As you know, your objective is to produce 300,000 lbs of Lucretex monomer at our Cambridge plant at minimum cost and minimum campaign time. We are anxious to test market the polymer as soon as possible. Please keep in mind the competing Cal Tech Industries estimate of 35 days at a cost of $10/lb. Your final design should be able to improve on this estimate.

I have collected essential economic information required for you to estimate the cost of your proposed design. In addition, I have summarized the various process information that has been developed by you and our associates at Research and Product Development in Blacksburg. Finally, I have specified a number of design constraints that must be imposed in order to assure safe and feasible operation.

A number of equipment units have been made available for your use in the plant. You may select the units you need from this inventory.
Summary of Process Information:

1. Reaction I: Use ABACUSS II (model ICE_Reactor1_Model.ABACUSS) to simulate the operation of Reaction I.

2. Reaction II: Reaction II is 1st order in methanol concentration and 1st order in the concentration of C.
   
   Stoichiometry: MeOH + C → E
   
   Rate expression: \( \frac{dC_E}{dt} = kC_{MeOH}C_C \)
   
   Relationship between concentrations and reaction time:
   \[
   \text{Time} = \frac{\ln\left(\frac{C_C C_M}{C_C C_C + C_M C_0}\right)}{k(C_C C_0 - C_M C_0)}
   \]  
   
   where:
   
   \( C_C C_0, C_C \) are initial and final conc of C
   
   \( C_M C_0, C_M \) are initial and final conc of MeOH
   
   \( k \) is the kinetic rate constant = 1.00 l/mol-h

3. Reaction III: Reaction is 2nd order in concentration of E:
   
   Rate Expression: \( \frac{dC_{H_2O}}{dt} = \frac{1}{2} \frac{dC_E}{dt} = -kC_E^2 \)
   
   Analytic Expression: \( \frac{1}{C_E} - \frac{1}{C_{E_0}} = 2kt \)
   
   Arrhenius Expression: \( k = k_0 e^{-\frac{E_a}{RT}} \)
   
   \( k_0 = 9.14215E11 \) l/(mol-hr), \( E_a = 83,354 \) J/mol = 19,922 cal/mol

4. Distillations: Use ABACUSS II to simulate the batch distillation tasks.
Equipment Inventory:

<table>
<thead>
<tr>
<th>Unit type</th>
<th>Volume (gal)</th>
<th>Usage cost ($/hr)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reactors</td>
<td></td>
<td></td>
</tr>
<tr>
<td>500</td>
<td>500</td>
<td>50</td>
</tr>
<tr>
<td>500</td>
<td>500</td>
<td>50</td>
</tr>
<tr>
<td>750</td>
<td>750</td>
<td>70</td>
</tr>
<tr>
<td>750</td>
<td>750</td>
<td>70</td>
</tr>
<tr>
<td>1000</td>
<td>1000</td>
<td>88</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Unit type</th>
<th># trays</th>
<th>Volume (gal)</th>
<th>Vapor (kmol/hr) Rate</th>
<th>Usage cost ($/hr)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Columns</td>
<td>8</td>
<td>750</td>
<td>15</td>
<td>90</td>
</tr>
<tr>
<td></td>
<td>12</td>
<td>750</td>
<td>20</td>
<td>110</td>
</tr>
<tr>
<td></td>
<td>8</td>
<td>1000</td>
<td>20</td>
<td>110</td>
</tr>
<tr>
<td></td>
<td>8</td>
<td>1250</td>
<td>15</td>
<td>125</td>
</tr>
<tr>
<td>Combination reactor/column</td>
<td>8</td>
<td>2000</td>
<td>10</td>
<td>175</td>
</tr>
</tbody>
</table>

Intermediate Storage is available in any total amount but only in increments of 250 gallons. Storage costs $5 / hr (250 gal increment). Other items of equipment may be made available on negotiation with management.

