

Memorandum

From: Jennifer Hsu and Kristie Stoneman

To: W. Green, Chief Technology Officer, *MegaBust Corporation*

G. Stephanopoulos, President, *OLED Inc.* (subsidiary of *MegaBust Corporation*)

Date: May 6, 2011

Re: Preliminary Process Design and Economic Assessment for the Production of Dyes for OLEDs

In response to your April 5, 2011 memorandum on “Establishing Business Opportunities in Dye-based OLEDs,” we have carried out a fairly detailed simulation of the dyes-producing batch process and an economic optimization of the overall process on an annual basis.

The principal results of our study can be summarized as follows:

- (a) Our company’s production facilities can accommodate the production of 20,776.05 kilograms of dyes per year.
- (b) The optimized production cost of dyes on an annual basis is \$ 9,729.92 per kilogram.
- (c) Assuming a selling price of \$20,000 per kilogram for the dyes, the net operating profit on an annual basis is estimated to be \$ 213,371,618.79. It corresponds to 51.35% return on sales and 105.55% return on the working capital (See Attachment-3).
- (d) The break-even price (where the profit is zero) for our dyes is in the range of \$9,600 and \$9,900 per kilogram (See Attachment-4).

We also carried out a series of economic sensitivity analyses to volatilities in materials prices and possible EPA waste treatment charges. The results are as follows:

1. There is significant volatility in the prices of specialty chemicals A and B that we use as the basic reagents. Specifically, these prices have been observed to vary as follows: Chemical A: From \$ 325 to \$675 per kilogram. Chemical B: From \$ 1,400 to \$2,600 per kilogram. In the worst case (where Chemical A costs \$675/kg and B costs \$2,600/kg), the Annual Operating Profit is \$187,452,994.92, the Return on Sales is 45.43%, the Return on Working Capital is 83.24%, and the new Break-Even price for our dyes is \$10,914.65 (See Attachment-5).
2. A competitor in the market for Reaction Solvent, S1, has recently filed for bankruptcy. The resulting surplus of S1 in the market is expected to drive the price from its current value of \$10 per kilogram to \$2.5 per kg. Lowering the price of S1 leads to an improvement of Annual Operating Profit by \$7,076,242.71, and increases the Return on Sales to 53.03% and the Return on Working Capital to 112.91%. The Break-Even price of our dyes is reduced by 3.46% (See Attachment-6).

3. EPA is considering of imposing tougher voluntary standards on vapor waste treatment. Research suggests that under current technology, implementation of these standards will lead to an additional charge of \$100 per kilogram of vapor wastes. This will reduce the Annual Operating Profit by \$2,386,624.52 and will decrease the Return on Sales to 50.76% and the Return on Working Capital to 103.08%. The Break-Even price of our dyes will be increased by 1.22% (See Attachment-7).
4. Within a few years the new EPA standards will become mandatory. However, anticipated improvements in our technology will allow us to recoup these charges, by charging \$4 per kilogram of liquid wastes, and \$1 per kilogram of vapor wastes. In such case the Annual Profit is expected to be reduced by \$12,362,721.06, the Return on Sales will decrease to 48.37%, and the Return on Working Capital to 93.67%. The Break-Even price of our dyes will be increased by 6.13% (See Attachment-8).
5. A patent infringement lawsuit has halted production of the extraction solvent, S2, for the foreseeable future. Though enough S2 is available from current inventories for several years' production, the manufacturer has raised the price of S2 to \$ 1,200 per kilogram. Under the new price, the Annual Profit for our dyes production is \$118,231,200.59, the Return on Sales will decrease to 28.46% and the Return on Working Capital decrease to 39.78%. The Break-Even price of our dyes will be increased by 47.05%.

The above results are fairly reliable and can be used as firm data in your discussions with OLED manufacturer.

More details on the batch process for the production of dyes and the associated operating conditions and economics can be found in the attached attachments, as follows:

- Attachment-1: Description of the batch process for the production of dyes.
- Attachment-2: Results of the simulation of the batch process for given nominal values of the optimization variables.
- Attachment-3: Results of the optimization of the batch process.
- Attachment-4: Results of the break-even point analysis.
- Attachment-5: Results of the economic sensitivity analysis to price volatility of A and B.
- Attachment-6: Results of the solvent, S1, price reduction
- Attachment-7: Results of the EPA additional charges on vapor waste treatment
- Attachment-8: Results of the analysis on the impact that the anticipated technological changes in the cost of liquid and vapor wastes treatment will have on the Annual Profit.
- Attachment-9: Results of the solvent, S2, price increase.
- Attachment-10: Further Analysis
- Attachment-11: MatLab files for the simulation and optimization of the batch process.

Attachment-1: Description of the batch process for the production of dyes.

The process for the manufacturing of the new dyes is shown in Figure 1. It is composed of the following batch operations:

- (a) Batch reactor for the chemical synthesis of the dyes.
- (b) Batch extractor for the recovery of the unreacted raw materials.
- (c) Batch distillation for the separation of the recovered raw materials from the extraction solvent.
- (d) Batch crystallizer for the recovery of high-purity dyes.
- (e) Batch dryer for the drying of the dye crystals.
- (f) The wastes of the process will be treated in our existing Waste Treatment unit.

Batch Reactor.

A liquid solution of the two primary reagents (raw materials), A and B, is loaded into the reactor vessel. The solvent of the solution is, S_1 .

The homogeneous catalyst, C, is then loaded into the reactor and the mixture is strongly stirred until perfect mixing of the catalyst in the reagents' solution is achieved.

The reactor vessel has the following features (Figure 2):

- It can handle material up to 2 m^3 volume per batch.
- An electric heater is available and can be used to heat the reaction mixture. The maximum power output of the electric heater is 500 KW.
- A cooling jacket surrounds the reacting vessel. Cooling water can flow through the jacket and can be used to cool the reacting mixture. The cooling system has a heat removal capacity of $20\text{ KW}/(\text{degree C})$.
- A stirrer is also available to stir the reacting mixture, operated by a 5 KW electric motor.
- It takes 3 hours for the turn around of the batch reactor, i.e. for the reacting mixture to be removed from the vessel, to cleaning of the vessel, and the charging of new raw materials and fresh catalyst.

The batch reactor is operated as follows:

- The raw materials, A and B, are first dissolved in Solvent, S_1 .
- The solution of the raw materials S_1 is loaded into the reactor vessel, and is fully mixed with the homogeneous catalyst, C. The initial temperature of the mixture is ambient of 25°Celsius .
- After the reagents and the catalyst have been fully mixed, the reacting mixture is heated for a certain period of time with the electric heater. [Note: The power output of the electric heater and the heating period are two optimization variables and have a significant effect on the production cost. They affect the temperature of the reacting mixture and the amount of dyes produced. These values are optimized so that they maximize the operating profit.]
- At the end of the reaction period, the content of the reactor is cooled back to the ambient temperature of 25°Celsius , using cooling water through the reactor's cooling jacket.
- The cooled reactor content is transferred to the extractor vessel.

- The reactor vessel is cleaned and is prepared for the next batch of dyes' production.

Figure 3 shows typical examples of the concentration and temperature profiles in the batch reactor over time.

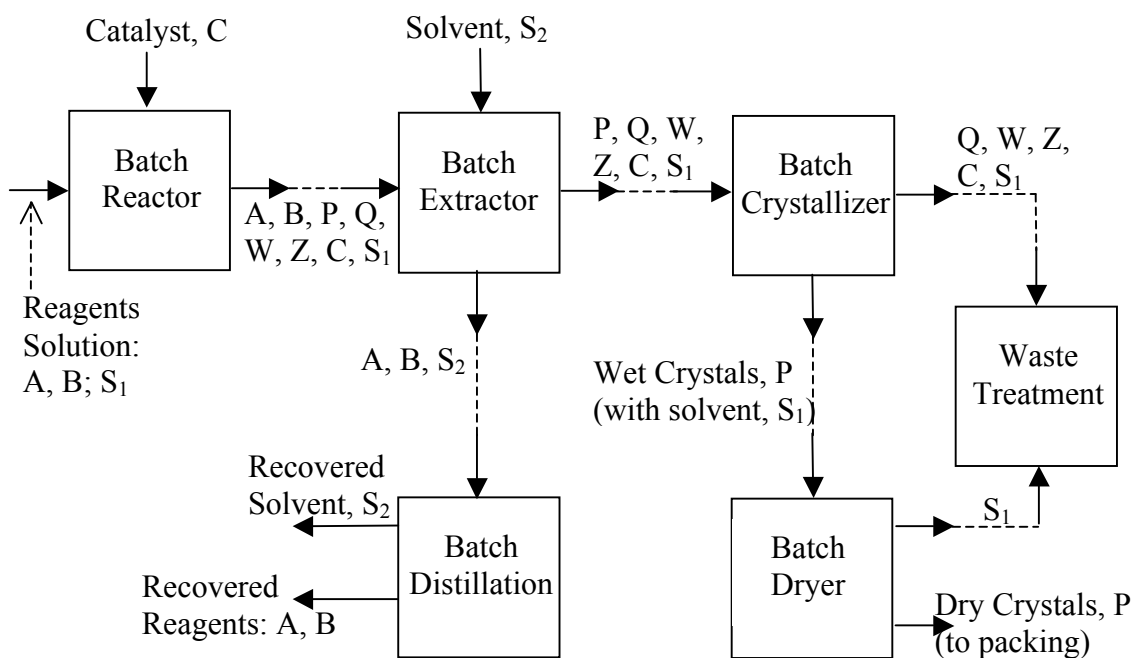


Figure 1. Process diagram for the manufacturing of dyes

Notes:

- Assume that the reagents, A and B, are liquid under normal conditions of temperature and pressure.
- Assume that the reagents, A and B, are mixed in a stoichiometric ratio, i.e. 1 to 2.
- Assume that when the liquid reagents, A and B, are dissolved in the Solvent S₁, the resulting volume of the liquid is equal to the sum of the three volumes. The volume of Solvent S₁, must be 10 times the combined volume of A and B.
- Assume that catalyst, C, is available in a liquid form and is fully dissolved in Solvent S₁. The volume of Catalyst, C, must be equal to the volume of A.
- As a result of the above notes,

$$\text{Total Volume of Reacting Mixture} = (\text{Volume of } S_1) + (\text{Volume of A}) + (\text{Volume of B}) + (\text{Volume of C}).$$
- The reaction starts as soon as you start the heating of the reacting mixture. The reaction rate is low at the beginning, but as the temperature increases, due to the heating with the electric heater and stirrer, the reaction rate increases. The reaction rate decreases after you start cooling the reacting mixture with cooling water.

- During the cooling with cooling water, the amount of heat transferred from the reacting mixture to the cooling water is given by:
Heat removed per unit of time = 20 KW/degree K.
- The cooling period is set to 2,000 seconds or the content of the reactor is cooled back to the ambient temperature of 25° Celsius.
- The cost of electricity for our plant is: 2.50 \$/KW-hr.
- The cost of cooling water is: 0.0001 \$/KJ of heat removed.

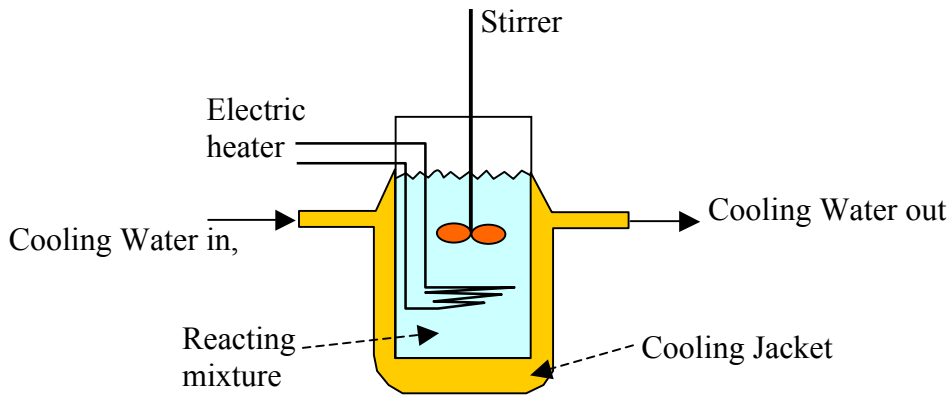


Figure 2. The Batch Reactor system

Batch Extractor

This is a simple vertical steel vessel (Figure 4), and it can handle batches of material with maximum initial volume of 6 m³. The batch extractor is operated as follows:

- The batch extractor vessel is loaded with the cooled content of the reactor vessel. Let's call this material *Phase-1*. It contains solvent, S₁, and the following materials which are dissolved in it: A, B, C, P (product), Q, and the two undesired by-products of the reaction, W and Z (see also below for the description of the chemical reactions).
- Solvent, S₂, is loaded into the extractor vessel. Solvent, S₂, is immiscible with solvent, S₁, and forms a separate liquid phase, which we will call, *Phase-2*.
- Raw materials, A and B, diffuse from Phase-1 to Phase-2 until they reach equilibrium conditions. The equilibrium constants are given below. When equilibrium conditions have been reached, no more A and B are transferred into Phase-2. The extraction solvent, S₂, is highly specific. Only A and B are transferred from Phase-1 to Phase-2 in appreciable amounts. We will assume that the amounts of C, P, Q, S₁, W and Z transferred from Phase-1 to Phase-2 are extremely small, i.e. zero for any practical considerations. [Note: The amount of solvent, S₂, used in the extractor, is an optimization variable. The more Solvent, S₂, we use the larger the amounts of A and B we can recover, but the larger the amount of solvent, S₂, we lose due to diffusion of S₂ in the solvent, S₁.]

- The two liquid phases, Phase-1 and Phase-2, are mechanically separated. Phase-2 is directed to a batch distillation, where the mixture, A and B, is separated from the solvent, S_2 . The recovered reagents are used in the subsequent batch reactions, while the recovered solvent, S_2 , is reused in a subsequent batch extraction.
- The modified Phase-1 is transferred to the batch crystallizer.

