρ indicates density (kg/m^3) , g is for the gravitational acceleration $[m^2/s]$, μ indicates viscosity of water [kg/ms] and VH designates hydraulic gradient. Due to the arbitrary choice of initial reactive surface for simulation the effective Damkohler numbers which indicate **the** relative importance of reaction to fluid flow were 0.14 and 1.4 for the first and the second simulation, respectively. Peclet number was **2.0** indicating **an** important role of advective fluid flow and less influence of diffusion/dispersion processes.

The above equations contain several simplifications which could be listed as follows:

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- concept of reactive surface; empirical and the most obscure feature of any model
- concept of single porosity; fracture porosity or dual porosity model would be more adequate depending **on** the actual situation
- simplified rate dependence; pH>7
- 1-D domain

The parameters used in the simulations are listed below:

 D_c - diffusiod dispersion coefficient; $D_c = D + 10q$; $D = 10^{-9} [m^2/s]$

q - Darcy velocity; [m/s]

VH - hydraulic gradient; 0.01 [m/m]

 k_p – permeability; initial permeability $k_{p0} - 10^{-12} [m^2]$

∮_m- mineral volume

L - length of the profile [50 m]

A_m - reactive surface per unit volume of rock; $[m^2/m^3]$

k - kinetic rate constant of the first order - pH>7; ~ 10^{-6} (25°C) [mol/m²/s] (PLUMMER et al., 1978; CHOU et al., 1987)

v - molar volume of CaCO₃;35*10⁻⁶[m³/mol]

T - absolute temperature [K]

Ceg - equilibrium concentration of calcium carbonate; 10⁻¹ [mol/m³]

C₀ - initial calcium carbonate concentration; 10⁻¹ [mol/m³]

C_B -boundary concentration; 10⁻³ [mol/m³]

E – activation energy [32 kJ/mol]

R - gas constant 8.314 [J/mol/K]

Pe - Peclet number defined as q/\u00f6Dc []

Da - apparent Damkohler number defined as Amkro/q []

Two empirical relations were used in the simulation, one relating permeability and porosity, and **the** second one relating reactive surface **of** the mineral and mineral volume:

$$\begin{aligned} k_{p} &= k_{p0} \left(\phi/\phi_{0} \right)^{3} [1.001 - \phi_{0}^{2}] / [1.001 - \phi^{2}] \quad (4) \\ &\text{and} \\ A_{m} &= A_{m0} (\phi_{m}/\phi_{m0})^{0.667} \quad (5) \end{aligned}$$

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where k_{p0} , k_{p} , are the initial permeability and actual permeability, A_{m0} and A_{m0} indicate reactive surface and initial reactive surface and finally ϕ_{m0} , ϕ_{m} , are initial mineral volume and actual mineral volume. A_{m} the reactive surface is the most critical parameter and it is expressed through effective Damkohler number. It is considered that hydraulic gradient of 0.01 sufficiently corresponds to a continuous cold water injection into the aquifer.



Figure I : A schematic diagramme for the advective-reactive system of interst

Discussion

When undersaturated cold solution replaces the original saturated solution within the carbonate aquifer (Fig. 1) a dissolution process provides enhanced porosity and permeability which in turn affect true velocity of fluid. At the same time the Ca^{2+} concentration evolves within the reaction length which is shown for consecutive time steps of 1 yr (Fig. 2a). For the initial $10m^{-1}$ of reactive surface, the Ca^{2+} concentration reaches saturation within the first 20m of the horizontal profile. Differently, for the reactive surface of $1m^{-1}$, the Ca^{2+} saturation is reached at approximately 40m. Figure 2b shows porosity changes occurring with length for the consecutive time steps as in Figure 2a. For the initial $10m^{-1}$ of reactive surface porosity evolved up to the value of 0.10 after 10 yrs. Porosity enhancement is largest upstream of the reaction front due to the relatively high reactive surface of $10m^{-1}$. This is in contrast to the case of relatively low reactive surface of $1m^{-1}$ where the maximum of porosity enhancement is shifted further along the profile and demonstrates that temperature increase up to 90° C does compensate for the effect of reactive surface.



Figure 2a $z Ca^{2+}$ concentration changes with length for the consecutive time steps of 1-10 years; continuous lines are for reactive surface of $10m^{-1}$ and broken lines are for reactive surface of $1m^{-1}$.

How the Ca^{2+} concentration changes with time for consecutive length is revealed on Figure 3a. For relatively high reactive surface of $10m^{-1}$, disequilibrium is apparent close to the undersaturated solution injection point, and for low reactive surface of $1m^{-1}$, the saturation level is kept downstream of the reaction front. Figure 3b indicates how porosity evolves in time with increasing length. It increases with time close to the injection point as it should for the reactive surface of $10m^{-1}$ and is much less developed for the reactive surface of $1m^{-1}$.



Figure 2b = Porosity changes with length for the consecutive time steps of **1-10** years; continuous lines are for reactive surface $\sigma 10m^{-1}$ and broken lines are for reactive surface $\sigma 1m^{-1}$.

Conclusions

The aquifer porosity to which cold water **is** injected can evolve dramatically in time due to dissolution of carbonate rocks. There are many important factors which affect the rate of porosity evolution but the most important are probably the reactive surface, the saturating state of injected waters and the true velocity of fluid. These parameters are all integrated in the effective Damkohler number.

It was found that dramatic changes in porosity extending from 0.05 to 0.10 occur even in the period of 10 years (Figs. 2b, 3b). This can be of great importance for existing geothermal installation and other hydro-engineering constructions. In the case of elevated risk of excavation the aquifer of interest could eventually be treated by some chemical agent to reduce the reactive surface. The above model is flexible enough and can be easily adapted to any other situation when predicting the porosity evolution is of interest.



Figure 3a : Ca^{2+} concentration changes with time for the consecutive length steps; continuous lines are for reactive surface $cf 10m^{2}$ and broken lines are for reactive surface of $1m^{2}$.



Figure 3b : Porosity changes with time for the consecutive length steps; continuous lines are for reactive surface of $10m^{-1}$ and broken lines are for reactive surface of $1m^{-1}$.

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