# An Alternate Way to Solve Equilibrium Problems

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In this essay we describe an alternative to solving equilibrium problems by the 'ICE' method (see *e.g*. problem 18-2 of your lecture notes). This alternative method is based on the conservation of mass and charge, concepts you have already used in the balancing of chemical equations. While a bit more trouble to use on simple problems, it clearly shows how the constraints of mass conservation enter into the solution.

We start by considering the following equilibrium system:

$$CO(g) + H_2O(g) = CO_2(g) + H_2(g) \tag{1}$$

Assume that the initial concentrations are

$$[CO]_0 = [H_2O]_0 = A_0; \quad [CO_2]_0 = [H_2]_0 = 0;$$

where $A_0$ is a constant, e.g. = 2.0 M.

Now define the sought for equilibrium concentrations in terms of abstract variables *u*, *v*, *x* and *y* as follows:

$$[\mathrm{CO}] = u; [H_2O] = v; [CO_2] = x; [H_2] = y \tag{2}$$

Then the abstract expression for K becomes:

$$K = \frac{[CO_2][H_2]}{[CO][H_2O]} = \frac{xy}{uv} \tag{3}$$

Equation 3 is a non-linear equation in four unknowns. We can obtain three more (linear) equations by considering the conservation of mass in the following manner:

$$\text{Conservation of carbon: } [\mathrm{CO}]_0 + [\mathrm{CO_2}]_0 = \mathrm{u} + \mathrm{x} \tag{4}$$

$$\text{Conservation of hydrogen: } 2[\mathrm{H_2O}]_0 + 2[\mathrm{H_2}]_0 = 2\mathrm{v} + 2\mathrm{y} \tag{5}$$

$$\text{Conservation of oxygen: } [\mathrm{CO}]_0 + [\mathrm{H_2O}]_0 + 2[\mathrm{CO_2}]_0 = \mathrm{u} + \mathrm{v} + 2\mathrm{x} \tag{6}$$

Equations 4-6 can be simplified to:

Conservation of carbon: $A_0 = u + x$ (7)

Conservation of hydrogen: $A_0 = v + y$ (8)

Conservation of oxygen: $2A_0 = u + v + 2x$ (9)

Now we have four equations (3, 7, 8 and 9) in four unknowns (u, v, x and y). We then proceed to solve these equations for the variable x by systematic elimination of the other three variables (y, u and v).

In the first step of the elimination process, we rearrange Equation 7 to $u = A_0 - x$ . Now we can eliminate *u* from Equations 3 and 9:

Equation 3 becomes: $K = \frac{xy}{(A_0 - x)v}$ (10)

Equation 8 remains as: $A_0 = v + y$ (11)

Equation 9 becomes: $A_0 = v + x$ (12)

The above are three equations (10, 11 and 12) in three unknowns (v, x and y). Next, we eliminate y from equations 10 and 12 by rearranging Equation 11 to $y = A_0 - v$ and substituting:

Equation 10 becomes: $K = \frac{x(A_0 - v)}{(A_0 - x)v}$ (13)

Equation 12 remains as: $A_0 = x + v$ (14)

This leaves two equations in two unknowns. Now we eliminate v from equation 13 by rearranging Equation 14 to $v = A_0 - x$ and substituting:

Equation 13 becomes:

$$K = \frac{x(A_0 - A_0 + x)}{(A_0 - x)(A_0 - x)} \quad (15)$$

Upon simplification Equation 15 becomes:

$$K = \frac{x^2}{(A_0 - x)(A_0 - x)} = \frac{x^2}{(A_0 - x)^2} \qquad (16)$$

This equation is identical to that of problem 18-2 obtained by the ICE method in Zumdahl.