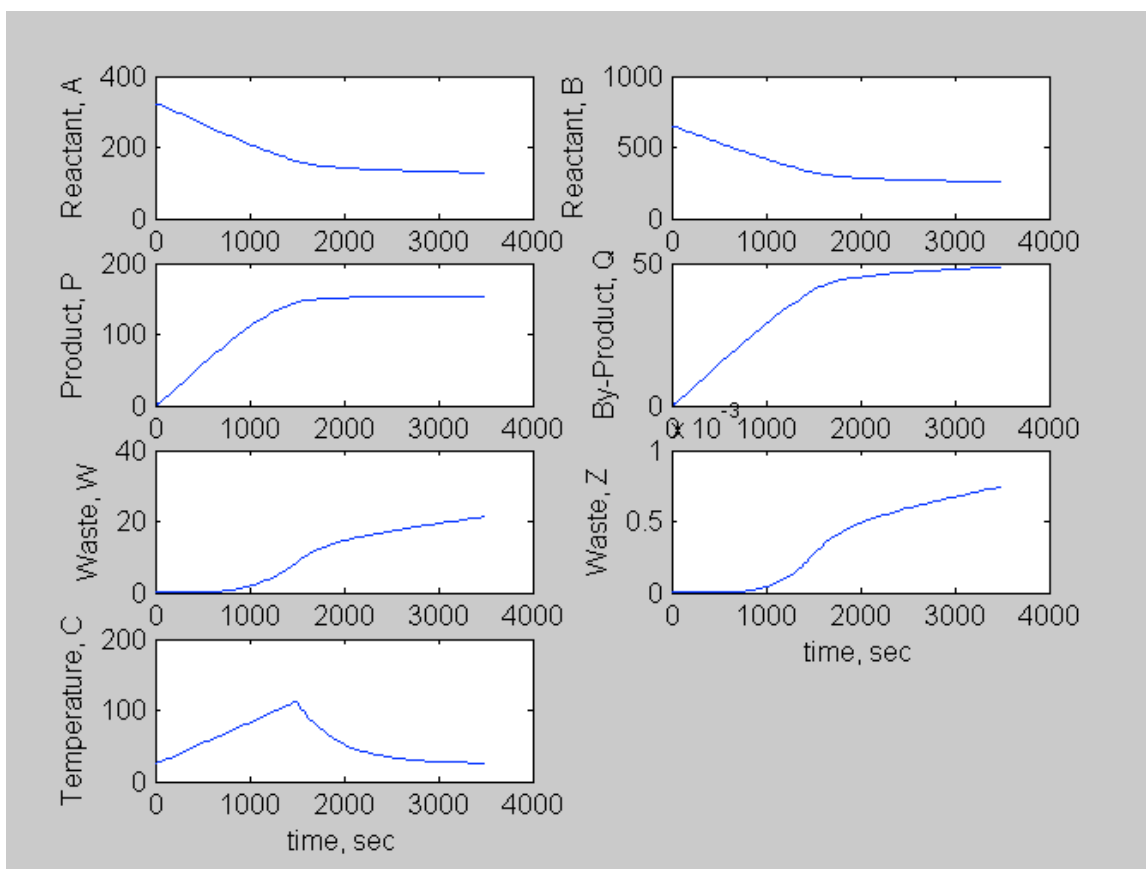


Figure 3. Typical profiles of chemicals (in moles) and temperature, over time, in the batch reactor

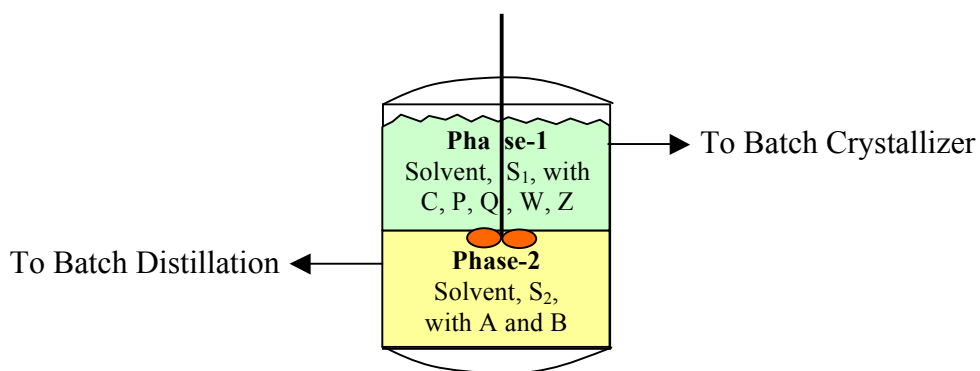


Figure 4. The Batch Extractor system

The equilibrium constants for A, B, and S₂ at 25° Celsius are given by the following relationships:

$$K_A = \frac{[A]_{Phase-2}}{[A]_{Phase-1}} = 10 \quad K_B = \frac{[B]_{Phase-2}}{[B]_{Phase-1}} = 8 \quad K_{S_2} = \frac{[S_2]_{Phase-2}}{[S_2]_{Phase-1}} = 10$$

Notes:

- Since no significant amounts of C, P, Q, W, Z, or S₁ are extracted into Phase-2, set the corresponding equilibrium constants to zero, i.e.
 $K_C = K_P = K_Q = K_W = K_Z = K_{S_1} = 0$.
- The turnaround time for the extractor is 2 hours.
- The extractor vessel is equipped with a 5 KW stirrer.

Batch Distillation

This unit is composed of the following elements (Figure 5):

- A spherical steel vessel, where the material to be separated is fed. It can handle up to 6 m³ of initial material load.
- A heat exchanger (reboiler), where the material is heated with steam to produce vapor.
- A heat exchanger (condenser), where the vapor is cooled to produced liquid enriched in the more volatile component.

Two liquid materials are produced from the operation of the batch distillation:

- The “overhead” or “distillate” product, which is 99 % by mole in A and B. We assume that all the amount of A and B is recovered through the “overhead” product.
- The “bottoms” or “residual” product, which is assumed to be pure solvent, S₂.

Notes:

- The period of batch distillation (seconds) is given by the equation,

$$\text{Distillation period} = (\text{Moles of A and B in the overhead}) * 18$$

- The heating required is equal to the total amount of heat needed to vaporize all the material that is collected in the distillate product, i.e.

Heating duty =

$$(\text{Moles}_{A_{\text{distillate}}}) * \Delta H_{\text{vap., A}} + (\text{Moles}_{B_{\text{distillate}}}) * \Delta H_{\text{vap., B}} + (\text{Moles}_{S_2_{\text{distillate}}}) * \Delta H_{\text{vap., S}_2}$$

- The turn around period for the batch distillation is 3 hours.
- The cooling duty in the condenser of the distillation is equal to the heating duty.
- The utilities costs are equal to:
 Heating: 0.03 \$/KJ of heat supplied.
 Cooling: 0.0001 \$/KJ of heat removed.

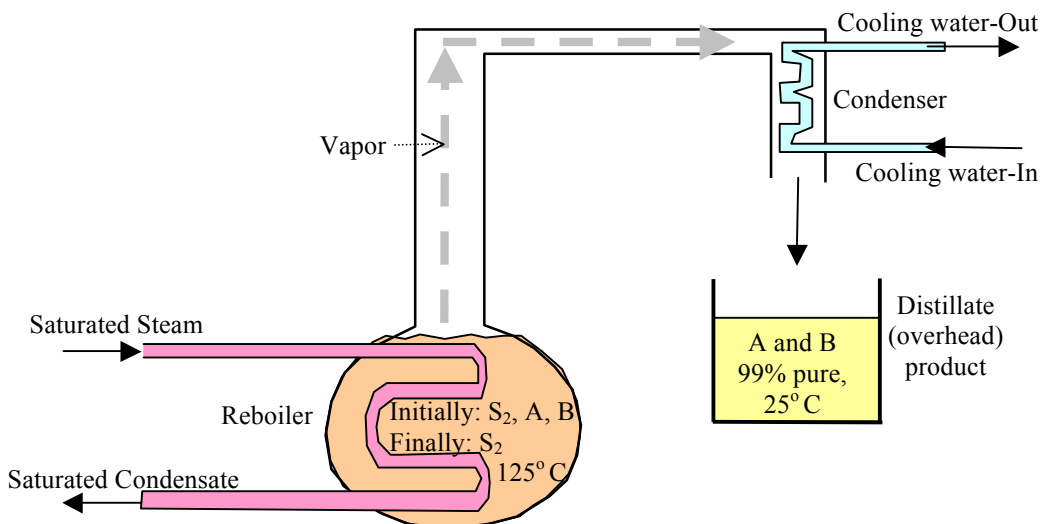


Figure 5. The Batch Distillation system

Batch Crystallizer

This is also a simple vertical steel vessel with a cooling jacket through which we can flow liquid refrigerant available at -20° Celsius (see Figure 6). The crystallizer can handle batches of material with maximum initial volume of 4 m³. The crystallizer is operated as follows:

- The material of Phase-1 is transferred from the batch extractor to the vessel of the batch crystallizer.
- Refrigerant is allowed to flow through the jacket and it cools the content of the vessel to -10° Celsius. At this temperature, crystals of the desired dyes (product, P) are formed, while all the other materials remain in solution. During crystallization the temperature of the liquid in the crystallizer remains at -10° C.
- When all the amount of product, P, has been crystallized, the crystals are separated from the liquid through a centrifuge.
- The crystals of P are “wet” crystals, i.e. they are coated with a thin liquid film, which has the same composition as the rest of the liquid in the crystallizer. The coating liquid is 10% by weight of the crystal weight. The composition of this coating liquid is the same as the composition of the liquid in the crystallizer.
- The “wet” crystals are sent to the batch dryer.
- The remaining liquid in the crystallizer contains, C, S₁, W, Z, S₂, and it is sent to the Waste Treatment unit.
- The turn around period for the crystallizer is 2 hours.
- The crystallizer is equipped with a stirrer, which is driven by a 3 KW motor.
- The cooling capacity of the refrigerant is, 10 KW.
- The cost of the refrigeration-based cooling is, 0.008 \$/KJ of heat removed. Notice that this is significantly higher than the cost of cooling with water.

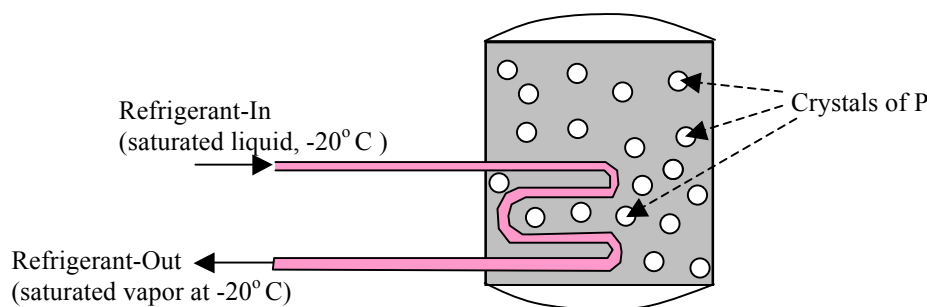


Figure 6. The Batch Crystallizer system

Batch Dryer

This unit contains a pulsing screen-bed through which hot air is passed. The hot air evaporates the liquid which is coating the crystals. The vapor is directed to the Waste Treatment unit. The dried crystals of our product, P, are sent to packaging.

- The dryer operates at a temperature which is 30° Celsius **higher** than the highest boiling point of a component in the liquid coating the crystals.
- The heating power of the dryer is 1.5 KW of heat supplied.
- The turn around period for the dryer is 2 hours.
- The cost of drying is, 0.10 \$/KJ of heat supplied.

Waste Treatment System

This system contains two distinct types of waste treatment: one for the treatment of vapors and another for the treatment of liquid wastes. The costs for each type of treatment are:

- 0.50 \$/Kg of vapor waste,
- 2.00 \$/Kg of liquid waste.

2. The Chemical Synthesis of Dyes

The two reagents, A and B, react in the presence of the homogeneous catalyst, C, to form the desired dye (P) according to the reaction,



The reaction is carried out in a solution of Solvent S₁, using a stoichiometric mixture of raw materials, A and B. By-product, Q, remains inert in all subsequent reactions.

Certain properties of the chemicals are given in Table 1, below.

Table 1. Properties of Chemicals

Chemical	Molecular Weight	Density (Kg/m ³)	Heat Capacity (KJ/Kg, °C)	Heat of Vaporization (KJ/mole)	Heat of Fusion (KJ/Kg)	Boiling Point (°K)
A	102	1030	4	300	-	453
B	163.5	720	2	50	-	450
P	459	1000	2	100	350	430
Q	133.5	1000	2	150	-	460
W	918	1000	2.5	200	-	470
Z	1377	1000	3	300	-	420
Catalyst, C	410	1010	2	100	-	450
Solvent, S ₁	76	1050	4.184	120	-	430
Solvent, S ₂	170	868	2	200	-	490

The rate of Reaction (1) is first-order in A and second-order in B, it has an Arrhenius activation energy, E_1 , and a pre-exponential constant, k_1 . Thus, the rate of production of P is given by the following kinetic expression. [Note: $[x]$ signifies the molar concentration of chemical, x, in moles per cubic cm]:

$$r_1 = \frac{dP}{dt} = k_1 \exp\left(\frac{-E_1}{RT}\right) [A][B]^2$$

Unfortunately, the following two reactions degrade product, P, and produce two undesired by-products, W and Z:



The kinetic rates for Reactions (2) and (3) are given by the following expressions:

$$r_2 = \frac{dW}{dt} = k_2 \exp\left(\frac{-E_2}{RT}\right) [P]^2$$

and

$$r_3 = \frac{dZ}{dt} = k_3 \exp\left(\frac{-E_3}{RT}\right) [P]^3$$

The pre-exponential coefficients and activation energies for the side-reactions are given in Table 2.

Table 2. Properties of the Reactions

Reaction	Pre-exponential Factor; k_i	Energy of Activation (KJ/mole); E_i	Heat of Reaction (KJ/mole)
Reaction (1)	Unknown (cm^3) ² /(second, (moles) ²)	unknown	30
Reaction (2)	1000 (cm^3)/(second, mole)	20	20
Reaction (3)	500 (cm^3) ² /(second, (moles) ²)	20	10

Unfortunately, the pre-exponential coefficient and activation energy for the main reaction (1) are not known and need to be estimated through a least-squares regression of experimental data.

Experimental Determination of Kinetic Parameters for the Main Reaction, Reaction-1.

Thirteen (13) experiments were carried out for the estimation of the pre-exponential factor, k_1 , and the activation energy, E_1 , of the main reaction, Reaction (1). Each experiment was carried out as follows:

A mixture of reagents A and B (dissolved in Solvent S_1 and mixed with catalyst, C) flows into a 10-liters vessel (Figure 7). The amounts of reagents (in moles) flowing into the reactor, per unit of time (one second), are known. The temperature in the reactor is kept constant at a desired value. The reacting material flows continuously out of the reactor and its composition is measured. It is assumed that the reacting mixture in the reactor is perfectly mixed, so the composition of the exit stream is the same as the composition of the reacting mixture in the reactor. Under such assumptions, the reactor is considered to be at steady-state. Table 3 lists the amounts (in moles) of A and B entering the reactor, and the amounts of A, and B, leaving the reactor, as well as the temperatures, for the thirteen (13) experiments.

