Chemical Engineering 323
Homework 8
Due 2:00pm, Friday June 3 in Catalysis Rm. 110
TA: *Manohar Murthi*

Download the zipped package of code available on the course website. Extract all the files into a single directory. Launch MATLAB and change the working directory to the location in which you installed the files. Run the simulation by typing 'kmc'.

Start with the base case (values already present in the main driver kmc.m). Note the results. Feel free to experiment with any of the simulation parameters or to extract various data from the program in order to further your understanding. Submit plots to support your arguments. Since this is a stochastic simulation, you may wish to run it several times for each datum to be sure that your results are consistent.

1. (20 points) Vary cp between 0.02 and 10.0. and the micropore fraction between 1.0 and 0.2. Examine the interplay between these parameters and explain the results. What is the physical interpretation of cp? It may be necessary to alter other simulation parameters (such as the time) in order to obtain a better understanding of the results.

2. (30 points) Due to time constraints, it was not possible to check that each cell remained connected to a wall through a cluster of other cells. The function check_cluster.m performs this check. Explain in detail how the routine works. Make the function call to perform the check and run the simulation with and without the check in place for the following scenarios (only values which differ from the base case are listed):
   (a) macro_size = 45; micro_fraction = 0.5; depth = 90; t_prolif = 12*60; s_prolif = 1.5*60; 50 time steps
   (b) other parameters as in (a), cp = 10.0
   Describe and explain the differences between the two models (i.e., with vs. without the check in place)

3. (20 points) What happens when you attempt to run the simulation with the base case parameters and check_cluster in place? Explain in detail the causes of the error.

4. (30 points) Using the check_cluster function is extremely timc-consuming. Discuss how using a better neighbor-searching algorithm may impact the simulation as a whole. Describe some of the different algorithms for neighbor searching. Include a discussion of their relative speeds.