Cost of Raw Materials:

<table>
<thead>
<tr>
<th>Material</th>
<th>Cost ($/unit)</th>
</tr>
</thead>
<tbody>
<tr>
<td>R1</td>
<td>4.11 /kg</td>
</tr>
<tr>
<td>R2</td>
<td>8.85 /kg</td>
</tr>
<tr>
<td>Toluene</td>
<td>1.464 /kg</td>
</tr>
<tr>
<td>Pt catalyst</td>
<td>35.0 /l slurry</td>
</tr>
<tr>
<td>MeOH</td>
<td>1.23 /kg</td>
</tr>
<tr>
<td>H2O</td>
<td>0.01 /kg</td>
</tr>
</tbody>
</table>

Cost of Waste Treatment:

<table>
<thead>
<tr>
<th>Wastes</th>
<th>Source</th>
<th>Cost ($/kg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Solids (Pt catalyst, I2, A)</td>
<td>Bottoms Distillation II</td>
<td>13.60</td>
</tr>
<tr>
<td>Aqueous (MeOH, H2O, Toluene, E)</td>
<td>Overheads Distillation III</td>
<td>1.70</td>
</tr>
<tr>
<td>Organic</td>
<td>Overheads Distillation I</td>
<td>Credit</td>
</tr>
</tbody>
</table>
Note the that overheads of distillation task I is organic waste, and the waste treatment facility can recover 90% by mass of the Toluene, Methanol, and R1 in this stream as pure solvent and reagent for recycle. The waste treatment facility will credit your design with 50% of the raw material cost for the mass it can recover.

**Cost of Utilities ($/batch):**

1. Reaction I heatup:

   \[ 3.171 \times 10^{-6} \left( \frac{\$}{KJ} \right) 4.18 \left( \frac{KJ}{L^{o}C} \right) (T_{\text{feed,C}} - 25)V_{\text{final}} \]

   where \( T_{\text{feed,C}}[^{o}C] \) is the temperature the reactor contents are preheated to, and \( V_{\text{final}}[l] \) is the volume of the reaction mass at the end of the reaction step (i.e., this figure includes preheating any material fed to the reactor during the reaction step).

2. Reaction I condenser cooling:

   \[ 7.9274 \times 10^{-7} \left( \frac{\$}{KJ} \right) \dot{Q}_{c,\text{max}}t_{\text{rxn,hr}} \]

   where \( \dot{Q}_{c,\text{max}}[KJ/hr] \) is the maximum condenser cooling rate required during the reaction step, and \( t_{\text{rxn,hr}}[hr] \) is the time the reaction step is run for.

3. Reaction I cooldown:

   \[ 7.9274 \times 10^{-7} \left( \frac{\$}{KJ} \right) 4.18 \left( \frac{KJ}{L^{o}C} \right) (T_{\text{final,C}} - 65)V_{\text{final}} \]

   where \( T_{\text{final,C}}[^{o}C] \) is the temperature the reactor contents at the end of the reaction, and \( V_{\text{final}}[l] \) is the volume of the reaction mass at the end of the reaction step.

4. Column boilup/condensing:

   Condenser: \( 3.171 \times 10^{-2} V t_{\text{dist,hr}} \)

   Reboiler: \( 0.12684 V t_{\text{dist,hr}} \)

   where \( V[kmol/hr] \) is the vapor rate in the column and \( t_{\text{dist,hr}}[hr] \) is the time over which the utility is used.

5. Vacuum:

   \[ 125 \ln(760/P_{mm\text{Hg}})(t_{\text{dist,hr}} + 0.3) \]

   where \( P_{mm\text{Hg}}[mm\text{Hg}] \) is the pressure in the column during the vacuum step, and \( t_{\text{dist,hr}}[hr] \) is the time period over which vacuum is applied.
Assumptions and Process Constraints:

1. Reaction I:
   (a) Reaction solvation. The total mass of R2 fed to the reactor over the entire cycle \((F_{R2} [kg])\) and the volume of toluene initially charged to the reactor \((V_{Toluene} [l])\) should satisfy the inequality:
   \[
   \frac{F_{R2}}{V_{Toluene}} \leq 0.84
   \]
   Note that at least the volume of toluene indicated by this inequality must be added in the initial charge to the reactor.
   (b) Consumption of key reactant. The mass of R2 remaining in the reactor at the end of a cycle \((M_{R2,final} [kg])\) and the volume of toluene initially charged to the reactor \((V_{Toluene} [l])\) should satisfy the inequality:
   \[
   \frac{M_{R2,final}}{V_{Toluene}} \leq 0.016
   \]
   (c) Reflux cooling duty. Each reactor is constrained by the maximum cooling duty of the overhead condenser used to condense and reflux solvent and reagent that is boiled off during the exothermic reaction. The maximum cooling duty that the condenser can supply is a function of the volumetric capacity of the reactor (in \([l]\)), and is expressed as:
   \[
   \text{Maximum Condenser Cooling Rate} = 150 \ [KJ/(hr \ l)]
   \]
   If this constraint is exceeded at any time, solvent and reagent will be vented to the flare with dire consequences.
   (d) Initial reaction heat up takes 0.5 hr.
   (e) Post reaction cool down requires 0.5 hr.
   (f) No reaction takes place during heat up or cool down.
   (g) Molar concentration of undiluted catalyst slurry is 5.0 \([mol/l]\).

2. Reaction II:
   (a) Reaction temperature is fixed and constant at 65°C.
   (b) Conversion of C \(\geq 0.98\).
   (c) Assume no volume change (use conservative estimate: the larger of the reactant volume or the product volume).
3. Reaction III:

(a) Feed ratio specification:
\[ \frac{N_{\text{H}_2\text{O},i}}{N_{\text{E},i}} \frac{[\text{mol}]}{[\text{mol}]} \geq 25 \]

(b) Reaction Temperature \( \leq 95^\circ\text{C} \)

(c) Assume no volume change (use conservative estimate).

(d) Assume mixture does not boil.

4. Distillations I and II:

(a) Lump components C, R2, I1, and R1 into R1. Use the properties of R1.

(b) Lump component I2 and catalyst into I2. Use the properties of I2.

(c) There is a maximum pot temperature of 140^\circ\text{C}. Exceeding this temperature allows unwanted byproduct reactions to be catalyzed. These reactions will rapidly degrade product A.

(d) An initial operating period of 0.5 hours is required at total reflux to bring the column trays to steady-state before distillate can be removed. At any later time it takes the column 0.25 hours to reach steady-state at total reflux (note that this transient is not modeled by the ABACUSS simulation).

(e) The pressure in the column may be reduced at a maximum rate of 0.4 mmHg/s. The time it takes to apply vacuum is included in the simulation time reported by ABACUSS.

(f) The second cut must be cooled before it can be transferred to reaction III. This cooling period will take 30 minutes.

(g) A minimum vacuum pressure of 5 mmHg may be applied to the column.

5. Distillation III:

(a) Do not model components that are not present in the charge to the pot, nor components that are only present in trace amounts. This will make the numerical solution much more robust.

(b) There is a purity specification on the product (A and D) from this distillation. The product should be at least 99% pure A and D on a mass basis.

(c) An initial operating period of 0.5 hours is required at total reflux to bring the column trays to steady-state before distillate can be removed. At any later time it takes the column 0.25 hours to reach steady-state at total reflux (note that this transient is not modeled by the ABACUSS simulation).

(d) The pressure in the column may be reduced at a maximum rate of 0.4 mmHg/s. The time it takes to apply vacuum is included in the simulation time reported by ABACUSS.

(e) A minimum vacuum pressure of 5 mmHg may be applied to the column.
(f) Use the Wilson model for the liquid phase fugacity and the ideal gas equation of state for the vapor phase fugacity. All necessary physical property parameters may be found in Memo #2. In fact, water and toluene are immiscible, but the Wilson model is incapable of predicting vapor-liquid-liquid equilibria. Neglect this inaccuracy in your model.

6. Additional Constraints and Assumptions:

(a) Transferring material between pieces of equipment will take 30 minutes. This should be taken into account when conducting the analysis of the simulation.

(b) Any density data that you require should be taken from the property file provided earlier or from standard references (e.g., Perry’s Chemical Engineers’ Handbook, CRC Handbook of Chemistry and Physics, etc.).

pib: August 30, 2005