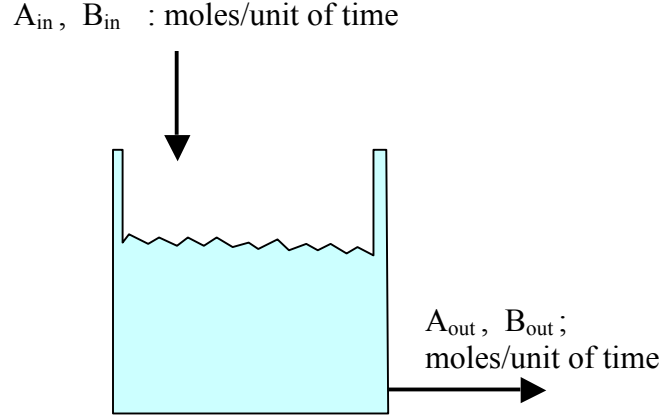


Figure 7. Experimental setup for the regression of the kinetic constants

For such reactor, the steady state material balance of reagent, A, is given by the following equation:

$$A_{in} - r_1^*(reactor\ volume) - A_{out} = 0$$

From the above equation, we can easily find that the experimental estimate (from experiment-i) of the reaction rate, r_1 , is given by the following expression:

$$r_{1,experiment-i} = (A_{in,experiment-i} - A_{out,experiment-i})/(reactor\ volume)$$

The model-based estimate of the rate was given above by the following equation:

$$r_{1,model} = k_1 \exp\left(\frac{-E_1}{RT}\right) [A][B]^2$$

The concentrations, $[A]$ and $[B]$, in the vessel can be approximated by the arithmetic mean of the entering and existing concentrations as follows:

$$[A] = [(A_{in,experiment-i} + A_{out,experiment-i})/2]/(reactor\ volume)$$

$$[B] = [(B_{in,experiment-i} + B_{out,experiment-i})/2]/(reactor\ volume)$$

Therefore, from each experiment we produce the following residual:

$$residual_{(experiment-i)} = r_{1,model} - r_{1,experiment-i}$$

Then, we can estimate the values of k_1 and E_1 by minimizing the sum of the squares of the thirteen (13) residuals.

Notes:

- MatLab has a special function, `lsqnonlin`, for non-linear least squares regression. When you use `lsqnonlin` it is very useful to provide a set of options in the arguments of the function, so that you can facilitate the minimization of the sum of the squares of the residuals. It is suggested that you call `lsqnonlin` as follows:
- The units of k_1 will be $[(\text{cm}^3)^2 / (\text{s}, (\text{mol})^2)]$ and the units of E_1 will be $[\text{J/mol}]$.

Table 3. Experimental Data for Reaction (1)

Experiment	Temperature (K)	A _{in} (moles/unit time)	B _{in} (moles/unit time)	A _{out} (moles/unit time)	B _{out} (moles/unit time)
1	300	10	20	9.30	18.60
2	310	10	20	9.21	18.42
3	320	10	20	9.12	18.24
4	330	10	20	9.03	18.06
5	340	10	20	8.93	17.86
6	350	10	20	8.83	17.66
7	360	10	20	8.72	17.44
8	370	10	20	8.63	17.26
9	380	10	20	8.53	17.06
10	390	10	20	8.42	16.84
11	400	10	20	8.33	16.66
12	410	10	20	8.23	16.46
13	420	10	20	8.13	16.26

3. Data for the Economic Analysis of the Dye-Manufacturing Process

The corporate overhead rate is, 50%, on all costs.

The annual production is based on 4,000 hours of operation.

The total operating cost, associated with the manufacturing of dyes, using the process of Figure 1, is given by the following relationships:

$$\begin{aligned}\text{Manufacturing cost per kilogram of P} &= \\ &= (\text{Total production cost}) / (\text{Amount of P in kilograms})\end{aligned}$$

$$\begin{aligned}\text{Total production cost} &= \\ &= (\text{Total cost of materials used}) + (\text{Total cost of utilities used}) \\ &+ (\text{Total "rental" cost of equipment engaged in production}) + (\text{Total cost of labor}) \\ &+ \text{Production overhead.}\end{aligned}$$

$$\text{Total cost of materials} =$$

$$= (\text{Cost of fresh reagents, A and B}) + (\text{Cost of solvent, } S_1, \text{ to create the solution of A and B for the reaction}) + (\text{Cost of Catalyst, C, used}) + (\text{Cost of fresh solvent, } S_2)$$

$$\begin{aligned} \text{Total cost of utilities used} &= \\ &= (\text{Cost of utilities used in reactor}) + (\text{Cost of refrigerant used in crystallizer}) \\ &+ (\text{Cost of utilities used in batch distillation}) + (\text{Cost of heating used in dryer}) \\ &+ (\text{Cost of waste treatment}). \end{aligned}$$

$$\begin{aligned} \text{Cost of utilities used in reactor} &= \\ &= (\text{Cost of electricity for heating the reacting mixture}) \\ &+ (\text{Cost of cooling the reacting mixture back to } 25^\circ \text{ Celsius}) \\ &+ (\text{Cost of electricity for operating the stirrer}). \end{aligned}$$

$$\text{Cost of utilities used in extractor} = \text{Cost of electricity to operate stirrer.}$$

$$\begin{aligned} \text{Cost of utilities used in batch distillation} &= \\ &= (\text{Cost of heating used in the reboiler}) + (\text{Cost of cooling used in condenser}) \end{aligned}$$

$$\begin{aligned} \text{Cost of utilities used in crystallizer} &= \\ &= (\text{Cost of refrigeration cooling}) + (\text{Cost of electricity to operate the stirrer}) \end{aligned}$$

$$\text{Cost of utilities used in dryer} = \text{Cost of heating}$$

$$\begin{aligned} \text{Cost of waste treatment} &= \\ &= (\text{Cost of treating the liquid from the crystallizer}) \\ &+ (\text{Cost of treating vapor from the batch dryer}) \end{aligned}$$

$$\text{Production overhead} = (0.50) (\text{Total production cost})$$

Table 5 shows the prices for all chemicals, utilities, and labor cost.

Table 5. Economic Data

	Price	Unit	Comments
Chemical			
A	500	\$/Kg	
B	2,000	\$/Kg	
P	20,000	\$/Kg	
Q	0	\$/Kg	
W	0	\$/Kg	
Z	0	\$/Kg	
Catalyst, C	1,000	\$/Kg	
Solvent, S_1	10	\$/Kg	
Solvent, S_2	30	\$/Kg	
Utility			

Electricity	2.50	\$/KW-hr	
Cooling Water	0.0001	\$/KJ	Cost per KJ of heat removed
Steam-based heating	0.03	\$/KJ	Cost per KJ of heat supplied
Refrigeration cooling	0.008	\$/KJ	Cost per KJ of heat removed
Dryer heating	0.10	\$/KJ	Cost per KJ of heat supplied
Waste Treatment-Liquid	2.00	\$/Kg	Cost per Kg of liquid treated
Waste Treatment-Vapor	0.50	\$/Kg	Cost per Kg of vapor treated
Other			
Labor	100	\$ per hour	Includes employee benefits
Equipment "Rental"			
Reactor	3,000	\$/hour of use	-----
Extractor	3,000	\$/hour of use	-----
Distillation	6,000	\$/hour of use	-----
Crystallizer	5,000	\$/hour of use	-----
Dryer	3,000	\$/hour of use	-----

Attachment-2: Results of the simulation of the batch process for given nominal values of the optimization variables.

A. Nominal Values of Optimization Variables:

- (a) Reactor Heater Power = 500 KW/hr;
- (b) Heating Period = 1500 sec;
- (c) Amount of S2 = 3.5 m³;

B. Estimation of Kinetic Parameters

The estimated kinetic parameter values are:

Pre-exponential factor = 2,422,200 cm⁶/mol²-sec

Activation energy = 12,100 J/mol

Performance of the least-squares function

Iteration	Func-count	f(x)	Norm of step	First-order optimality	CG-iterations
0	3	2.66496e-05		0.00112	
1	6	2.44469e-05	10	0.00108	0
2	9	1.93017e-05	20	0.00116	0
3	12	2.74028e-06	40	0.000948	0
4	15	2.36308e-07	29.6123	5.78e-05	0
5	18	2.36308e-07	60.2262	5.78e-05	0
6	21	1.73473e-07	15.0566	4.46e-05	0
7	24	1.1541e-07	30.1131	7e-05	0
8	27	5.36453e-08	30.1131	3.57e-05	0
9	30	2.83383e-08	37.8911	2.96e-05	0
10	33	9.97237e-09	23.5113	7.27e-06	0
11	36	7.54215e-09	17.4332	3.12e-06	0
12	39	7.25813e-09	4.5714	1.87e-07	0
13	42	7.25637e-09	0.557668	2.73e-09	0
14	45	7.25637e-09	0.0124485	1.33e-12	0
15	48	7.25637e-09	0.00019168	5.04e-14	0
16	51	7.25637e-09	4.38319e-06	3.18e-14	0
17	54	7.25637e-09	7.69497e-07	3.18e-14	0

Optimization terminated successfully:

C. TABLE OF PROCESS STREAMS PER BATCH OF PRODUCTION

Stream	A	B	P	Q	W	Z	C	S1	S2	Temp
Reactor										
Feed	323.4	646.8	0.0	0.0	0.0	0.0	78.9	24717.4	0.0	298.0
Effluent	67.3	134.7	174.7	64.0	40.7	0.0	78.9	24717.4	0.0	299.1
Extractor										
Fresh S2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	17870.6	298.0

S1 Phase	3.6	8.9	174.7	64.0	40.70	0.0	78.9	24717.4	958.9	301.9
S2 Phase	63.7	125.8	0.0	0.0	0.0	0.0	0.0	0.0	16911.7	301.9
Distillation										
Overhead	63.7	125.8	0.0	0.0	0.0	0.0	0.0	0.0	1.9	298.0
Bottoms	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	16909.8	458.0
Crystallizer										
Crystal,Sol	0.0	0.0	157.2	0.0	0.0	0.0	0.0	0.0	0.0	263.0
Crystal,Liq	0.0	0.0	0.1	0.2	0.1	0.0	0.3	83.7	3.2	263.0
Liquid	3.6	8.9	17.4	63.8	40.6	0.0	78.6	24633.6	955.6	263.0
Dryer										
Crystal	0.0	0.0	157.2	0.0	0.0	0.0	0.0	0.0	0.0	520.0
Vapor	0.0	0.0	0.1	0.2	0.1	0.0	0.3	83.7	3.2	520.0

D. NET UTILIZATION OF MATERIALS PER BATCH

Reagent, A (Kgs) = 26.49
 Reagent, B (Kgs) = 85.19
 Catalyst, C (Kgs) = 32.35
 Solvent, S1 (Kgs) = 1878.52
 Solvent, S2 (Kgs) = 163.33

E. AMOUNT OF PRODUCT

P, (Kilograms per Batch) = 72.15

F. TABLE OF PROCESS ECONOMICS PER BATCH

	Reactor	Extractor	Distillation	Crystall- ization	Dryer	Waste Treatment
MATERIALS COSTS PER BATCH (\$)						
A	16493.69	0.00	0.00	0.00	0.00	0.0000
B	211507.33	0.00	0.00	0.00	0.00	0.0000
C	32346.85	0.00	0.00	0.00	0.00	0.0000
S1	18785.20	0.00	0.00	0.00	0.00	0.0000
S2	0.00	91140.00	0.00	0.00	0.00	0.0000

 Total Materials Cost (\$ per batch) = **370,273.07**

UTILITIES COSTS PER BATCH (\$)

Electricity-Heat	520.83	0.00	0.00	0.00	520.83	0.00
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Electricity-Cool	12.15	44.57	0.00	106.93	12.15	44.57
Water Cooling	352.36	0.00	2.58	0.00	352.36	0.00
Steam Heating	0.00	0.00	774.66	0.00	0.00	0.00
Refrigerant Cooling	0.00	0.00	0.00	4106.19	0.00	0.00
Fuel Heating-Dryer	0.00	0.00	0.00	0.00	0.00	0.00
Waste Treatment	0.00	0.00	0.00	0.00	0.00	0.00

Total Utilities Cost (\$ per batch) = **33,478.25**

LABOR COSTS PER BATCH (\$)

Unit Labor Cost	397.22	356.57	394.75	1625.76	582.85	0.00
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Total Labor Cost (\$ per batch) = **3,357.15**

EQUIPMENT RENTAL COSTS PER BATCH (\$)

Vessel Rental Cost	11916.67	10697.10	23685.07	81287.94	17485.55	0.00
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Total Rental Costs (\$ per batch) = **145,072.33**

TOTAL OPERATING COST PER BATCH (\$) = 552,180.81

MATERIALS CREDITS PER BATCH (\$)

Recovered, A	0.00	0.00	3250.22	0.00	0.00	0.00
Recovered, B	0.00	0.00	41127.61	0.00	0.00	0.00
Recovered, S2	0.00	0.00	86240.06	0.00	0.00	0.00

TOTAL MATERIALS CREDITS PER BATCH (\$) = 130,617.89

NET OPERATING COST PER BATCH (\$) = 843,125.85

COST PER KILOGRAM, P (\$/Kg) = 11,685.51

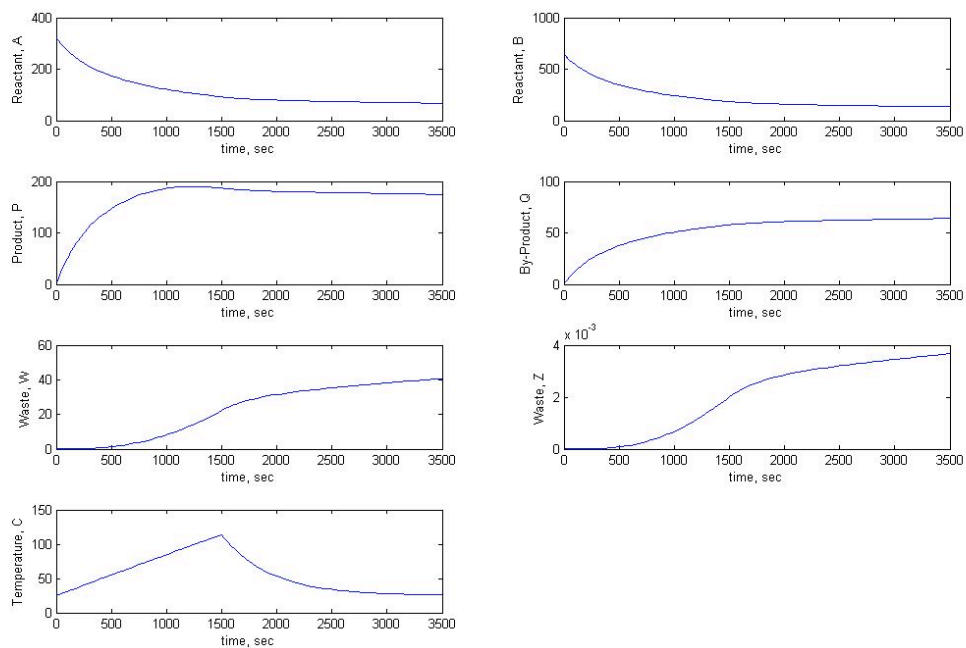
PROFIT PER KILOGRAM, P (\$/Kg) = 8,314.49

**G. SUMMARY OF PROCESS ECONOMICS ON AN ANNUAL BASIS (In \$ for a
4,000 hours Annual Operation)**

NUMBER OF BATCHES PER YEAR = 246.04
ANNUAL PRODUCTION OF P, Kgs = 17,752.05

MATERIALS COST (Net), \$ =	58,964,509.29
UTILITIES COST, \$ =	8,236,954.05
LABOR COST, \$ =	825,990.67
EQUIPMENT "RENTAL" COST =	35,693,444.82
NET OPERATING COST, \$ =	207,441,797.65
ANNUAL INCOME, \$ =	355,041,007.37
OPERATING PROFIT, \$ =	147,599,209.72

H. The Dynamic Response of the Batch Reactor.



Attachment-3: Results of the optimization of the batch process.

