

MODELLING COPPER MOBILIZATION FROM LOW-GRADE ORE CONTROLLED BY MINERAL SURFACE REACTIONS

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1. DETAILS OF FLUID FLOW AND TRANSPORT MODELING:

The Navier-Stokes equation (Eq. S1) and mass conservation equation (Eq. S2) are used to define the local velocity distribution:

$$\rho \frac{\partial \mathbf{u}}{\partial t} = \mu \nabla^2 \mathbf{u} - \rho (\mathbf{u} \cdot \nabla) \mathbf{u} - \nabla p \Big|_{\Gamma_{\text{pores}}} \quad (\text{S1})$$

$$\nabla \cdot (\rho \mathbf{u}) = 0 \Big|_{\Gamma_{\text{pores}}} \quad (\text{S2})$$

Here $\mathbf{u}$ (m s^{-1}) is the velocity of the fluid, μ ($\text{kg m}^{-1} \text{s}^{-1}$) is the fluid viscosity, ρ (kg m^{-3}) is the fluid density and p (Pa) is the pressure field.

Together with the above-mentioned equations, the Brinkman equation is solved which is a combination of the continuity equation and the momentum equation and is defined for an incompressible flow according to (3):

$$\frac{\rho}{\phi} \left(\frac{d\mathbf{u}}{dt} + (\mathbf{u} \cdot \nabla) \frac{\mathbf{u}}{\phi} \right) = \nabla \cdot \left[-p + \frac{\mu}{\phi} (\nabla \mathbf{u} + (\nabla \mathbf{u})) - \frac{2}{3} \mu (\nabla \cdot \mathbf{u}) \right] - \left(\mu K^{-1} + \frac{Q}{\phi^2} \right) \mathbf{u} \Big|_{\Gamma_{\text{quartz} + \text{jarosite}}} \quad (\text{S3})$$

$$\nabla \cdot (\rho \mathbf{u}) = Q \Big|_{\Gamma_{\text{quartz} + \text{jarosite}}} \quad (\text{S4})$$

Here ϕ is the porosity and K (m^2) is the permeability of the porous media and Q is a mass source/sink term.

2. DETAILS OF THE ADVECTION-DIFFUSION-REACTION EQUATION:

The standard reactive-transport equation is used combining terms for advection, diffusion and reaction:

$$\frac{\partial c_i}{\partial t} = \underbrace{-\nabla \cdot (\mathbf{u} c_i)}_{\text{Advection}} + \underbrace{\nabla \cdot (\nabla D_{\text{diff}} c_i)}_{\text{Diffusion}} + \underbrace{R_i}_{\text{Reaction}} \Big|_{\Gamma_{\text{quartz} + \text{jarosite} + \text{pores}}} \quad (\text{S5})$$

Here, $\mathbf{u}$ (m s^{-1}) is the fluid velocity, c_i (mol m^{-3}) is the concentration of species i transported through the pore scape and porous media domains ($\Gamma_{\text{quartz} + \text{jarosite} + \text{pores}}$), D_{diff} ($\text{m}^2 \text{s}^{-1}$) is the diffusion coefficient and R_i ($\text{mol m}^{-3} \text{s}^{-1}$) is the rate of a chemical reaction contributing to the

concentration of the species i through homogeneous reaction like aqueous speciation and kinetic reactions taking place in the bulk fluid. Advection and diffusion are accounted for by the first and the second term on the right-hand side of the equation. A multi-component reactive transport formulation where the transport equation is solved for each element in the chemical system is used. Reactions occurring at the boundary are not included in this equation, explicit definition of these reactions are defined in the following section.

