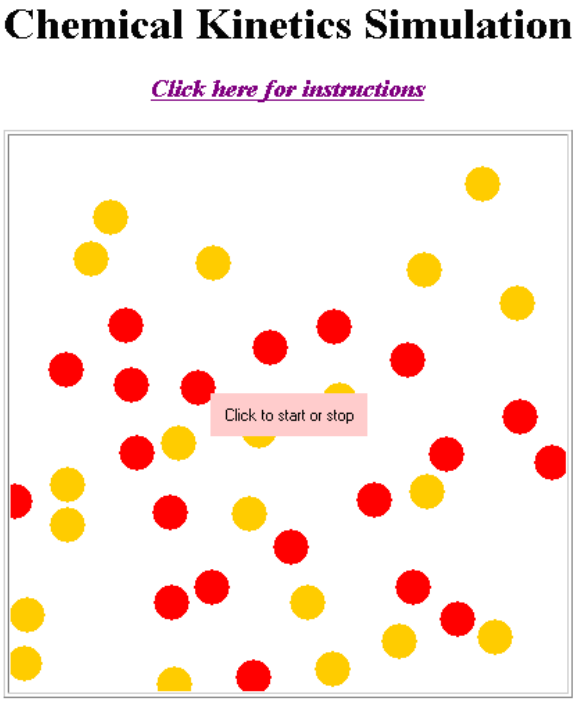
ChE 344
Week 3
Problem Set 3
Due Tuesday, January 22, 2013 (Lecture 4)

Individual Assignment

1. PLQ4 - Each group member is to individually define θ_i, θ_A, θ_B, and δ. Submit to CTools before class

Group Assignment

1. P2-11_B
2. P3-3_B and then write a paragraph describing activation energy, its origin, and how it affects chemical reaction rates.
3. P3-6_B
4. P3-10_A
5. P3-11_A
6. As a group explain what each member of the group did in the active learning role, i.e. manager, recorder, checker, and critic.
7. Go to the website: http://www.chem.uci.edu/undergraduate/applets/sim/simulation.htm. Note: make sure your browser supports Java. When you access the website, you should see something very similar to this:



The reaction is

$$(A + B \leftrightarrow C + D)$$
$$\text{Red} + \text{Yellow} \leftrightarrow \text{Green} + \text{Blue}$$

In the upper left-hand corner of the screen should be a box, which is the "simulation control panel". The numbers in the boxes next to red/yellow/green/blue represent the initial number of molecules (i.e. initial concentration or number density) present in the simulation. The values k_f and k_r are the forward and reverse reaction rate constants respectively. These are expressed as a probability between 0 and 1 that a collision between reactants will result in a reaction. The "Stripchart ON" button allows you to track changes in the number of molecules over time. Detailed instructions for operating the simulation are available by clicking on the link displayed above the graphic.

(a) Run a simulation with $k_f = k_r$, and beginning with equal numbers of red and yellow balls. Track the changes in numbers of molecules using the stripchart. What is observed? Now run the simulation again in the cases when $k_f > k_r$ and $k_f < k_r$. How do these simulations differ from the original case?

(b) How does the time to reach equilibrium change when you increase the number of red and yellow balls? Why?

(c) How does the time to reach equilibrium change when k_f and k_r are increased? Why?

(d) Once equilibrium is reached are reactions taking place? What does this result say about chemical equilibrium?

(e) Describe what you learned from this simulation.