A. Nominal Values of Optimization Variables:

(a) Reactor Heater Power = 0.00 KW/hr;

(b) Heating Period = 934.66 sec;

(c) Amount of S2 = 3.98 m³;

B. Estimation of Kinetic Parameters

The estimated kinetic parameter values are:

Pre-exponential factor = 2,422,200 cm⁶/mol²-sec

Activation energy = 12,100, J/mol

Performance of the least-squares function

Iteration	Func-count	f(x)	Norm of step	First-order optimality	CG-iterations
0	3	2.66496e-05		0.00112	
1	6	2.44469e-05	10	0.00108	0
2	9	1.93017e-05	20	0.00116	0
3	12	2.74028e-06	40	0.000948	0
4	15	2.36308e-07	29.6123	5.78e-05	0
5	18	2.36308e-07	60.2262	5.78e-05	0
6	21	1.73473e-07	15.0566	4.46e-05	0
7	24	1.1541e-07	30.1131	7e-05	0
8	27	5.36453e-08	30.1131	3.57e-05	0
9	30	2.83383e-08	37.8911	2.96e-05	0
10	33	9.97237e-09	23.5113	7.27e-06	0
11	36	7.54215e-09	17.4332	3.12e-06	0
12	39	7.25813e-09	4.5714	1.87e-07	0
13	42	7.25637e-09	0.557668	2.73e-09	0
14	45	7.25637e-09	0.0124485	1.33e-12	0
15	48	7.25637e-09	0.00019168	5.04e-14	0
16	51	7.25637e-09	4.38319e-06	3.18e-14	0
17	54	7.25637e-09	7.69497e-07	3.18e-14	0

Optimization terminated successfully:

C. TABLE OF PROCESS STREAMS PER BATCH OF PRODUCTION

Stream	A	B	P	Q	W	Z	C	S1	S2	Temp
Reactor										
Feed	323.41	646.81	0.00	0.00	0.00	0.00	78.89	24717.37	0.00	298.0
Effluent	91.37	182.75	203.51	58.01	14.26	0.00	78.89	24717.37	0.00	298.3
Extractor										
Fresh S2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	20346.12	298.0

S1 Phase	4.34	10.72	203.51	58.01	14.26	0.00	78.89	24717.37	965.84	301.3
S2 Phase	87.04	172.03	0.00	0.00	0.00	0.00	0.00	0.00	19380.28	301.3
Distillation										
Overhead	87.04	172.03	0.00	0.00	0.00	0.00	0.00	0.00	2.62	298.0
Bottoms	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	19377.67	458.0
Crystallizer										
Crystal, Sol	0.00	0.00	183.16	0.00	0.00	0.00	0.00	0.00	0.00	263.0
Crystal, Liq	0.02	0.04	0.08	0.23	0.06	0.00	0.31	98.60	3.85	263.0
Liquid	4.32	10.67	20.27	57.78	14.20	0.00	78.58	24618.77	961.98	263.0
Dryer										
Crystal	0.00	0.00	183.16	0.00	0.00	0.00	0.00	0.00	0.00	520.0
Vapor	0.02	0.04	0.08	0.23	0.06	0.00	0.31	98.60	3.85	520.0

D. NET UTILIZATION OF MATERIALS PER BATCH

Reagent, A (Kgs) = 24.11
 Reagent, B (Kgs) = 77.63
 Catalyst, C (Kgs) = 32.35
 Solvent, S1 (Kgs) = 1878.52
 Solvent, S2 (Kgs) = 164.64

E. AMOUNT OF PRODUCT

P, (Kilograms per Batch) = 84.07

F. TABLE OF PROCESS ECONOMICS PER BATCH

	Reactor	Extractor	Distillation	Crystall- ization	Dryer	Waste Treatment
MATERIALS COSTS PER BATCH (\$)						
A	16493.69	0.00	0.00	0.00	0.00	0.00
B	211507.33	0.00	0.00	0.00	0.00	0.00
C	32346.85	0.00	0.00	0.00	0.00	0.00
S1	18785.20	0.00	0.00	0.00	0.00	0.00
S2	0.00	103765.22	0.00	0.00	0.00	0.00

 Total Materials Cost (\$ per batch) = **382,898.29**

UTILITIES COSTS PER BATCH (\$)

Electricity-Heat	0.00	0.00	0.00	0.00	0.00	0.00
Electricity-Cool	10.19	48.31	0.00	106.39	0.00	0.00
Water Cooling	3.47	0.00	3.52	0.00	0.00	0.00
Steam Heating	0.00	0.00	1058.17	0.00	0.00	0.00
Refrigerant Cooling	0.00	0.00	0.00	4085.46	0.00	0.00
Fuel Heating-Dryer	0.00	0.00	0.00	0.00	2421.68	0.00
Waste Treatment	0.00	0.00	0.00	0.00	0.00	4202.25

Total Utilities Cost (\$ per batch) = **32,950.72**

LABOR COSTS PER BATCH (\$)

Unit Labor Cost	381.52	386.50	429.53	1618.56	648.46	0.00
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Total Labor Cost (\$ per batch) = **3,464.57**

EQUIPMENT RENTAL COSTS PER BATCH (\$)

Vessel Rental Cost	11445.55	11595.06	25772.01	80928.08	19453.78	0.00
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Total Rental Costs (\$ per batch) = **149,194.48**

TOTAL OPERATING COST PER BATCH (\$) = 568,508.06

MATERIALS CREDITS PER BATCH (\$)

Recovered, A	0.00	0.00	4438.84	0.00	0.00	0.00
Recovered, B	0.00	0.00	56254.04	0.00	0.00	0.00
Recovered, S2	0.00	0.00	98826.10	0.00	0.00	0.00

TOTAL MATERIALS CREDITS PER BATCH (\$) = 159,518.99

NET OPERATING COST PER BATCH (\$) = 817,978.16

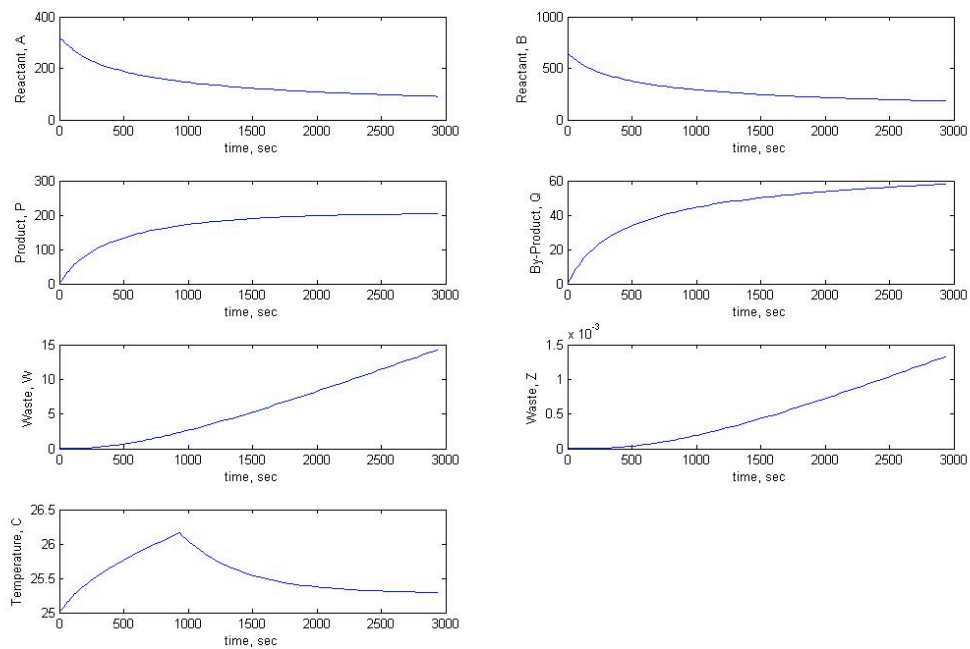
COST PER KILOGRAM, P (\$/Kg) = 9,729.92

PROFIT PER KILOGRAM, P (\$/Kg) = 10,270.08

G. SUMMARY OF PROCESS ECONOMICS ON AN ANNUAL BASIS (In \$ for a
4,000 hours Annual Operation)

NUMBER OF BATCHES PER YEAR =	247.13
ANNUAL PRODUCTION OF P, Kgs =	20,776.05
MATERIALS COST (Net), \$ =	55,204,400.68
UTILITIES COST, \$ =	8,143,210.54
LABOR COST, \$ =	856,210.80
EQUIPMENT "RENTAL" COST =	36,870,880.75
NET OPERATING COST, \$ =	202,149,405.56
ANNUAL INCOME, \$ =	415,521,024.34
OPERATING PROFIT, \$ =	213,371,618.79

H. The Dynamic Response of the Batch Reactor.



Attachment-4: Results of the Break-Even Analysis.

In the initial optimization scenario, the break-even price of the dyes is in the range of \$9,600/kg to \$9,900/kg. This allows penetration into the automobile displays, cellphones, and computer monitors markets. Our potential sales will be approximately \$2.2 billion. However, our production costs are still too high (by roughly \$4,700/kg) to enter the television market.

Even in the case where the volatility of prices in A and B bring costs to a minimum, the cost of producing the dyes is still in the range of \$8,400 to \$8,600. This suggests that we will not be able to break into the TVs market solely based on the volatility of material costs. Much further refinement of the production process will be necessary to penetrate that market.

In all of the scenarios analyzed, the highest breakthrough cost found is where the price of S2 increased to \$1,200. The breakthrough price increased to \$14,300, still low enough to penetrate into the automobile displays and cellphone markets. However, we will no longer be able to compete in the computer monitors market, where potential sales are valued at \$1 million.

Market	Potential Sales	Breakthrough Price (\$/kg)
Automobile Displays	\$500,000,000	\$18,000/kg
Cellphones	\$700,000,000	\$15,000/kg
Computer monitors	\$1,000,000,000	\$10,000/kg
TVs	\$5,000,000,000	\$5,000/kg

Scenario	Approximate Break-even Price (\$/kg)
Initial Simulation	\$11,685.51/kg
Initial Optimization	\$9,729.92/kg
Price of A = \$ 325.00 Price of B = \$ 1400.00	\$8,530.83/kg
Price of A = \$ 675.00 Price of B = \$ 2000.00	\$9,831.24/kg
Price of A = \$ 500.00 Price of B = \$ 2600.00	\$10,816.23/kg
Price of A = \$ 675.00 Price of B = \$ 2600.00	\$10,914.65/kg
Price of S1 = \$2.50	\$9,393.47/kg
Cost of vapor treatment = \$100.50	\$9,848.40/kg
Cost of liquid treatment = \$4.00 Cost of vapor treatment = \$1.00	\$10,326.73/kg
Price of S2 = \$1200.00	\$14,308.14/kg

Attachment-5: Results of the economic sensitivity analysis to the price volatility of chemicals A and B.

A. WORST CASE SCENARIO - A AND B AT HIGHEST COST

COST A (\$/Kg) = 675

COST B (\$/Kg) = 2600

NET OPERATING COST PER BATCH (\$) = 913,565.03

COST PER KILOGRAM, P (\$/Kg) = 10,914.65

PROFIT PER KILOGRAM, P (\$/Kg) = 9,085.35

SUMMARY OF PROCESS ECONOMICS ON AN ANNUAL BASIS (In \$ for a 4,000 hours Annual Operation)

NUMBER OF BATCHES PER YEAR = 246.50

ANNUAL PRODUCTION OF P, Kgs = 20,632.45

MATERIALS COST (Net), \$ = 66,710,575.29

UTILITIES COST, \$ = 8,145,868.60

LABOR COST, \$ = 855,553.31

EQUIPMENT "RENTAL" COST = 36,885,973.17

NET OPERATING COST, \$ = 225,195,940.72

ANNUAL INCOME, \$ = 412,648,935.64

OPERATING PROFIT, \$ = 187,452,994.92

**DECREASE IN ANNUAL PROFIT COMPARED TO INITIAL OPTIMIZATION,
\$ 25,918,623.87**

RETURN ON SALES, % = 45.43

RETURN ON WORKING CAPITAL, % = 83.24

BREAK-EVEN PRICE, \$ = 10,914.65

B. INCREASE IN A ONLY

COST A (\$) = 675

COST B (\$) = 2000

NET OPERATING COST PER BATCH (\$) = 823,696.97

COST PER KILOGRAM, P (\$/Kg) = 9,831.24

PROFIT PER KILOGRAM, P (\$/Kg) = 10,168.76

**SUMMARY OF PROCESS ECONOMICS ON AN ANNUAL BASIS (In \$ for a 4,000
hours Annual Operation)**

NUMBER OF BATCHES PER YEAR =	246.64
ANNUAL PRODUCTION OF P, Kgs =	20,664.43
MATERIALS COST (Net), \$ =	55,715,442.96
UTILITIES COST, \$ =	8,149,643.84
LABOR COST, \$ =	855,130.00
EQUIPMENT "RENTAL" COST =	36,858,319.55
NET OPERATING COST, \$ =	203,157,072.67
ANNUAL INCOME, \$ =	413,288,609.77
OPERATING PROFIT, \$ =	210,131,537.10

**DECREASE IN ANNUAL PROFIT COMPARED TO INITIAL OPTIMIZATION,
\$ 3,240,081.69**

C. INCREASE IN B ONLY

**COST A (\$) = 500
COST B (\$) = 2600**

NET OPERATING COST PER BATCH (\$) = 908,376.85

COST PER KILOGRAM, P (\$/Kg) = 10,816.23

PROFIT PER KILOGRAM, P (\$/Kg) = 9,183.77

RETURN ON SALES, % = 50.84

RETURN ON WORKING CAPITAL, % = 103.43

BREAK-EVEN PRICE, \$ = 9,831.24

**SUMMARY OF PROCESS ECONOMICS ON AN ANNUAL BASIS (In \$ for a 4,000
hours Annual Operation)**

NUMBER OF BATCHES PER YEAR =	247.01
ANNUAL PRODUCTION OF P, Kgs =	20,744.95
MATERIALS COST (Net), \$ =	66,296,706.84
UTILITIES COST, \$ =	8,142,837.82
LABOR COST, \$ =	856,422.73
EQUIPMENT "RENTAL" COST =	36,895,057.35

NET OPERATING COST, \$ =	224,382,049.49
ANNUAL INCOME, \$ =	414,898,938.94
OPERATING PROFIT, \$ =	190,516,889.45

DECREASE IN ANNUAL PROFIT COMPARED TO INITIAL OPTIMIZATION,
\$ 22,854,729.33

RETURN ON SALES, % = 45.92
RETURN ON WORKING CAPITAL, % = 84.91
BREAK-EVEN PRICE, \$ = 10,816.23

D. COMMENTS

From the above data, we can see that the cost of Reagent B has a much greater effect on the economics of the project than the cost of Reagent A. Increasing the cost of B by 30%, from 2000 \$/Kg to 2600 \$/Kg decreases the annual profit by 10%. On the other hand, increasing the cost of A from 500 to 675, a 35% increase, decreases annual profit by only 1.5%. In the worst case scenario, where both A and B have increased in cost, annual profit decreases by 12%.