The initial conditions in the model were defined as follows:

$$\begin{bmatrix} u_x = 0 \\ u_y = 0 \\ p = 0 \end{bmatrix} \quad (S6)$$

3. RATE EQUATIONS FOR REACTIONS USED IN THE STUDY:

The rate of chalcopyrite dissolution according to the ferric iron dissolution mechanism is defined as:

$$\dot{R}_{Fe} = 10^{1.88} e^{-48100/RT} [H^+]^{0.8} (Fe(III))^{0.42} \Big|_{\gamma_{chalcopyrite}} \quad (S7)$$

The rate of chalcopyrite dissolution according to the proton-promoted dissolution mechanism is defined as:

$$\dot{R}_H = 10^{-1.52} e^{-28200/RT} [H^+]^{1.68} \Big|_{\gamma_{chalcopyrite}} \quad (S8)$$

Here, $\dot{R}_{Fe}$ and $\dot{R}_H$ are the reaction rates for [Equations 8](#) and [9](#) in the manuscript, respectively. $[H^+]$ and $(Fe(III))$ are the activity of protons and ferric ions, respectively, R is the ideal gas constant ($8.314 \text{ J mol}^{-1} \text{ K}^{-1}$) and T (K) is the temperature.

The kinetically controlled dissolution of quartz can be defined as:



And the reaction rate can be defined as:

$$R_{quartz} = SA_{quartz} \left[A_i^{298} e^{-\frac{E_a}{R}} \prod (a_{ij}^n) (1 - \Omega_{quartz}^{p_i})^{q_i} \right] \Big|_{\Gamma_{quartz}} \quad (S10)$$

R_{quartz} is the reaction rate in mol s^{-1} . SA_{quartz} is the surface area of the quartz mineral, which is calculated as $22.64 \text{ m}^2 \text{ kgw}^{-1}$ assuming the quartz grain is a sphere with a diameter of 0.0001 m , it has a smooth surface and a density of 22.65 Kg m^{-3} . Given the short simulation times and the slow dissolution rate of quartz, the geometry of the quartz grain did not evolve with time. The Arrhenius pre-exponential factor A_i^{298} ($\text{mol m}^2 \text{ s}^{-1}$), is calculated from k_i the log rate constant ($\log \text{mol m}^2 \text{ s}^{-1}$) and Arrhenius activation energy E_a (kJ mol^{-1}) at 25°C and a $\text{pH}=0$. T is the temperature in K and R is the ideal gas constant ($8.314 \text{ J mol}^{-1} \text{ K}^{-1}$). Here Ω is the saturation state of the quartz, n represents the reaction order with respect to the species H^+ . The chemical affinity parameters p_i and q_i in most cases is unity unless specified. The parameters used for the kinetic dissolution at different reaction conditions are listed in [Table S1](#) below.

Table S1: Parameters used for the reaction rate of quartz (adopted from (1)).

	Acid	Neutral	Base
$A_i^{298} (\text{mol m}^2 \text{ s}^{-1})$	0	1.98	1.97E+04
$E_a (\text{kJ mol}^{-1})$	0	77	80
n	0	0	0.34

The rate equation for the oxidation of ferrous iron is given as:

$$R_{Fe^{2+}} = -(2.91e^{-9} + 1.33e^{12} \alpha_{OH^-}^2 P_{O_2}) m_{Fe^{2+}} \big|_{\Gamma_{\text{quartz+pores+jarosite}}} \quad (\text{S11})$$

Here $\alpha_{OH^-}^2$ is the activity of the hydroxyl ion, $m_{Fe^{2+}}$ is the total molality of ferrous iron in solution, and P_{O_2} is the oxygen partial pressure (atm).

Table S2: Aqueous speciation reactions used in the model (adopted from the phreeqc.dat database (2)).

Reaction	$\log K_{eq}$
$Fe^{2+} + H_2O = FeOH^-$	-9.5
$Fe^{2+} + 3H_2O = Fe(OH)_3^-$	-31.0
$Fe^{3+} + H_2O = Fe(OH)^{2+}$	-2.19
$Fe^{3+} + 2H_2O = Fe(OH)_2^+$	-5.67
$Fe^{3+} + 3H_2O = Fe(OH)_3$	-12.56
$SO_4^{2-} + H^+ = HS^- + 2O_2$	-125.0

REFERENCES

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