

Evolution of H₂O and CO₂ contents in silicate melt inclusions during post-entrapment crystallization

R. ESPOSITO, M.J. STEELE-MACINNIS, L. FEDELE
AND R.J. BODNAR

Department of Geosciences, Virginia Tech, Blacksburg, VA
24061 USA
(nonac004@vt.edu, mjmaci@vt.edu, rjb@vt.edu)

Concentrations of H₂O and CO₂ in silicate melt inclusions are often interpreted to represent magmatic 'degassing paths,' in which depressurization of the magma during ascent leads to volatile saturation and release of CO₂ and H₂O from the melt [1]. This interpretation explicitly assumes that melt inclusions are trapped under conditions of volatile saturation. If the trapped melt is saturated in volatiles, then the melt must exsolve a volatile phase if any post-entrapment crystallization occurs on the walls of the inclusion (which happens to greater or lesser extent in all melt inclusions). As a result, the pressure inside the MI may differ from the confining pressure during post-entrapment cooling, and the PT path of the MI may be calculated knowing the solubility of H₂O and CO₂ in the melt as a function of temperature and pressure, as well as the PVT properties of the H₂O-CO₂ volatile phase and the partial molar volumes of H₂O and CO₂ in the melt.

Using PVTX data for the systems NaAlSi₃O₈-H₂O and NaAlSi₃O₈-H₂O-CO₂ [3, 4], we investigate the effect of small fractions of post-entrapment crystallization on the dissolved volatile content in an albitic melt inclusion entrapped under conditions of volatile saturation. The model is constrained to be a closed, isochoric system. As small amounts of albite crystallize on the inclusion walls, nucleation and growth of an H₂O or H₂O-CO₂ vapor bubble occurs and the pressure inside the MI is estimated from the difference between the molar volume of the volatile phase and the partial molar volume of the volatile in the melt using the EOS for H₂O-CO₂.

Model results show that dissolved volatile contents in the melt vary in a systematic manner during low degrees of post-entrapment crystallization. More importantly, the H₂O and CO₂ contents of the melt (glass) in the inclusion define trends that are similar to those produced during open system degassing. Thus, melt inclusions that all trap a volatile-saturated melt, but experience varying degrees of post-entrapment crystallization on the walls, will define an H₂O-CO₂ volatile trend similar to an open-system degassing path.

[1] Lowenstern (1994) *Geology* **22**, 893–896. [2] Roedder (1984) *Rev. Mineral.* **12**. [3] Burnham & Davis (1974) *Am. J. Science* **274**, 902–940. [4] Holloway & Blank (1994) *Rev. Mineral.* **30**, 187–225.

Geochemical modeling of speciation and the prediction of bioaccessibility: Can the former lead to the latter?

M.E. ESSINGTON*

Biosystems Engineering and Soil Science, University of
Tennessee, USA (*correspondence: messington@utk.edu)

It has long been recognized that the chemical speciation of an element in the terrestrial environment is an important determinant of bioavailability. Valence (redox status), aqueous speciation, solid-phase speciation (mineralogy), and adsorbed phase speciation (exchangeable vs. non-exchangeable) all play a role in dictating the ability of an organism to assimilate a potentially toxic element. Mechanisms to predict the distribution of an element between and within the various phases of soil and other environments are commonly based on the Laws of Thermodynamics through the application of the ion associate model. This model, which is executed by various geochemical computer codes, requires two generally distinct datasets: (1) the chemical characteristics of the environment in question, and (2) the thermodynamic data that described elemental distribution. As the Laws of Thermodynamics are assumed immutable, the quality of the ion speciation computations is due to the quality and completeness of the two datasets.

For natural systems, the determination of the salient chemical characteristics of an environment that affect elemental fate and behavior can be a daunting, if not impractical (or impossible) exercise. Also implicit to the model predictions are the robustness and accuracy of the accompanying thermodynamic database. The satisfactory determination of aqueous phase speciation is required for the prediction of mineral solubility and adsorption equilibria. Although geochemical models are meagerly equipped to predict the stability a small number of pure and macrocrystalline minerals, and to consider the surface complexation of a limited number of metals and ligand, the coupling of geochemical model predictions to bioaccessibility remains a challenge.

This presentation will examine the requirements for predicting the fate and behavior of the emerging contaminant antimony. The information necessary to delineate aqueous, solid, and adsorbed phase speciation of antimony will be identified. Mechanisms to translate geochemical modeling results to predictions of bioaccessibility will be discussed.