Attachment-6: Results of the economic impact of Solvent, S1, price reduction.

A. ECONOMIC RESULTS

COST S1 (\$/Kg) = 2.5

NET OPERATING COST PER BATCH (\$) = 789,700.37

COST PER KILOGRAM, P (\$/Kg) = 9,393.47

PROFIT PER KILOGRAM, P (\$/Kg) = 10,606.53

**SUMMARY OF PROCESS ECONOMICS ON AN ANNUAL BASIS (In \$ for a 4,000
hours Annual Operation)**

NUMBER OF BATCHES PER YEAR =	247.23
ANNUAL PRODUCTION OF P, Kgs =	20,784.16
MATERIALS COST (Net), \$ =	51,743,306.99
UTILITIES COST, \$ =	8,145,918.92
LABOR COST, \$ =	856,217.97
EQUIPMENT "RENTAL" COST =	36,872,245.85
NET OPERATING COST, \$ =	195,235,379.47
ANNUAL INCOME, \$ =	415,683,240.97
OPERATING PROFIT, \$ =	220,447,861.50

**CHANGE IN ANNUAL PROFIT COMPARED TO INITIAL OPTIMIZATION,
INCREASE BY \$ 7,076,242.71**

RETURN ON SALES, % = 53.03

RETURN ON WORKING CAPITAL, % = 112.91

BREAK-EVEN PRICE, \$ = 9,393.47

B. COMMENTS

A decrease in solvent cost by 75% as a result of changes in the market will increase the annual profit by 3.3%.

Attachment-7: Results of the Economic Impact of the EPA Voluntary Standards on vapor waste treatment.

A. ECONOMIC RESULTS

VAPOR TREATMENT COST (\$/Kg) = 100.5

NET OPERATING COST PER BATCH (\$) = 827,932.17

COST PER KILOGRAM, P (\$/Kg) = 9,848.40

PROFIT PER KILOGRAM, P (\$/Kg) = 10,151.60

SUMMARY OF PROCESS ECONOMICS ON AN ANNUAL BASIS (In \$ for a 4,000 hours Annual Operation)

NUMBER OF BATCHES PER YEAR =	247.22
ANNUAL PRODUCTION OF P, Kgs =	20,783.43
MATERIALS COST (Net), \$ =	55,220,127.82
UTILITIES COST, \$ =	9,392,873.75
LABOR COST, \$ =	856,219.25
EQUIPMENT "RENTAL" COST =	36,872,567.14
NET OPERATING COST, \$ =	204,683,575.92
ANNUAL INCOME, \$ =	415,668,570.19
OPERATING PROFIT, \$ =	210,984,994.26

**CHANGE IN ANNUAL PROFIT COMPARED TO INITIAL OPTIMIZATION,
DECREASE BY \$ 2,386,624.52**

RETURN ON SALES, % = 50.76

RETURN ON WORKING CAPITAL, % = 103.08

BREAK-EVEN PRICE, \$ = 9,848.40

B. COMMENTS

By participating in the voluntary EPA program, the cost of vapor treatment increases from \$0.50 per Kg to \$100.50 per Kg. This decreases the annual profit by 1.1% and brings the break-even price to \$9,848.40.

Attachment-8: Results of the Economic Impact of the EPA Mandatory Standards on vapor waste treatment.

A. ECONOMIC RESULTS

VAPOR TREATMENT COST (\$/Kg) = 1.00

LIQUID TREATMENT COST (\$/Kg) = 4.00

NET OPERATING COST PER BATCH (\$) = 868,064.38

COST PER KILOGRAM, P (\$/Kg) = 10,326.73

PROFIT PER KILOGRAM, P (\$/Kg) = 9,673.27

SUMMARY OF PROCESS ECONOMICS ON AN ANNUAL BASIS (In \$ for a 4,000 hours Annual Operation)

NUMBER OF BATCHES PER YEAR =	247.20
ANNUAL PRODUCTION OF P, Kgs =	20,779.83
MATERIALS COST (Net), \$ =	55,184,515.69
UTILITIES COST, \$ =	14,378,340.83
LABOR COST, \$ =	856,234.04
EQUIPMENT "RENTAL" COST =	36,874,744.01
NET OPERATING COST, \$ =	214,587,669.13
ANNUAL INCOME, \$ =	415,596,566.86
OPERATING PROFIT, \$ =	201,008,897.72

**CHANGE IN ANNUAL PROFIT COMPARED TO INITIAL OPTIMIZATION,
DECREASE BY \$ 12,362,721.06**

RETURN ON SALES, % = 48.37

RETURN ON WORKING CAPITAL, % = 93.67

BREAK-EVEN PRICE, \$ = 10,326.73

B. COMMENTS

Once the EPA program becomes mandatory, the cost of vapor treatment in the long-term increases from \$0.50 per Kg to \$1.00 per Kg and the liquid treatment cost increases from \$2.00 to \$4.00 per Kg. This decreases the annual profit by 5.79%.

Attachment-9: Results of the Economic Impact of the solvent S2 price increase

A. ECONOMIC RESULTS

COST S2 (\$/Kg) = 1,200.00

NET OPERATING COST PER BATCH (\$) = 1,202,519.34

COST PER KILOGRAM, P (\$/Kg) = 14,308.14

PROFIT PER KILOGRAM, P (\$/Kg) = 5,691.86

**SUMMARY OF PROCESS ECONOMICS ON AN ANNUAL BASIS (In \$ for a 4,000
hours Annual Operation)**

NUMBER OF BATCHES PER YEAR =	247.15
ANNUAL PRODUCTION OF P, Kgs =	20,771.99
MATERIALS COST (Net), \$ =	102,722,710.09
UTILITIES COST, \$ =	8,144,856.51
LABOR COST, \$ =	856,294.78
EQUIPMENT "RENTAL" COST =	36,880,426.83
NET OPERATING COST, \$ =	297,208,576.43
ANNUAL INCOME, \$ =	415,439,777.03
OPERATING PROFIT, \$ =	118,231,200.59

**CHANGE IN ANNUAL PROFIT COMPARED TO INITIAL OPTIMIZATION,
DECREASE BY \$ 95,140,418.19**

RETURN ON SALES, % = 28.46

RETURN ON WORKING CAPITAL, % = 39.78

BREAK-EVEN PRICE, \$ = 14,308.14

B. COMMENTS

The increase in the cost per kg of S2 has dramatic effects on the profitability of the process, decreasing annual profit by 44.6%.

Attachment-10: Further Analysis

In the following attachment (Attachment-11), we have included an additional function, “Results_To_Excel.m”. This function should be run after the results of the simulation or optimization is complete. Its results will be printed to the file “data.xls”. Hopefully, this format will allow for easier reading. The results of our work have been attached electronically in the “Optimizations.xls” file in separate sheets.

In analyzing the process, we found the three parameters to be the most important in affecting the annual operating profit. We determined these through close examination of the most expensive costs.

First, reagent B has the highest cost per batch of all the materials used, even after some of it is recycled. Therefore, fluctuations in the prices of reagent B up to 20% will have dramatic effects on the cost of production and as a result, the profit. The following table shows that its cost is several times that of every other material used.

Material	Net Cost per Batch
Reagent A	\$12,054.85
Reagent B	\$155,253.29
Catalyst C	\$32,346.85
Solvent S1	\$18,785.20
Solvent S2	\$4,939.12

Secondly, in reviewing each of the units, we found that the crystallizer to be the most costly to rent at \$80,928.08 per batch. Thus, if variations on the rental cost will significantly impact our profits. Additionally, the crystallizer is also the time limiting step. The unit adds approximately 8.5 hours to the total process time per batch. Adding a second crystallizer to the process would allow us to nearly double the number of batches annually, while the cost per batch remains the same.

Time per Batch (hours)				
Reactor	Extractor	Distiller	Crystallizer	Dryer
3.74	12.06	4.35	20.64	6.47

Third, the rate of reactions used in these optimizations need to be calculated with a larger set of data. In the kinetics regression performed for the primary reaction, only 13 experiments were performed. Because this set of experimental data is small and several rough estimations were made, the accuracy of the calculated pre-exponential factor and activation energy should be brought into question. Furthermore, the rates for both side reactions were given to us from the reactions lab without experimental data so their validity should also be examined. As these reactions determine the amounts of each material we consume and produce, changes in these values will likely have dramatic effects on production costs.

In addition to the parameters discussed, we should reexamine the following assumptions:

The optimized value of the reactor heater output shows us that the reaction proceeds at room temperature. Therefore, the desired reaction will continue as long as the Reagents A and B are in contact, through the Extractor and Distiller units, and even more so when they are heated. Furthermore, the degradation of Product, P, into Waste Products, W and Z, will continue in all of the units following the reactor. This means that the values of P produced from the process are incorrect, as are the amounts of waste generated.

Although corporate overhead is 50% on all costs, we have assumed 100% overhead in our simulation. The additional 50% covers all additional costs that we haven't considered. This is a very conservative assumption that potentially has great effects on the amount of profit. If the true overhead value were less than this – let's assume 50% - the increase in profit would be very large, decreasing the break even price from \$9,729.92/kg to \$7,306.82/kg, pushing us even closer to penetrating the television market. Below are the values based on 50% overhead costs.

Annual Operating Profit, \$	264,093,270.10
Return on Sales, %	63.47
Return on Working Capital, %	173.72
Break-even Price, \$	7,306.816749

Attachment-11: MatLab files for the simulation and optimization of the batch process.

The MatLab functions used for the Simulation and Optimization of the batch process are as follows (for the code see attached files):

Project_10_10_Spring_2003; (function represents the top-level routine of the entire program.)

Set_Parameters; (sets the parametric values of the Project.)
MaterialsProperties; (sets properties of all materials)

ReactionsProperties; (sets properties of all reactions)
KineticsRegression; (regresses kinetic parameters of main reaction)

ProcessUnitsParameters; (sets properties of all batch unit operations)
EconomicData; (sets values of economic parameters)
ReactorFeed; (defines characteristics of reactor feed)

Simulator(X) ; (calls the various functions which simulate the batch units)
Reactor; (Simulate the Batch Reactor)
Reactions; (defines material and energy balances of batch reactor)
ReactorEvents;

Extractor; (Simulate the Batch Extractor)
Distillation; (Simulate the Batch Distillation)
Crystallizer; (Simulate the Batch Crystallizer)

Dryer; (Simulate the Batch Batch Dryer)
Waste_Treatment; (Compute economics of the Waste Treatment Unit)
F = Overall_Process_Economic_Objective(X) ; (Process Economics)

fminsearch(@Simulator,, options) ; (MatLab system function. No code given)

Results_Displayer; (organizes the display of the simulation or optimization results.)
TransientPlots; (plots the dynamic behavior of the batch reactor)

Results_To_Excel (Tabulates all of the results into an excel file for easy access.)

```

function Set_Parameters
%
% 10.10 Project. Spring 2011.
% Prepared by George Stephanopoulos.
%
% This function calls several other functions, which activate the
% assignment of values to the parameters associated with various
components
% of the project. Each of these other functions put the saved values in
the
% corresponding parameters of the project and makes them available to
% whatever function needs them through the appropriate GLOBAL
% characterization of the parameters.
%
% INPUT Global Variables. None.
% OUTPUT Global Variables. None.
%
% STEP-1(A): Set the Physical Properties values for all materials in
the
% project.
MaterialsProperties;
%
% STEP-1(B): Set the values for all properties of the three chemical
% reactions in the project.
%
ReactionsProperties;
%
% STEP-1(C): Set the values for the various characteristics of all the
% processing unites in the process of the project.
%
ProcessUnitsParameters;
%
% STEP-1(D): Set economic parameters
%
EconomicData;
%
% STEP-1(E): Set the characteristics of the feed to the reactor.
%
ReactorFeed;

global Materials_Properties
global Reactions_Properties
global ExtractorTurn
global Distillation_rental_cost_per_hour
global Reactor_feed

% To test if global variables are set:
% fprintf('Materials_Properties(2,2) = %d\n',
Materials_Properties(2,2));
% fprintf('Reactions_Properties(3,1) = %d\n',
Reactions_Properties(3,1));
% fprintf('ExtractorTurn = %d\n', ExtractorTurn);
% fprintf('Distillation_rental_cost_per_hour = %d\n',
Distillation_rental_cost_per_hour);
% fprintf('Reactor_feed(10) = %d\n', Reactor_feed(10));

end

```

```

function MaterialsProperties
%
% 10.10 Project. Spring 2011.
% Prepared by George Stephanopoulos.
%
% This function assigns the physical properties values of all the
% materials in the process, onto the elements of a matrix and makes the
% matrix available to all other functions as a GLOBAL variable.
%
% The name of the matrix is: Materials_Properties(i,j).
%   The first index signifies a material, i.e.
%       i = 1, signifies reagent, A
%       i = 2, signifies reagent, B
%       i = 3, signifies main product, P
%       i = 4, signifies by-product, Q
%       i = 5, signifies waste, W
%       i = 6, signifies waste, Z
%       i = 7, signifies catalyst, C
%       i = 8, signifies reaction solvent, S1
%       i = 9, signifies reaction solvent, S2
%   The second index signifies the specific property, i.e.
%       j = 1, molecular weight of the material
%       j = 2, density of the material, kg/m3
%       j = 3, heat capacity of the material, kJ/kg, C
%       j = 4, heat of vaporization of the material, kJ/mole
%       j = 5, heat of fusion of the material, kJ/kg
%       j = 6, boiling point, degrees Kelvin
%
% INPUT Global Variables. None.
% OUTPUT Global Variables
%
global Materials_Properties % This matrix contains the
physical properties of all materials in the process
%
% Assign property values for the various materials
%
%   Chemical, A
Materials_Properties(1,1) = 102;
Materials_Properties(1,2) = 1030;
Materials_Properties(1,3) = 4;
Materials_Properties(1,4) = 300;
Materials_Properties(1,6) = 453;
%
%   Chemical, B
Materials_Properties(2,1) = 163.5;
Materials_Properties(2,2) = 720;
Materials_Properties(2,3) = 2;
Materials_Properties(2,4) = 50;
Materials_Properties(2,6) = 450;
%
%   Product, P
Materials_Properties(3,1) = 459;
Materials_Properties(3,2) = 1000;
Materials_Properties(3,3) = 2;
Materials_Properties(3,4) = 100;
Materials_Properties(3,5) = 350;
Materials_Properties(3,6) = 430;
%

```

```

% By-product, Q
Materials_Properties(4,1) = 133.5;
Materials_Properties(4,2) = 1000;
Materials_Properties(4,3) = 2;
Materials_Properties(4,4) = 150;
Materials_Properties(4,6) = 460;
%
% Waste, W
Materials_Properties(5,1) = 918;
Materials_Properties(5,2) = 1000;
Materials_Properties(5,3) = 2.5;
Materials_Properties(5,4) = 200;
Materials_Properties(5,6) = 470;
%
% Waste, Z
Materials_Properties(6,1) = 1377;
Materials_Properties(6,2) = 1000;
Materials_Properties(6,3) = 3;
Materials_Properties(6,4) = 300;
Materials_Properties(6,6) = 420;
%
% Catalyst, C
Materials_Properties(7,1) = 410;
Materials_Properties(7,2) = 1010;
Materials_Properties(7,3) = 2;
Materials_Properties(7,4) = 100;
Materials_Properties(7,6) = 450;
%
% Reaction solvent, S1
Materials_Properties(8,1) = 76;
Materials_Properties(8,2) = 1050;
Materials_Properties(8,3) = 4.184;
Materials_Properties(8,4) = 120;
Materials_Properties(8,6) = 430;
%
% Extraction solvent, S2
Materials_Properties(9,1) = 170;
Materials_Properties(9,2) = 868;
Materials_Properties(9,3) = 2;
Materials_Properties(9,4) = 200;
Materials_Properties(9,6) = 490;

