D.1 Practical Applications of Geochemical Modeling

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PRACTICAL APPLICATIONS OF GEOCHEMICAL MODELING

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I. OVERVIEW OF GEOCHEMICAL MODELING
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   Goal to further understanding; integrate and constrain possibilities
   Complexity paradox (see Oreskes paper)

II. ORIGIN AND EVOLUTION OF GEOCHEMICAL MODELS
   Concepts and computer programming evolved from early 1960's
   Numerous codes available but *the model makes the code - the code is NOT a model*
   Speciation; mass balance; reactive-transport

III. SPECIATION AND SATURATION INDICES
   Definitions
   The problem of supersaturation - ferrihydrite

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   Remediation scenarios
   Long-term research should lead to new and improved remediation

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I. OVERVIEW OF GEOCHEMICAL MODELING

Geochemical models are used extensively for contaminant source characterization, contaminant transport, and remediation scenarios. Their limitations, however, are not well known and sometimes it is not clear what a model is or how it can be appropriately used.

``Every area of science uses models as intellectual devices for making natural processes easier to understand. The model that reliably predicts the outcome of real events, or that continues to fit new data, is essentially a kind of theory, a broad statement of how nature works.''
   - Jay Lehr (1990) editorial in Ground Water

What is a model? A model is an idea, a hypothesis, a theory, or a combination of theories that provide new insight into a challenging problem. Retired UBC geology professor Hugh Greenwood (1989) put it very well when he said that a model ``is a well-constrained logical proposition, not necessarily mathematical, that has necessary and testable consequences.''

The key phrases here are ``logical proposition'' and ``necessary and testable consequences.'' These phrases help to separate science from religion, liberal arts, or mere statistical exercises.

A geochemical model is a theoretical construct based on principles of physical chemistry applied to hydrogeologic systems. Geochemical models do not usually provide unique answers but they do constrain the possibilities and they often integrate a large amount of information. One of the limitations that has been pointed out by Naomi Oreskes (2000) is the Complexity Paradox: the more general and sophisticated models (and their associated codes) become, the less we know about their reliability. Conversely, the simpler a model, the easier it is to test.

A related concern is the use of the word ``prediction.'' When science predicts something, it is a logical prediction, i.e. it follows the logic that if one accepts principles A and B, and assumptions C-F then the result will be X. It is not temporal prediction in the sense that science can predict exactly when some event will happen in the future except for relatively simple, repeating events such as the orbits of the planets.

II. ORIGIN AND EVOLUTION OF GEOCHEMICAL MODELS AND CODES

The evolution of computer codes and models from the early 1960's has been impressive but thermodynamic property measurement and data evaluation has not kept pace with model and code developments. Even worse, the field measurements are often inadequate to apply the model and many codes are run without necessary constraints to make the model useful. Assumptions regarding whether equilibrium or non-equilibrium processes are dominant often do not have a firm basis.

``Models'' should not be used interchangeably with ``codes.'' The model is a conceptual understanding (along with its relevant mathematics or scaled down 3-D representation) whereas the code is the algorithm, the translation of the mathematics and related features embodied in a software program.

A thorough review of geochemical models useful for mine waste environments is available (Alpers and Nordstrom, 1999) and evolutionary lines of many different codes are shown in this paper. With regard to geochemical models the following definitions are helpful:

Speciation: equilibrium distribution of aqueous species among free ions, ion pairs, and complexes.

Mass transfer: transfer of mass between two or more phases (such as dissolution or precipitation of minerals).

Mass transport: solute movement by fluid flow.

Reactive transport: combined mass transfer and speciation with fluid flow.

III. SPECIATION AND SATURATION INDICES

Once speciation has been done with an appropriate algorithm, the output will contain the aqueous activity of various free ions and ion pairs or complexes. These activities can then be used to calculate the saturation index or the tendency of the water to dissolve or precipitate minerals. The saturation index is defined as:

$$S.I. = \log (IAP/K_{sp})$$