



the
 Drake
 the iron
 tween (0.
 used in the
 The other
 the values of A

2.2.2. Oxidation li
 Initially, when
 ferrous content in b
 trolled by dissolution
 strained by diffusive
 serially, with an overa
 action steps. The overa
 expressions ($R_{diss} = R_{ox}$)

$$c_2' = c_{20}' \frac{k_2}{k_2 + k_1 c_1'}$$

where $k_1 = (k_r/k_H)c_{20}'c_1'$
 Substituting Eq. (4) in the
 pseudo-steady-state, whi
 equation for oxygen (Eq.

$$D_p \frac{\partial^2 c_1'}{\partial z^2} = f \frac{c_1' k_1}{1 + c_1' k_1/k_2}$$

The right-hand side
 gradually changes from
 dissolved oxygen conc

$$\text{For } \frac{k_1}{k_2} c_1' \gg 1 \quad \frac{c_1' k_1}{1 + c_1' k_1/k_2} \approx c_1'$$

$$\text{For } \frac{k_1}{k_2} c_1' = 1 \quad \frac{c_1' k_1}{1 + c_1' k_1/k_2} = \frac{c_1' k_1}{1 + c_1' k_1/k_2}$$

processes, resulting in a sharp reaction front. In the future, the reaction front location will change in correlation with the change in concentration in the pores of the cement, the concentration of the reaction front location. As derived in [Sidborn et al., 2018](#) and [derived by Rajaram et al., 2018](#), the reaction front propagation

2.3. Numerical experiments

The inter-granular reaction front propagation is here using a micro-Discrete Fracture Network (DFN) with three different fracture sets. The DFNs are used to mimic grain-boundary fractures that transect different mineral grains. The DFNs are continuous porous media. The DFNs are generated using the finite element method (FEM) using the software [Tools \(Svensson et al., 2018\)](#) (Svensson et al., 2018). The parameters are listed in [Table 2](#). These parameters are used to mimic diffusive properties of the KFM02A of Forsmark. The DFN model differs from the DFN model used in [Svensson et al. \(2018\)](#) in the fact that the model should be regarded as a porous media model, which are distributed in a tight granitic rock, with a high surface area.

DFN-derived porosity is assigned to all the a



Fig. 4. Top: distribution of biotite grains in case 1 (VC1) with higher grain size. Bottom: distribution of biotite grains for the variant case 2 (VC2) with smaller grain size. The distribution of biotite grains in case 1 is more uniform than in case 2, whereas the distribution of transparent volume is more uniform in case 2. The grain size δ_{grain} is equal to δ_{cont} (see Table 3). The model is based on the Voronoi model. (For interpretation of the references to this model, the reader is referred to the web version of this article.)

$118 \times 19 \times 500 = 1,121,100$ cells. The grain size $\delta_{cont} = 2.5 \cdot 10^{-7}$ m.

Biotite grain distribution is modeled using binary random unimodal distribution. The presence or absence of a biotite grain in each cell is determined by the different considered cases. The different considered cases are: (1) uniform distribution (uniformization) of the biotite grain size (δ_{grain}) of the considered biotite grain size.

In the continuum model, the surface area is given by assuming that for a grain of size δ_{grain} , the surface area is given by

$$A_{s_i} = \epsilon_i \cdot S_{F_i} / \delta_{cont}^3$$

Fig. 6. Normalis

First, the penetration
analysed in order to infe
used in the subsequent
penetration profiles of th
analytical solution for di
[1959](#); [Crank, 1979](#)) (Fig.
diffusivity of $3.5 \cdot 10^{-13}$
porosity is used as input

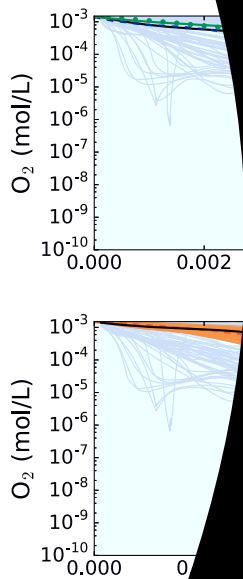
Table 3
List of numerical experim

Numerical experiment
Base case (BC)
Variant case 1 (VC1)
Variant case 2 (VC2)
Variant case 3 (VC3)

concentration
line 1
(1959);
figure leg

Table 1. The
experiments.

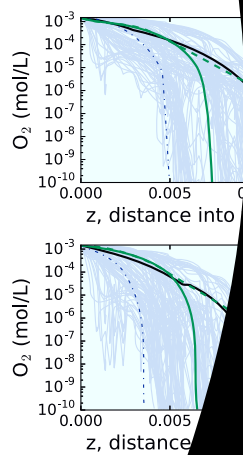
In Fig. 8a, the
is also shown. The
capacity of the root
perturbation). The
concentration profile



The scaling of the concentration of oxygen with the distance of diffusion in the VC2 model is shown in Fig. 10b. For the case of a single pathway (green dashed line), the concentration of oxygen at the surface area of 60 μm^2 was set to 0.99 and

3.3. VC2 numerical experiment

The results of the VC2 numerical experiment are shown in Fig. 10. The single pathway and



BC and VC3, and in these cases the diffusivity is homogeneous and the oxygen concentration smooths out the heterogeneous available for reaction.

Other interesting mineral grain size of amount of biotite is oxygen is slightly low sensitive to mineral grain considered (VC3 vs. BC) is observed as a surface.

An equivalent value A_s^{bulk} , which is the average whole bulk volume of the concentration profiles computed estimate the actual oxygen estimation is significant köhler number. On the order provides a reasonable approximation, particularly agreement is due to the numerical experiment, with actions.

In a practical application corrosion of a copper relatively high oxygen corrosion rate is limited (et al., 2012). Thus

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