```

end

```

function ReactionsProperties
%
% 10.10 Project. Spring 2011.
% Prepared by George Stephanopoulos.
%
% This function assigns the values of various properties of the three
reactions,
% onto the elements of a matrix, and makes the matrix available to all
other
% functions as a GLOBAL variable.
%
% The name of the matrix is: Reactions_Properties(i,j).
%     The first index signifies the reaction, i.e.
%         i = 1, signifies the main reaction,  $A + 2B = P + (1/4)Q$ 
%         i = 2, signifies the first of the side reactions,  $2P = W$ 
%         i = 3, signifies the second of the side reactions,  $3P = Z$ 
%     The second index signifies the specific property value of the
corresponding
%     reaction, i.e.
%         j = 1, Pre-exponential factor;
%         j = 2, Activation Energy of the reaction; KJ/mol
%         j = 3, Heat of reaction; KJ/mol
%     INPUT Global variables. None
%     OUTPUT Global variables
%
global Reactions_Properties % This matrix
contains the properties of the three reactions in the process
%
Reactions_Properties = zeros(3,3);
% Assign property values for the various reactions
%
% Properties of the Main Reaction, Reaction 1
%
% Estimate kinetic paraters for Reaction-1 through regression
parameters = KineticsRegression; % Use the
"KineticsRegression" function to estimate the kinetic parameters
%
Reactions_Properties(1,1) = parameters(1,1); % Estimate of the
pre-exponential constant, in:  $(\text{cm}^3)^2/(\text{second}, (\text{moles})^2)$ 
Reactions_Properties(1,2) = parameters(1,2)/1000; % Estimate of the
activation energy, in KJ/mole
Reactions_Properties(1,3) = 30; % in KJ/moles
%
% Properties of the First Side-Reaction, Reaction-2
%
Reactions_Properties(2,1) = 1000; % in
 $(\text{cm}^3)^2/(\text{second}, (\text{moles})^2)$ 
Reactions_Properties(2,2) = 20; % in KJ/moles
Reactions_Properties(2,3) = 20; % in KJ/moles
%
% Properties of the Second Side-Reaction, Reaction-3
%
Reactions_Properties(3,1) = 500; % in
 $(\text{cm}^3)^2/(\text{second}, (\text{moles})^2)$ 
Reactions_Properties(3,2) = 20; % in KJ/moles
Reactions_Properties(3,3) = 10; % in KJ/moles

end

```

```

function [parameters] = KineticsRegression
%
% determines the Arrhenius paraters for A + 2B = P
% parameters(1) = Arrhenius pre-exponential factor A, in cm6/mole2-sec
% parameters(2) = E_act, in J/mol
%
% Prepared by George Stephanopoulos
% Modified by Jennifer Hsu
% Modified: 4/13/2011
%
% This function regresses a set of experimental data for Reaction(1)
(the
% main reaction) of the process and computes the Least Squares estimate
of
% the (a) Pre-Exponential factor, and (b) Activation Energy of the
% reaction.
%
% OUTPUT
%   Parameters = [Pre-exponential factor    Activation energy] for
%   Reaction-1
%
% Initial guesses
parameters_0(1) = 2000; % Initial guess of the pre-exponential factor
of the main reaction
parameters_0(2) = 12000; % Initial guess of the activation energy of
the main reaction
% Call the MatLab function that carries out Non-Linear Least Squares
% estimates
[parameters, resnorm] = lsqnonlin(@residuals, parameters_0, [1;2000],
[1e8; 40000], [optimset('Display','iter','TolFun', 1e-30)]);
end

```

```

function ProcessUnitsParameters
%
% 10.10 Project. Spring 2011.
% Prepared by George Stephanopoulos.
%
% This function sets the parametric values for the various processing
units
% in the process of the project. Makes these values available to other
% MATLAB functions through the command, GLOBAL.
%
% INPUT Global Variables
% OUTPUT Global Variables
global ReactorVolume ReactorStir ReactorCool ReactorTurn
ReactorCoolTemp TimeReactorCool
global ExtractorVolume ExtractorTurn ExtractorStir
global DistillationTurn DistillationVolume
global CrystallizerVolume CrystallizationStir CrystallizationTurn
CrystallizerCool
global DryerTurn DryerHeatingPower
%
% Set the parametric values for the Batch Reactor
%
ReactorVolume = 2;           % Reactor filling volume in cubic meters
(m3)
ReactorStir = 5;             % Reactor stirring power, KW
ReactorCool = 20;           % Reactor water cooling heat transter
coefficient, KW/(degree C)
ReactorTurn = 3;            % Reactor turn around time, hr
ReactorCoolTemp = 25;       % Temperature to which the reactor is to be
cooled at the end of the batch
TimeReactorCool = 2000;     % Time that the reactor cooling is on,
seconds
%
% Set the parametric values for the Batch Extractor
%
ExtractorVolume = 6;        % Extractor filling volume in cubic meters
(m3)
ExtractorTurn = 2;          % Extractor turn around time, in hours.
ExtractorStir = 5;          % Extractor stirring power, KW
%
% Set the parametric values for the Batch Distillation system
%
DistillationVolume = 6;     % Distillation volume in cubic maters (m3)
DistillationTurn = 3;       % Distillation turn around time, in hours
%
% Set the parametric values for the Batch Crystallizer
%
CrystallizerVolume = 4;     % Volume of the crystallization vessel, in
cubic meters (m3)
CrystallizationStir = 3;    % Crystallization vessel stirring power, KW
CrystallizationTurn = 2;    % Crystallizer's turn around time, in hours
CrystallizerCool = 10;     % Capacity of the refrigeration-based
cooling, KW
%
% Set the parametric values for the Batch Dryer
%
DryerTurn = 2;              % Dryer's turn around time, in hours
DryerHeatingPower = 1.5;    % Heating power of the dryer, in KW

```



```
%  
% No parameters for the waste treatment system  
%  
end
```

```

function EconomicData
%
% 10.10 Project. Spring 2011.
% Prepared by George Stephanopoulos.
%
% This function prepares the economic data and makes them available
through
% global variables to all the routines that use them.
%
% INPUT Global Variables
% OUTPUT Globla Variables
global Overhead Annual_operating_period
global Electricity_cost Water_cooling_cost Steam_heating_cost
Refrigeration_cooling_cost Dryer_heating_cost
global Liquid_waste_treatment_cost Vapor_waste_treatment_cost
global Labor_unit_cost
global Extractor_rental_cost_per_hour Reactor_rental_cost_per_hour
Distillation_rental_cost_per_hour
global Crystallizer_rental_cost_per_hour Dryer_rental_cost_per_hour
global Materials_Prices
%
%   Annual Operating Period
Annual_operating_period = 4000;           % Hours of operation per year
%
%   Overhead
Overhead = 0.5;                           % 50% overhead to the total
production cost
%
%   Labor Cost
Labor_unit_cost = 100;                    % In $ per hour, including
labor-associated overhead
%
%   Utilities
Water_cooling_cost = 0.0001;              % Cost of water cooling, $/kJ
of heat removed
Electricity_cost = 2.5;                    % Cost of electricity, %/kW-hr
(used for heating and the stirrer)
Dryer_heating_cost = 0.10;                 % $ per kJ of heat supplied
Steam_heating_cost = 0.03;                 % $ per kJ of heat supplied
Refrigeration_cooling_cost = 0.008;       % $ per kJ of heat removed
%
%   Vessel rental costs
Reactor_rental_cost_per_hour = 3000;      % Rental cost for the
reactor vessel, $ per hour of use
Extractor_rental_cost_per_hour = 3000;     % Rental cost for the
extractor vessel, $ per hour of use
Distillation_rental_cost_per_hour = 6000; % Rental cost for
crystallizer vessel, $ per hour of use
Crystallizer_rental_cost_per_hour = 5000; % Rental cost for the dryer
system, $ per hour of use
Dryer_rental_cost_per_hour = 3000;        % Rental cost for the
%
%   Materials prices
Materials_Prices(1) = 500;                 % price of reagent, A, $/kg
Materials_Prices(2) = 2000;                % price of reagent, B, $/kg
Materials_Prices(3) = 20000;               % price of the product, P,
$/kg
Materials_Prices(4) = 0;                   % price of the by-product,

```

```

Q, $/kg
Materials_Prices(5) = 0;           % price of waste, W, $/kg
Materials_Prices(6) = 0;           % price of waste, Z, $/kg
Materials_Prices(7) = 1000;        % price of catalyst, C,
$/kg
Materials_Prices(8) = 10;          % price of solvent, S1,
$/kg
Materials_Prices(9) = 30;          % price of solvent, S2,
$/kg
%
%   Waste treatment costs
Liquid_waste_treatment_cost = 2;   % $ per kilogram of liquid
waste
Vapor_waste_treatment_cost = 0.5;  % $ per kilogram of vapor
waste

end

```

```

function ReactorFeed
%
% 10.10 Project. Spring 2011.
% Prepared by George Stephanopolous.
% Transcribed by Kristie Stoneman.
%
% This function determines the composition and volume of the reacting
% mixture, before the reaction starts.
%
% INPUT Global Variables.
global Materials_Properties % Provided from the
"Materials_Properties" function
global ReactorVolume % Provided from the
"ProcessUnitsParameters" function
% OUTPUT Global Variables
global Reactor_feed % Describes the composition,
temperature, total mass, and volume of feed
%
% Basic assumptions:
% (a) Total Volume of Reactive Mixture = (Volume of Solvent,S1) +
(Volume of A) + (Volume of B) + (Volume of C).
% (b) (Volume of C) = (Volume of A)
% (c) (Volume of Solvent,S1) = 10*[(Volume of A) + (Volume of B)]
% (d) The molar amounts of A and B in the mixture are in their
stoichiometric ratio.
% (e) Total Volume of Reacting Mixture = Capacity of the reactor
vessel.
% This requirement will maximize the amount of the desired
product per batch.
%
% Compute the amounts of the required A, B, C, and Solvent-S1.
%
total_volume_of_reacting_mixture = ReactorVolume; % This satisfies
requirement (e), above.
%
% Note: Requirement (d), above, implies the following
relationship
% between volume_A and volume_B:
%  $(\text{volume\_B}/\text{volume\_A}) = 2 \cdot (\text{MW\_B}/\text{MW\_A}) \cdot (\text{density\_A}/\text{density\_B})$ 
%
a =
2*(Materials_Properties(2,1)/Materials_Properties(1,1))*(Materials_Prop
erties(1,2)/Materials_Properties(2,2));
volume_A = (total_volume_of_reacting_mixture)/(12+11*a);
volume_B = volume_A*a;
volume_C = volume_A;
volume_S1 = 10*(volume_A + volume_B);
%
% Compute the amounts (in kilograms and moles) of all the materials
in the
% reactor feed.
%
Reactor_feed_kilograms(1) = volume_A*Materials_Properties(1,2); %
Reactor feed: Amount of A in kilograms.
Reactor_feed_kilograms(2) = volume_B*Materials_Properties(2,2); %
Reactor feed: Amount of B in kilograms.
Reactor_feed_kilograms(7) = volume_C*Materials_Properties(7,2); %
Reactor feed: Amount of C in kilograms.

```

```

Reactor_feed_kilograms(8) = volume_S1*Materials_Properties(8,2);      %
Reactor_feed: Amount of S1 in kilograms.
%
Reactor_feed(1) =
1000*Reactor_feed_kilograms(1)/Materials_Properties(1,1); % Reactor
feed: Amount of A in g-moles.
Reactor_feed(2) =
1000*Reactor_feed_kilograms(2)/Materials_Properties(2,1); % Reactor
feed: Amount of B in g-moles.
Reactor_feed(7) =
1000*Reactor_feed_kilograms(7)/Materials_Properties(7,1); % Reactor
feed: Amount of C in g-moles.
Reactor_feed(8) =
1000*Reactor_feed_kilograms(8)/Materials_Properties(8,1); % Reactor
feed: Amount of S1 in g-moles.
%
%   Add the following for vector consistency, despite the fact that the
%   Reactor Feed does not contain the chemicals, P,Q,W,Z, and Solvent
S2.
%
Reactor_feed_kilograms(3) = 0;      % Reactor feed: Amount of P in
kilograms.
Reactor_feed_kilograms(4) = 0;      % Reactor feed: Amount of Q in
kilograms.
Reactor_feed_kilograms(5) = 0;      % Reactor feed: Amount of W in
kilograms.
Reactor_feed_kilograms(6) = 0;      % Reactor feed: Amount of Z in
kilograms.
Reactor_feed_kilograms(9) = 0;      % Reactor feed: Amount of Solvent,
S2, in kilograms.
Reactor_feed(3) = 0;      % Reactor feed: Amount of P in g-moles.
Reactor_feed(4) = 0;      % Reactor feed: Amount of Q in g-moles.
Reactor_feed(5) = 0;      % Reactor feed: Amount of W in g-moles.
Reactor_feed(6) = 0;      % Reactor feed: Amount of Z in g-moles.
Reactor_feed(9) = 0;      % Reactor feed: Amount of Solvent, S2, in
g-moles.
%
%   Set the temperature, total kilograms, and total volume of the
reactor
%   feed.
Reactor_feed(10) = 298;      % in degrees, K.
Reactor_feed(11) = sum(Reactor_feed_kilograms); % The total mass of
reactor feed in kilograms.
Reactor_feed(12) = total_volume_of_reacting_mixture; % In cubic meters
(m3).

%
end

```

```

function F = Simulator(X)
%
% 10.10 Project. Spring 2011.
% Prepared by George Stephanopoulos.
% Transcribed by Kristie Stoneman
% Updated by: Jennifer Hsu, 04/28/2011
%
% This function directs the sequential simulation of the processing
units
% in the process.
%
% INPUT:
%     X ---- Vector of Optimization Variables
%           X(1) = ReactorHeater
%           X(2) = ReactionHeatingPeriod
%           X(3) = AmountSolvent_S2
% OUTPUT: Global Variable
global ReactorHeater ReactionHeatingPeriod AmountSolvent_S2
% OUTPUT:
%     F ---- The value of the Net Operating Profit
%
ReactorHeater = X(1);
ReactionHeatingPeriod = X(2);
AmountSolvent_S2 = X(3);
%
%..... STEP-2(A)-1: Simulate Batch Reactor
Reactor;
%
%..... STEP-2(A)-2: Simulate the Batch Extractor
Extractor;
%
%..... STEP-2(A)-3: Simulate the Batch Distillation
Distillation;
%
%..... STEP-2(A)-4: Simulate the Batch Crystallizer
Crystallizer;
%
%..... STEP-2(A)-5: Simulate the Batch Dryer
Dryer;
%
%..... STEP-2(A)-6: Simulate the Waste Treatment Unit
Waste_Treatment;
%
%..... STEP-2(A)-7: Compute Process Economics
F = Overall_Process_Economic_Objective(X);
%
end

