

## Alternative Activity 3.2

### Description

In this activity the students will “explore and learn” using three chemical reaction equilibrium simulators.

### Objective

The objectives of this activity are for the students to (a) begin to develop a qualitative “feel” for how composition, temperature and pressure affect chemical equilibrium and the equilibrium constant, (b) to realize that the heat of reaction dictates whether increasing temperature leads to increasing or decreasing equilibrium conversion, (c) to recognize that the equilibrium constant is not affected by pressure, but the equilibrium conversion can be affected if the total number of moles changes as a consequence of reaction and (d) to realize that when the number of moles does change as a consequence of reaction, then increasing pressure will always move the reaction toward fewer total moles.

### Preparation

Arrangements should be made so that small groups of students can simultaneously use the three simulators provided with the unit in class. That is, either have students bring laptops to class with the simulators already installed and operating or hold class in a computer-equipped classroom.

1. Familiarize yourself with the use of the simulators (there is a user's guide under the help menu).

### Lesson Plan

1. Display the first slide and describe the activity and its objectives.
2. Have the students work in groups of two to four. Assign one-third of the groups the methyl chloride reaction, one-third the methanol synthesis reaction and one-third the reverse water-gas shift.
3. Let the groups use the simulators to gather “data” making sure they record all trends that they observe.
4. For each reaction, have the students who studied it arrive at a consensus on the effects of temperature, pressure and composition upon the thermodynamic quantities and the equilibrium conversion. This might be done by letting all the groups who worked on a given reaction compare notes and summarize, it could be done by calling on groups to report, etc.
5. The trends will not be the same for all of the groups. Allow them time to discuss, check each other's results, etc. with the goal of explaining all of the observations of all the groups.
6. Call on groups to report their findings and their explanations for them. Record their results and interpretation, leading to the formulation of a set of “rules of thumb” such as those presented on the final slide.
7. At the end of the activity, point out that if the Gibbs free energy change is expressed in terms of the enthalpy and entropy changes and if the latter quantities are assumed to be constant, equation (4.3)

will take the form of  $K = K_0 \exp\left(\frac{-\Delta H}{RT}\right)$

### Variations

Have the students work in groups of 3 with all of them recording the trends initially. Then re-form the groups so that in each new group there is one person who worked initially on each of the three reactions.

Have them compare notes and rationalize the differences as in step 5 above. Then call on groups to report while you record their findings and generate an overall summary.

#### **Tips and Suggestions**

To try to relate this information to that from Unit 3, have them discuss or debate whether (or when) the heat of reaction at 298K would be sufficient to predict the effect of temperature (at a temperature other than 298K) upon the equilibrium constant or whether the heat of reaction at the prevailing temperature is needed. {If the heat of reaction at 298 K is much greater than the sensible heat of cooling and heating between 298K and T, then the heat at 298 K is an acceptable predictor}.