
Check for updates

mic

B

erogene

distributi

rock, a p

$(Mg,Fe)_3A1S$

tential to retai

et al., 2014) and

waters (Sidborn a

As exemplified by

dispersed in a rando

with microscopy in a

suggest that typical

$\sim 400 \times 200\,\mu m^2$ (0.0

$2\,mm^2$ can also be fou

The influence of the

rock matrix on bufferi

tration is studied in this

micro-DFN model comb

grains. An analytical so

th

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 overal

expressions ($R_{diss} = R_{ox}$

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

where $k_1 = (k_r/kH'')c_{20}'c_{20}'$

Substituting Eq. (4) in th

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 fro

dissolved oxygen conc

For $\frac{k_1}{k_2} c_1' \gg 1$ $\quad \frac{c_1' k$

$1 + c_1'$

For $\frac{k_1}{k_2} c_1' = 1$ $\quad \frac{c$

$1 +$

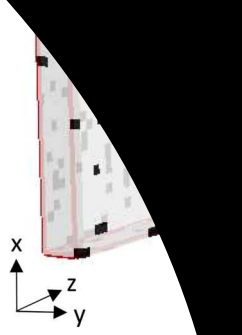


Fig. 4. Top: distribution
case 1 (VC1) with highe
for the variant case 2 (VC
distribution of biotite grai
the biotite grains is doub
whereas transparent volum
equal to δ_{grain} (see Table 3).
model. (For interpretation
reader is referred to the we

$118 \times 19 \times 500 = 1{,}121$
finement $\delta_{cont} = 2.5 \cdot 10^{-7}$

Biotite grain distribut
using binary random un
sence or absence of a bio
the different considered
considered cases are
cretization (δ_{grain}) of t
sidered biotite grain s

In the continuum
by assuming that fo
face area is given b

$$A_{si} = \varepsilon_i \cdot S_{Fi} / \delta_{cont}^3$$

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

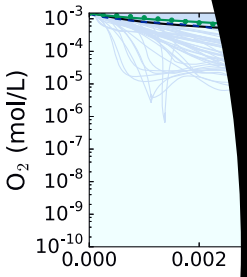
Table 3
List of numerical experim

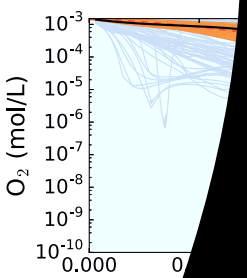
Numerical experiment
Base case (BC)
Variant case 1 (VC1)
Variant case 2 (VC2)
Variant case 3 (VC3)

co
line
(1959);
figure leg

Table 1. The
experiments.

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

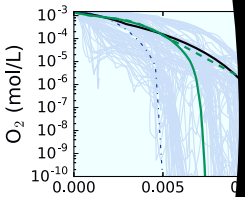


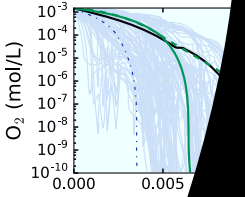


scaling
of diffusi
diffusion in
with the dif
Fig. 10b. For th
continuous line)
surface area of 60
green dashed line),
was set to 0.99 and

3.3. VC2 numerical ex

The results of the V
The single pathway an





BC
and
in thes
diffusive
geneity in
higher diffu
smooths out
homogeneous a
used (Table 4) a
available for react

Other interestin
mineral grain size o
amount of biotite is
oxygen is slightly low
sitive to mineral grai
considered (VC3 *vs.* BC
tration is observed as a
surface.

An equivalent value
A_s^{bulk}, which is the avera
whole bulk volume of th
tration profiles computed
mate the actual oxygen
estimation is significant
köhler number. On the c
vides a reasonable appr
periment, particularly
agreement is due to the
merical experiment, wh
actions.

In a practical appl
corrosion of a coppe
latively high oxygen
corrosion rate is li
et al., 2012). Thus,

or
for d
investig

Acknowle

PT, MS, US
Management C
gratefully acknov
on the supercomp

References

Antonellini, M., Mollema, P.,
outcrop observations: Imp
Water Resources Research
Andersson, J., Skagius, K., Win
elling for a final repository
1045–1060.
Auqué, L., Gimeno, M., Gómez,
Groundwater chemistry arou
TR-06-31. Svensk Kärnbräns
Banwart, S.A., Wikberg, P., Puig
repository: Concepts, results
Metcalfe, R., Rochelle, C.A. (
157. Geological Society, Lon
Bomberg, M., Nyyssönen, M., Pit
communities inhabit sulphat
Olkiluoto, Finland. BioMed.
Carslaw, H., Jaeger, J., 1959. Co
Oxford.
Crank, J., 1979. The Mathemati
Drake, H., Sandström, B., Tullb
Fracture Fillings from Fors
06-109. Svensk Kärnbräns
Drake, H., Ivarsson, M., Tillbe
activity in deep hydraulic
geological nuclear waste
Glynn, P., Voss, C., Provost
based ice sheets into th
Testing Groundwater