```

```

function Reactor
%
% 10.10 Project. Spring 2011.
%
% Prepared by George Stephanopoulos
% Updated by: Kristie Stoneman, 04/08/2011
% Updated by: Jennifer Hsu, 04/20/2011
%
% This function simulates the performance of the Batch Reactor and
computes
% its associated economics. It is called by the function "Simulator.m".
%
% INPUT Global Variables
global ReactionHeatingPeriod ReactorHeater
global Reactor_feed
global TimeReactorCool ReactorCoolTemp ReactorTurn ReactorCool
ReactorStir
global Reactor_rental_cost_per_hour Electricity_cost Water_cooling_cost
global Labor_unit_cost
global Materials_Prices
global Materials_Properties
%
% OUTPUT Global Variables
%
global ReactorTimeVector Reactor_dynamics Reactor_effluent
global Materials_Costs Utilities_Costs Vessel_Rental_Costs Labor_Costs
Material_Credits
global Vessel_Occupancy
%
% Set initial reactor parameters
%
X = ReactionHeatingPeriod;           % Sets the value of the reactor
heating period
% Y = [molesA, molesB, molesP, moles Q, molesW, molesZ, molesC,
molesS1, molesS2, T_Reactor, total kg/moles(?), total volume]
Y0 = Reactor_feed;                   % Sets the initial conditions to be equal
to the conditions of the Reactor Feed
P = [1; -1];                         % The P(1)>0, P(2)<0 imply that heating is
ON and cooling is OFF for the integrator
TimeSpanHeat = [0 X];                % Set range of integration from 0 until the
heater is turned off
%
% Period-1 of integration
% Solve dynamic balance equations for the Bath Reactor (see equations
in
% file, Reactions.m) keeping the reactor heater ON and the reactor
cooler
% OFF.
%
[TimeVecHeat Y1] = ode45(@Reactions,TimeSpanHeat,Y0,[],P); % integrate
%
% Turn off the heater and turn on the cooler
P = [-1; 1];                         % The P(1)<0, P(2)>0 imply that heating is
OFF and cooling is ON for the integrator
%
% Period-2 of integration
% Solve dynamic balance equations for the Batch Reactor (see equations
in

```

```

% file, Reactions.m) keeping the reactor heater OFF and the reactor
cooler
% ON.
%
% Set the start and the end time-points of cooling
TimeVecHeatLength = length(TimeVecHeat); % Determine the length of the
time vector
TimeSpanCool = [X X+TimeReactorCool]; % Set the start and stop times
of the cooling
% Set the initial conditions for the Period-2 to be the same as the
final
% conditions of Period 1:
Y0 = Y1(TimeVecHeatLength,:);
Y0 = Y0';
% Set conditions for ending integration when the temperature of the
% reactor's content has reached ReactorCoolTemp
OPTIONS = odeset('Events',@ReactorEvents); % set for events to stop at
ReactorCoolTemp
%
[TimeVecCool Y2] = ode45(@Reactions,TimeSpanCool,Y0,OPTIONS,P); %
Integrate and use OPTIONS to stop integration
%
% Collate the solutions of integration in Period-1 and Period-2
ReactorTimeVector = [TimeVecHeat; TimeVecCool]; % Form a single time
vector of reactor heating and cooling
Y = [Y1; Y2]; % Form a single Y vector containing the molar amounts at
times corresponding to tvec vector
%
% Assign values to the vector, ReactorEffluent. These values will
become
% available to other processing units, e.g. Batch Extractor, through a
% GLOBAL assignment.
%
TimeVecCoolLength = length(TimeVecCool); % Determine the length of the
time vector from the integration
k = length(ReactorTimeVector);
% !!!!
% plot(ReactorTimeVector, Y(:,10));
%
% Put the results of the dynamic simulation of the batch reactor into
one
% variable, "reactor_effluent" and make it globally available.
Reactor_dynamics = Y;
Reactor_effluent = Reactor_dynamics(k,:);
%
% Compute the Economics of the Reactor per batch.
%
reaction_period = ReactorTimeVector(k)/3600;
% in hours
reactor_rental_cost =
(reaction_period+ReactorTurn)*Reactor_rental_cost_per_hour; % in $
amount_of_heat_used = TimeVecHeat(length(TimeVecHeat))*ReactorHeater;
% in KW
reactor_heating_cost = amount_of_heat_used/3600*Electricity_cost; % in
$
amount_of_cooling_used = (ReactorCool*(Y1(TimeVecHeatLength,10) -
Y2(TimeVecCoolLength,10)))*TimeReactorCool; % in KJ
reactor_cooling_cost = Water_cooling_cost*amount_of_cooling_used;

```



```

% in $
reactor_stirrer_electricity_cost =
ReactorTimeVector(k)/3600*ReactorStir*Electricity_cost;           % in
$
%
% Materials Cost, in $
reagent_materials_cost_A =
Reactor_feed(1)*Materials_Prices(1)/1000*Materials_Properties(1,1);
reagent_materials_cost_B =
Reactor_feed(2)*Materials_Prices(2)/1000*Materials_Properties(2,1);
catalyst_cost_C =
Reactor_feed(7)*Materials_Prices(7)/1000*Materials_Properties(7,1);
solvent_cost_S1 =
Reactor_feed(8)*Materials_Prices(8)/1000*Materials_Properties(8,1);
%
product_value_from_P =
Reactor_effluent(3)*(Materials_Properties(3,1)/1000)*Materials_Prices(3
);
product_value_from_Q =
Reactor_effluent(4)*(Materials_Properties(4,1)/1000)*Materials_Prices(4
);
product_value_from_W =
Reactor_effluent(5)*(Materials_Properties(5,1)/1000)*Materials_Prices(5
);
product_value_from_Z =
Reactor_effluent(6)*(Materials_Properties(6,1)/1000)*Materials_Prices(6
);
%
% Labor Cost
reactor_labor_cost = Labor_unit_cost*(reaction_period + ReactorTurn); %
in $
%
% SUMMARY OF REACTOR ECONOMICS
%
Materials_Costs(1,1) = reagent_materials_cost_A;
Materials_Costs(1,2) = reagent_materials_cost_B;
Materials_Costs(1,3) = catalyst_cost_C;
Materials_Costs(1,4) = solvent_cost_S1;
Materials_Costs(1,5) = 0; % Cost of Solvent S2 (zero, because it is not
present)
Utilities_Costs(1,1) = reactor_heating_cost;
Utilities_Costs(1,2) = reactor_stirrer_electricity_cost;
Utilities_Costs(1,3) = reactor_cooling_cost;
Utilities_Costs(1,(4:7)) = 0; % No steam heating, refrigeration
cooling, fuel heating, or waste treatment
Vessel_Rental_Costs(1) = reactor_rental_cost;
Labor_Costs(1) = reactor_labor_cost;
Material_Credits(1,(1:5)) = 0;
Vessel_Occupancy(1) = reaction_period + ReactorTurn; % Total occupancy
time of the reactor vessel, per batch

end

```

```

function dYdt = Reactions(t,Y,P)
%
%
% Prepared by George Stephanopoulos
%
% This function provides the values of the derivatives of the batch
reactor
% mass and energy balances. It is called by the MATLAB Integration
routine,
% ode45.m, from the function, Reactor.m
%
% INPUTS
% Y -- [molesA, molesB, molesP, molesQ, molesW, molesC, molesS1,
molesS2,
%       T_Reactor, total moles, total volume]
% P -- [heat_on, cooling_on]
%       If heat_on > 0, then the reactor heater is on.
%       If cooling_on > 0. then the reactor cooler is on.
% INPUT Global Variables
global Materials_Properties           % This matrix contains the
physical properties of all materials in the process
global Reactions_Properties           % This matrix contains the
properties of the three reactions in the process
global Reactor_feed                   % Characteristics of the
reactor feed
global ReactorVolume ReactorCool ReactorCoolTemp ReactorStir
ReactorHeater
%
% OUTPUTS
% dYdt -- Vector of derivatives of moles of species and temperature
in
%       the reactor
% OUTPUT Global Variables
%       None
%
% Assign Reaction properties to Local Variables
Reaction1PreExp = Reactions_Properties(1,1);
Reaction1Eact = Reactions_Properties(1,2);
HeatRxn1 = Reactions_Properties(1,3);
Reaction2PreExp = Reactions_Properties(2,1);
Reaction2Eact = Reactions_Properties(2,2);
HeatRxn2 = Reactions_Properties(2,3);
Reaction3PreExp = Reactions_Properties(3,1);
Reaction3Eact = Reactions_Properties(3,2);
HeatRxn3 = Reactions_Properties(3,3);

dYdt = zeros(12,1); % Zero vector for integration
%
% Set Concentration for each chemical species
conc_A = Y(1)/(ReactorVolume*1000000); % moles of A/cm3
conc_B = Y(2)/(ReactorVolume*1000000); % moles of B/cm3
conc_P = Y(3)/(ReactorVolume*1000000); % moles of P/cm3
conc_Q = Y(4)/(ReactorVolume*1000000); % moles of Q/cm3
conc_W = Y(5)/(ReactorVolume*1000000); % moles of W/cm3
conc_Z = Y(6)/(ReactorVolume*1000000); % moles of Z/cm3
conc_C = Reactor_feed(7); % moles/cm3 of Catalyst C; This stays
constant.
conc_S1 = Reactor_feed(8); % moles/cm3 of Solvent, S1; This stays

```

```

constant.
conc_S2 = 0; % moles/cm3 of Solvent, S2;
This is not present
T = Y(10); % Set temperature
%
H(1) = HeatRxn1; % Set the vector containing the
heats of the three reactions
H(2) = HeatRxn2;
H(3) = HeatRxn3;
H = H';
%
rate = zeros(1,3); % Zero differentials
%
% As rate(i) we signify the total production rate of a product by
% reaction-i, e.g. (rate of reaction-i)*(reactor volume)
rate(1) = Reaction1PreExp*exp(-
Reaction1Eact/(0.008314*T))*conc_A*(conc_B^2)*ReactorVolume*1000000;
% Compute total rate of reaction 1
rate(2) = Reaction2PreExp*exp(-
Reaction2Eact/(0.008314*T))*(conc_P^2)*ReactorVolume*1000000; %
Compute total rate of reaction 2
rate(3) = Reaction2PreExp*exp(-
Reaction2Eact/(0.008314*T))*(conc_P^3)*ReactorVolume*1000000; %
Compute total rate of reaction 3
% Formulate the Material Balances for the Batch reactor
dYdt(1) = -rate(1); % change in moles/cm3 of A
dYdt(2) = -2*rate(1); % change in moles/cm3 of B
dYdt(3) = rate(1)-2*rate(2)-3*rate(3); % change in moles/cm3 of P
dYdt(4) = rate(1)/4; % change in moles/cm3 of Q
dYdt(5) = rate(2); % change in moles/cm3 of W
dYdt(6) = rate(3); % change in moles/cm3 of Z
dYdt(7) = 0; % change in moles/cm3 of
Catalyst, C; this stays constant
dYdt(8) = 0; % change in moles/cm3 of
Solvent, S1; this stays constant
dYdt(9) = 0; % change in moles/cm3 of
Solvent, S2; S2 is not present
dYdt(11) = 0; % there is no change in the
total mass, i.e. kilograms, of the reacting mixture.
component_mass = dYdt(1:9).*Materials_Properties((1:9),1)/1e3; % in
kilograms
component_volume = component_mass./Materials_Properties((1:9),2); % in
m3.
dYdt(12) = sum(component_volume(1:9)); %
change in total volume, m3
%
% Formulate the Energy Balance for the Batch Reactor
%
% The Energy Balance has the following form:
% d(mass in the reactor*heat capacity*temperature)/dt
% = (work of the stirrer)
% + (heat exchanged with the surroundings)
% - (sum of heats consumed by the three endothermic reactions)
% Energy conservation equation
%
mass_of_reacting_mixture = Reactor_feed(11); % in
kilograms
total_heat_capacity_reacting_mixture =

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```

(mass_of_reacting_mixture)*Materials_Properties(8,3);
% assumes that heat capacity is the same as of Solvent S1
%
% Qdot: Heat exchanged with surrounding environment
% If the Reactor Heater is ON and Water-cooling is OFF, then Qdot is
given
% by the following equation.
if (P(1)>0) % i.e. the reactor heater is on
    Qdot = ReactorHeater + ReactorStir; % Add stirrer energy to
heater energy, when heater is on, KW
end
% If Reactor Water-cooling system is ON and the Reactor Heater is OFF,
then
% Qdot is given by the following equation.
if (P(2)>0)
    Qdot = ReactorCool*(ReactorCoolTemp+273 - T) + ReactorStir; % Add
stirrer energy to cooler when it is on, KW
end

%
% Total heat rate produced by the three exothermic reactions
DH = rate*H;
%
% Complete Energy Balance and compute the derivative of tempature with
% time
dYdt(10) = (Qdot + DH)/total_heat_capacity_reacting_mixture;

end

```

```

function [value, isd, dir] = ReactorEvents(t,Y,P,K)
%
% Prepared by Herb Swain
% Transcribed by Kristie Stoneman
%
% This function stops the ode45 integration of the differential
equations
% in the file, reactions.m, when the temperature in the reactor reaches
the
% ReactorCoolTemp(C).
% It is called by the function, Reactor.m, which simulates the Batch
% Reactor.
%
%
global ReactorCoolTemp
%
% Check if the reactor temperature has reached the final temperature,
% ReactorCoolTemp(C).
value = Y(10)-(ReactorCoolTemp+273);
%
isd = 1; % This switch determines whether ode45 stops once it reaches
the 'event'.
%      'event' is given by the value of the variable, 'value' (see
%      previous line. Since we'd like it to stop, we'll set this to
1,
%      implying that the switch is ON.
%
dir = -1; % This switch determines the direction from which we approach
our zero.
% Since we want to detect cooling, we will set it to -1 to detect when
it
% has cooled to ReactorCoolTemp.
end

