Problem Set 1

This problem set reviews reactor engineering and batch processing topics. Later, we will do similar problems, but more complicated, so that we will require a process simulation code to reach an answer. Here, a spreadsheet suffices.

Problem 1: Data Analysis and Parameter Estimation (40 points)
One reaction in the Lucretex process is the hydrolysis of E to give D. The chemistry of the reaction (also given in the problem statement) is

$$2E + H_2O \rightarrow D + 2MeOH \qquad (1)$$

The chemists conducted batch experiments in the laboratory to generate kinetic data. They carried out Reaction (1) in a flask at three different temperatures, and measured the concentration of E in the flask over time. The flask initially contained 1.3 mol/liter of E and 26 mol/liter of water, along with inert materials. The data for the experiments are shown in Table 1.

- From their measurements, determine a rate expression for the hydrolysis reaction. (The chemists feel that the reaction is either first order in E and water, or second order in E).
- Calculate the kinetic rate constant at the three different temperatures.
- Determine the pre-exponential factor and the activation energy in the Arrhenius expression for the rate constant for this reaction.

Table 1: Concentration of E (molar)

	temperature (ºC)		
time(h)	94	88	80
0	1.3	1.3	1.3
0.25	0.599	0.732	0.911
0.5	0.380	0.523	0.714
1	0.226	0.319	0.481
1.5	0.159	0.244	0.384
2	0.116	0.182	0.297
2.5	0.104	0.151	0.264
3	0.084	0.124	0.209
3.5	0.075	0.106	0.194
4	0.064	0.108	0.163
4.5	0.065	0.100	0.150
5	0.063	0.086	0.139
5.5		0.065	0.122
6		0.074	0.129
6.5		0.061	0.110
7		0.066	0.107
7.5		0.049	0.086
8			0.086
8.5			0.098
9			0.073
9.5			0.084
10			0.072

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Problem 2: Batch Reactor Sizing (30 points)

It is desired to produce 1000 Mg of D in 200-day operating campaign via batch reaction. The reactor is to be charged with reactants in the proportions of Problem 1 and run at 84ºC. The stopping criterion is 97% conversion of E. A complete batch consists of fill/react/empty. The flow rate for pumping reactants in and products out is 200 L min^{-1}. Calculate the required volume of a reactor vessel, assuming it is to run no more than 80% full.

Problem 3: Back-of-the-Envelope Calculation (30 Points)

Raw material costs for the Lucretex process are given in Table 2. Given the information currently available to you, estimate a lower bound on the cost of manufacturing 280,000 lb_m of Lucretex. List and explain your assumptions.

Table 2: Raw Material Costs for the Lucretex Process

R1	4.25	\$ kg^{-1}
R2	9.2	\$ kg^{-1}
toluene	1.52	\$ kg^{-1}
Pt cat	55	\$ L^{-1}
MeOH	1.34	\$ kg^{-1}
H_2O	0.015	\$ kg^{-1}