A Short Program for Teaching Chemical Equilibrium

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Abstract

A short GW/BASIC program for the automatic calculation of equilibrium concentrations is presented. This program can be used to solve problems with an arbitrary number of reactants and products. The program uses an iterative algorithm. Common and sometimes hard to understand simplifications are avoided. Once the calculation have been carried out, the equilibrium concentrations of reactants and products are shown and a Kc is computed from these concentrations.

Teaching chemical equilibrium takes up a large part of the chemistry curriculum. The problems and questions related to chemical equilibrium can be presented in various ways, often involving ionic species in solution. One of the main objectives of chemical education is that students understand chemical equilibrium as a dynamic equilibrium in which two semi-reactions, direct and inverse, take place. It is also desirable that students learn to use the mass action law and Le Chatelier's principle to predict the result of the possible variations of variables (pressure, volume,...) involved in chemical equilibria. Another main objective is that intermediate level students learn how to compute equilibrium concentrations from initial concentrations of chemical species involved in a given reaction. To do so students are generally taught to write the Kc formula with the dissociation rate, $\propto$, as an unknown. Typical problems are carefully chosen to obtain easily-solved first grade or, at the most, second grade equations. The numerical values of Kc and initial concentrations are also chosen in such a way that, if necessary, and its powers are small and can be ignored with regard to initial concentrations. Students sometimes do not understand properly when this can and cannot be done. All of the above result from the students using rote instead of meaningful learning strategies for calculation. Thus many students have misconceptions about chemical equilibrium (Wheeler and Kass, 1978), even though they are able to solve the numeric problem properly. The situation is even worse: these misconceptions can be identified also in some preservice science teachers (Furiò and Ortiz, 1983).

$$Kc = \frac{\prod_{i=1}^{M} (C_{2i})_{eq}^{a_{2i}}}{\prod_{i=1}^{N} (C_{1i})_{eq}^{a_{1i}}}$$

Consider the reaction of some chemical species (A_{1i} y A_{21}), with initial concentrations of C_{1i} y C_{2i}. Depending on the values of these initial concentrations, three situations are found: (1) The chemical species on the left side (reactants), A_{1i}, react and transform into the chemical species on the right, A_{2i}, until equilibrium is reached; (2) the chemical species on the right side (products), A_{2i}, react and transform into the chemical species on the left, A_{1i}; and (3) the initial concentrations, C_{1i} and C_{2i}, may be such that the system is already in equilibrium.

If we define K(x) as: