

## Chapter 11 Answers

2. One input file for PHREEQC is supplied, which can be edited to do the various steps. Note, however, that there are several database files available, which may use different mineral names. For example phreeqc.dat uses K-mica, but llnl.dat uses Muscovite. You must of course use the appropriate name for the database you are using.

In the solution in which PHREEQC is instructed to equilibrate five phases in a four component system, it chooses to undersaturate Gibbsite. In calculating values of SI, PHREEQC does not solve a system of linear or non-linear equations, but uses an optimization routine. There is no requirement that equations be linearly independent or even that the number of equations must equal the number of unknowns. The inequalities are the objective functions, and the method tries to satisfy them as equalities but otherwise minimizes the residuals of the inequality equations. The equations for phase equilibria are put into the inequality relations so that  $SI \leq 0$  are the relations that are solved. Mass-balance relations are included as equalities, as the system composition is known.

The result in this case is that Gibbsite cannot equilibrate with the relatively K-rich solution produced by the other minerals, and is unstable. The SI is the result of the mass balance calculations.