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Reaction Menu

This menu can be used to create a new reaction or to exit the program.

Temperature Item

Clicking on this item will allow the user to change the temperature of the reaction vessel. The reaction can be run at 25°C or 35°C. The starting temperature for any new reaction is 25°C. The temperature may be changed to 35°C by selecting the desired temperature from the dialog box. The time will be reset to zero and the user can see which way the equilibrium will shift (Le Chatelier's principle) when the temperature is changed. This will give an indication as to whether the reaction is endothermic (absorbs heat) or exothermic (evolves heat). The temperature can be reset to 25°C if desired. This option does not work with the unregistered version of the program. See register.doc for more information.

Concentration Item

By clicking on Concentration the user can change the number of molecules of A, B, and/or C. The time will be reset to 0 and a new graph will be started. Changing the number of molecules will allow the user to see Le Chatelier's principle at the molecular level. There can be no more than 80 total molecules. This option does not work with the unregistered version of the program. See register.doc for more information.

Purpose of the program

Equilibrium can be a difficult subject because it is hard to visualize what is occurring at the molecular level as a reversible reaction at equilibrium proceeds. This program allows the user to view equilibrium while it is being achieved. Le Chatelier's principle can also be examined by changing the temperature or concentration of the reaction mixture. A lab which can be used with the program is included with the registered copy.

Pause Item

Clicking on this item freeze the action so that data and observations can be made. The reaction may be restarted by using restart This option does not work with the unregistered version. See register.doc for more information.

Restart Item

This item will restart a reaction that has been stopped with pause This option does not work with the unregistered version. See register.doc for more information.

New Item

Choosing this menu item will allow the user to start a new reaction with a user determined number of molecules of A, B, and X. Enter the number of molecules of each substance desired into the boxes provided. Use the mouse or Tab key to move around the dialog box. You may have no more that a total of 80 molecules. The reaction will start.

Exit

To quit the program select this menu item or press Alt-x.

Window Appearance

When a reaction is started by selecting new from the reaction menu a box will appear in the upper left hand corner of the window. This is the reaction vessel. The molecules of A , B , and X will move at various speeds in a manner similar to that which would occur at the molecular level during an actual chemical reaction. The equilibrium being illustrated is:

$$A(g) + B(g) <-> 2\ X(g)$$

This reaction is similar in mechanism to the classic equilibrium example which occurs between hydrogen and iodine vapor to produce gaseous hydrogen iodide. When molecules of A and B collide they may react to form, two X molecules. (Not all collisions result in a reaction). When two X molecules collide they may form an A and a B molecule.

The actual number of molecules of each species can be found on a table below the reaction vessel. In the upper right hand corner A table including The elapsed time since the beginning of the reaction and the average number of A, B, and X molecules is presented. When doing calculations involving equilibrium constants the average number of molecules gives a more statistically consistent result form student to student. Constants will not match exactly (statistics!!) , but if a class average of all constants is taken the correlation is very consistent.

In the lower right hand corner of the screen there is a graph which relates the average number of molecules present vs. time. The graph shows the student a very clear representation of what is happening as equilibrium is established. Every 100 seconds the graph will be refreshed.