Chemistry
Excel Equilibrium Activity

Name _____ Date _____ Period _____
equiexcelac05.doc

Show all calculations.

Introduction:

Given the following chemical equation:

$3H_{2(g)} + CO_{(g)} \leftrightarrow H_2O_{(g)} + CH_{4(g)}$ $K_c = 190$ @ 1000K

written in the form $aA + bB \leftrightarrow cC + dD$

You will use an Excel spreadsheet to investigate and determine equilibrium conditions given a set of initial concentrations.

Open the appropriate Excel spreadsheet (excelequilact2005.xls). Familiarize yourself with the layout of the application. For the moment, **focus on the boxed area in dark blue**. The boxes in this area are where you will input coefficients, initial concentrations, K_c values and make manual changes to the concentrations. This area also keeps you informed about the current Q (mass-action expression) value for the reaction. The light purple area will show the current concentrations for each chemical component.

Procedure:

1. Examine the K_c value given above. Does this reaction appear to be spontaneous? Explain.

2. You will begin by inputting initial concentrations of .15M for each substance. Using the format $aA + bB \leftrightarrow cC + dD$, enter the initial concentrations and coefficients from the balanced chemical equation into the proper boxes of the input area (in blue) on the form (Remember that A/B are the reactants and C/D are the products). Also enter the *Desired K_c Value*, and make sure that the *Concentration Change* value is set to zero.

3. Determine the initial reaction quotient Q value.

   Q = _____

4. Predict the direction that the reaction will proceed in.

5. Determine the value of the concentration change required to bring the system to equilibrium either by successive approximations (manually entering various values for the *concentration change* parameter until $Q = K_c$) or by using the Solver function. (See instructor for help on using the Solver function.). Try to get Q as close to K_c as you can. You should carry out the concentration change to ***five decimal places***.

Remember that the *Concentration Change* value is equivalent to the variable x in an equilibrium table and has not been multiplied by the coefficients of the equation. (However, the table does this internally as it updates the equilibrium expression.)

Best value of Concentration Change parameter (when $Q = K_c$): _____ mol/L

6. Write down the final equilibrium concentrations determined by the spreadsheet from your Q value (lavender box):

H_2 = _____M CO = _____M H_2O = _____M CH_4 = _____M

7. Calculate the actual concentration **change** for each component of the reaction (i.e. with respect to their initial concentrations).

$\Delta[H_2]$ = _____M Δ[CO] = _____M $\Delta[H_2O]$ = _____M $\Delta[CH_4]$ = _____M

Based on this information, was your prediction from step 4 confirmed?

8. Would this be an easy equilibrium expression to solve by hand? Why or why not?

9. Add an additional .05M to your initial concentration of CO, then alter the *Concentration Change* parameter to bring the system back into equilibrium.

What is the new value for the concentration change parameter that brings Q back to K_c?

Are the new equilibrium concentrations what you expected based on putting this kind of "stress" on the system? Explain.

10. Enter the concentration values from the lavender box into the initial condition boxes for A thru D (blue area). Change the "Concentration Change" parameter to zero. Is the system in equilibrium? How do you know? Explain.

10. Calculate the value of K_p from K_c. Show your calculations.

K_p = _____

11. If this reaction took place inside a sealed container that was suddenly expanded after equilibrium was established, describe what would happen to the system and why.