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

$$2E + H_2O \rightarrow D + 2\text{MeOH} \quad (1)$$

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)

<table>
<thead>
<tr>
<th>time(h)</th>
<th>94</th>
<th>88</th>
<th>80</th>
</tr>
</thead>
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<tr>
<td>0</td>
<td>1.3</td>
<td>1.3</td>
<td>1.3</td>
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<tr>
<td>0.25</td>
<td>0.599</td>
<td>0.732</td>
<td>0.911</td>
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<td>0.5</td>
<td>0.380</td>
<td>0.523</td>
<td>0.714</td>
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<td>1</td>
<td>0.226</td>
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<td>0.481</td>
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<tr>
<td>1.5</td>
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<td>0.244</td>
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<td>0.151</td>
<td>0.264</td>
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<td>0.124</td>
<td>0.209</td>
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<tr>
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<tr>
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<td>0.100</td>
<td>0.150</td>
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<tr>
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<td>0.086</td>
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<td></td>
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<td></td>
<td>0.084</td>
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<td>10</td>
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<td></td>
<td>0.072</td>
</tr>
</tbody>
</table>

revised 2006 Sep 7
**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 lbm of Lucretex. List and explain your assumptions.

*Table 2: Raw Material Costs for the Lucretex Process*

<p>| | | |</p>
<table>
<thead>
<tr>
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<td>R1</td>
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<tr>
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<tr>
<td>Pt cat</td>
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<td>$ L⁻¹</td>
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<tr>
<td>MeOH</td>
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<td>$ kg⁻¹</td>
</tr>
<tr>
<td>H₂O</td>
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<td>$ kg⁻¹</td>
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