```

```

function Extractor
%
%
% Prepared by George Stephanopoulos
% Modified by Jennifer Hsu on 04/26/2011
% Updated by: Jennifer Hsu, 04/28/2011
%
% This function simulates the performance of the Batch Extractor and
% computes its associated economics. It is called by the function
% "Simulator.m"
%
% INPUT Global Variables
global Reactor_effluent          % Provides the molar amounts for all
materials and temperature
global Materials_Properties      % This matrix contains the physical
properties of all materials in the process
global Labor_unit_cost Extractor_rental_cost_per_hour Electricity_cost
global ExtractorVolume ExtractorTurn ExtractorStir
global Materials_Prices
global AmountSolvent_S2
% OUTPUT Global Variables
global Extractor_Phase_1_exit_stream Extractor_Phase_2_exit_stream
global Materials_Costs Utilities_Costs Vessel_Rental_Costs Labor_Costs
Materials_Credits
global Vessel_Occupancy
global Solvent_S2
%
% Characterizes the Extraction Solvent, S2
%
volume_solvent_S2 = AmountSolvent_S2; % sets the solvent volume, in m3,
to a value given from outside.
mass_solvent_S2 = volume_solvent_S2*Materials_Properties(9,2); % in
kilograms
moles_solvent_S2 = 1000*mass_solvent_S2/Materials_Properties(9,1); % in
g-moles
Solvent_S2 =
[0;0;0;0;0;0;0;0;0;moles_solvent_S2;298;mass_solvent_S2;volume_solvent_S2
];
%
% Characterize the input to the Batch Extractor as identical to the
Reactor
% Effluent
%
Extractor_feed = Reactor_effluent;
Phase_1_initially = Extractor_feed;
Phase_2_initially = Solvent_S2; % This vector contains the molar
amounts of all chemicals in S2
volume_Phase_1 = Phase_1_initially(12); % in m3
volume_Phase_2 = volume_solvent_S2; % in m3
%
% Check if the volume of Solvent, S2, can be accommodated by the
Extractor
% vessel.
total_volume = volume_Phase_1 + volume_Phase_2;
if total_volume > ExtractorVolume
    disp('WARNING: The volume of Solvent, S2, is larger than what can
be accommodated by the extractor vessel, given the volume of material
from the reactor. The volume of Solvent, S2, has been reset to equal

```

```

the difference, (Extractor vessel volume) - (Volume of material from
reactor)');
    volume_Phase_2 = ExtractorVolume - volume_Phase_1;
end
% Set the Equilibrium constants for the distribution of A, B, P, Q, W,
Z,
% C, S1, S2, between the two solvents.
EquilibriumConstants = [10;8;0;0;0;0;0;0;0;10];
% Equilibrium Constant = [concentration of a species of Solvent
% S2]/[concentration of a species in Solvent S1]
%
% Carry out the equilibrium calculations.
% At equilibrium, [species, in Phase-2]/[species, in Phase-1] =
Equilibrium
% constant of x. where, [x] is the molar concentration of a species.
%
K = EquilibriumConstants;
volume_ratio = volume_Phase_2/volume_Phase_1; % volume of phase-2 over
volume of phase-1
divider = volume_ratio*K+1;
moles_transferred(1:8) =
(Phase_1_initially(1:8).*volume_ratio.*K(1:8)')./divider(1:8)'; % moles
of A,B,P,Q,W,Z,C,S1, transferred from phase-1 to phase-2
moles_transferred(9) = Phase_2_initially(9)/divider(9); % moles of S2
transferred from phase-2 to phase-1
% Number of Moles at equilibrium, at the end of the extraction
Phase_1_equilibrium(1:8) = Phase_1_initially(1:8) -
moles_transferred(1:8); % A,B,P,Q,W,Z,C,S1
Phase_1_equilibrium(9) = Phase_1_initially(9) + moles_transferred(9); %
S2
Phase_2_equilibrium(1:8) = Phase_2_initially(1:8)' +
moles_transferred(1:8); % A,B,P,Q,W,Z,C,S1
Phase_2_equilibrium(9) = Phase_2_initially(9) - moles_transferred(9); %
S2
%
% Specify the characteristics of the exiting two streams from batch
% extractor
%
Extractor_Phase_1_exit_stream(1:9) = Phase_1_equilibrium(1:9); % Assign
amounts in moles to the Phase_1_exit_stream
Extractor_Phase_2_exit_stream(1:9) = Phase_2_equilibrium(1:9); % Assign
amounts in moles to the Phase_1_exit_stream
% Compute total masses in kilograms
component_amounts_in_kilograms_1 =
Extractor_Phase_1_exit_stream(1:9)'.*Materials_Properties(1:9,1)/1000;
% Kgs for each component
Extractor_Phase_1_exit_stream(11) =
sum(component_amounts_in_kilograms_1); % Total mass, kgs
component_amounts_in_kilograms_2 =
Extractor_Phase_2_exit_stream(1:9)'.*Materials_Properties(1:9,1)/1000;
% Kgs for each component
Extractor_Phase_2_exit_stream(11) =
sum(component_amounts_in_kilograms_2); % Total mass, kgs
% Compute total volume, in m3.
component_volumes_1 =
component_amounts_in_kilograms_1./Materials_Properties(1:9,2); %
densities = Materials_properties(1:9,2), in Kgs/m3
Extractor_Phase_1_exit_stream(12) = sum(component_volumes_1);

```

```

component_volumes_2 =
component_amounts_in_kilograms_2./Materials_Properties(1:9,2);
Extractor_Phase_2_exit_stream(12) = sum(component_volumes_2);
% Compute the Extraction Time, hours
extraction_period =
(((Extractor_Phase_2_exit_stream(2))/(Extractor_Phase_2_exit_stream(12)
*1e6))*(1.5*1e8))/3600; % k*deltaC_B
% Assign temperatures
heat_produced_by_stirrer = extraction_period*3600*ExtractorStir; % heat
input into system by stirrer over the period of stirring
total_mass_in_extractor = Extractor_Phase_1_exit_stream(11) +
Extractor_Phase_2_exit_stream(11);
temperature_rise_due_to_stirrer =
heat_produced_by_stirrer/(total_mass_in_extractor*Materials_Properties(
9,3));
Extractor_Phase_1_exit_stream(10) = Extractor_feed(10) +
temperature_rise_due_to_stirrer;
Extractor_Phase_2_exit_stream(10) = Extractor_feed(10) +
temperature_rise_due_to_stirrer;
%
% Compute the Economics of the Extractor per batch.
%
% Equipment rental cost
extractor_rental_cost = (extraction_period +
ExtractorTurn)*Extractor_rental_cost_per_hour; % in $
extractor_stirrer_electricity_cost =
Electricity_cost*(extraction_period+ExtractorTurn)*ExtractorStir; % in
$
%
% Materials Cost
solvent_cost_S2 = Materials_Prices(9)*mass_solvent_S2; % in $
%
% Labor Cost
extractor_labor_cost = (extraction_period +
ExtractorTurn)*Labor_unit_cost; % in $
%
% SUMMARY OF EXTRACTOR ECONOMICS
%
Materials_Costs(2,(1:4)) = 0;
Materials_Costs(2,5) = solvent_cost_S2;
Utilities_Costs(2,(1:7)) = 0;
Utilities_Costs(2,2) = extractor_stirrer_electricity_cost;
Vessel_Rental_Costs(2) = extractor_rental_cost;
Labor_Costs(2) = extractor_labor_cost;
Materials_Credits(2,(1:5)) = zeros(1,5);
Vessel_Occupancy(2) = extraction_period + ExtractorTurn; % Total
occupancy time of the extractor vessel, per batch
%
end

```



```

function Distillation
%
% 10.10 Project. Spring 2011.
% Prepared by: George Stephanopoulos
% Updated by: Jennifer Hsu, 04/28/2011
%
% INPUT Global Variables
global Materials_Properties
global DistillationTurn Distillation_rental_cost_per_hour
global Electricity_cost Water_cooling_cost Steam_heating_cost
global Labor_unit_cost
global Extractor_Phase_2_exit_stream
% OUTPUT Global Variables
global Materials_Costs Utilities_Costs Vessel_Rental_Costs Labor_Costs
Materials_Credits Materials_Prices
global Distillation_overhead_product Distillation_bottoms_product
global Vessel_Occupancy
%
% SIMULATION
%
distillation_feed = Extractor_Phase_2_exit_stream;
% Description of Distillation Overhead stream
Distillation_overhead_product(1) = distillation_feed(1); % moles of A
Distillation_overhead_product(2) = distillation_feed(2); % moles of B
Distillation_overhead_product(9) = (0.01/0.99)*(distillation_feed(1) +
distillation_feed(2)); % moles of S2
Distillation_overhead_product(3:8) = 0; % moles of P,Q,W,Z,C,S1
Distillation_overhead_product(10) = 298; % temperature in degrees K
Distillation_overhead_product(11) =
(Distillation_overhead_product(1:9)*Materials_Properties((1:9),1)/1e3);
% total amount in kilograms
% Description of Distillation Bottoms stream
Distillation_bottoms_product(1) = distillation_feed(1) -
Distillation_overhead_product(1); % moles of A
Distillation_bottoms_product(2) = distillation_feed(2) -
Distillation_overhead_product(2); % moles of B
Distillation_bottoms_product(9) = distillation_feed(9) -
Distillation_overhead_product(9); % moles of S2
Distillation_bottoms_product(3:8) = distillation_feed(3:8); % moles of
P,Q,W,Z,C,S1
Distillation_bottoms_product(10) = 458; % temperature in degrees K
Distillation_bottoms_product(11) =
(Distillation_bottoms_product(1:9)*Materials_Properties((1:9),1)/1e3);
% total amount in kilograms
% Utilities
% Heating duty in the reboiler
heating_duty_for_sensible_heating =
sum((distillation_feed(1:9)'./(1e3*Materials_Properties((1:9),1))).*Mat
erials_Properties((1:9),3)*(458-Extractor_Phase_2_exit_stream(10))); %
in KJ. Heat used to heat distillation feed from its temperature to 458
degrees Kelvin
heating_duty_for_vaporization =
Distillation_overhead_product(1:9)*Materials_Properties((1:9),4); % in
KJ. Heat used to vaporize the moles of A, B, and S2, which go to the
distillate stream
total_heating_duty = heating_duty_for_sensible_heating +
heating_duty_for_vaporization;

```

```

% Cooling duty in the condenser
% cooling_duty_for_sensible_cooling = xxxxxxxxx; % in KJ. Heat removed
during cooling of the distillate from 458 to 298 degrees Kelvin
total_cooling_duty = heating_duty_for_vaporization; % in KJ. The
cooling duty is equal to the amount of heating used for vaporization
%
% Compute the Economics of the Distillation per batch
%
distillation_period = 18/3600*(distillation_feed(1) +
distillation_feed(2)); % in hours
distillation_rental_cost = (distillation_period +
DistillationTurn)*Distillation_rental_cost_per_hour; % in $
distillation_heating_cost = (total_heating_duty)*(Steam_heating_cost);
% in $
distillation_cooling_cost = (total_cooling_duty)*(Water_cooling_cost);
% in $
%
% Materials Credits
credit_from_recovered_A =
((Distillation_overhead_product(1)*Materials_Properties(1,1))/1e3)*Mate
rials_Prices(1); % $ of credit from recovered A
credit_from_recovered_B =
((Distillation_overhead_product(2)*Materials_Properties(2,1))/1e3)*Mate
rials_Prices(2); % $ of credit from recovered B
credit_from_recovered_S2 =
((Distillation_bottoms_product(9)*Materials_Properties(9,1))/1e3)*Mate
rials_Prices(9); % $ of credit from recovered S2
% Labor Cost
distillation_labor_cost = (distillation_period +
DistillationTurn)*Labor_unit_cost; % in $
%
% SUMMARY OF DISTILLATION ECONOMICS
%
Materials_Costs(3:(1:5)) = 0;
Utilities_Costs(3,(1:7)) = 0;
Utilities_Costs(3,3) = distillation_cooling_cost;
Utilities_Costs(3,4) = distillation_heating_cost;
Vessel_Rental_Costs(3) = distillation_rental_cost;
Labor_Costs(3) = distillation_labor_cost;
Materials_Credits(3,1) = credit_from_recovered_A;
Materials_Credits(3,2) = credit_from_recovered_B;
Materials_Credits(3,(3:4)) = 0; % No credit for C and S1 since none has
been recovered
Materials_Credits(3,5) = credit_from_recovered_S2;
Vessel_Occupancy(3) = distillation_period + DistillationTurn; % Total
occupancy time of the distillation system, per batch

end

```

```

function Crystallizer
%
% 10.10 Project. Spring 2011.
% Prepared by: Kristie Stoneman, 04/08/2011
% Updated by: Kristie Stoneman, 04/08/2011
% Updated by: Jennifer Hsu, 04/26/2011
% Updated by: Jennifer Hsu, 04/28/2011
%
% This function simulates the performance of the Batch Crystallizer and
% computes its associated economics. It is called by the function
% "Simulator.m"
%
% INPUT Global Variables
global Extractor_Phase_1_exit_stream
global Materials_Properties
global CrystallizerVolume CrystallizationStir CrystallizationTurn
CrystallizerCool
global Electricity_cost Refrigeration_cooling_cost
global Labor_unit_cost
global Crystallizer_rental_cost_per_hour
% OUTPUT Global Variables
global Materials_Costs Utilities_Costs Vessel_Rental_Costs Labor_Costs
Materials_Credits
global Crystal_phase_Coating_Liquid_from_crystallizer
Crystal_phase_from_crystallizer Liquid_phase_from_crystallizer
global Vessel_Occupancy
%
% Mass Balances
Feed_to_crystallizer = Extractor_Phase_1_exit_stream; % The stream of
Phase-1 from the extractor is the feed to the crystallizer.
crystals_from_crystallizer = (0.9)*Feed_to_crystallizer(3); % 90% of
moles of P crystallize
weight_of_crystals =
crystals_from_crystallizer*Materials_Properties(3,1)/1000; % Kilograms
of crystals, P
liquid_coating_crystals = (0.1)*weight_of_crystals; % kg of liquid
coating the crystals in the crystallizer
liquid_after_removal_of_crystals(1:9) = Feed_to_crystallizer(1:9) - [0
0 crystals_from_crystallizer 0 0 0 0 0];
% The next line computes the mole fractions of all components in the
liquid
% at the end of crystallization, e.g. (mole fraction of A) = (moles of
% A)/(sum of moles of all components)
mole_fractions_in_liquid_after_removal_of_crystals(1:9) =
liquid_after_removal_of_crystals(1:9)/sum(liquid_after_removal_of_cryst
als(1:9));
% The next line computes the weight ratios of all components in the
liquid
% with respect to chemical, A, e.g.(weight ratio of B) = (weight of
% B)/(weight of A).
weight_ratios_in_liquid_after_removal_of_crystals(1:9) =
(mole_fractions_in_liquid_after_removal_of_crystals(1:9)).*Materials_Pr
operties((1:9),1))/(mole_fractions_in_liquid_after_removal_of_crystals(
1)*Materials_Properties(1,1));
% The next line computes the sum of the weight ratios, i.e. sum(weight
% ratio of A, weight ratio of B, etc.)
sum_of_weight_ratios =
sum(weight_ratios_in_liquid_after_removal_of_crystals(1:9));

```

```

% The next line computes the moles of A in the liquid coating of the
% crystals as follows: The sum of the weights of all components in the
% liquid coating the crystals is equal to the
"liquid_coating_crystals",
% computed in line 28, above. Therefore, (weight,A) =
% (liquid_coating_crystals)/(sum(weight ratios*ratios of molecular
weights),
% and (moles,A) = (weight,A)*1000/(molecular weight, A); moles of A in
the
% liquid coating the crystals.
moles_in_the_liquid_coating_the_crystals(1) =
1000*(liquid_coating_crystals)/(sum_of_weight_ratios*Materials_Properti
es(1,1));
% The next line yields the moles of B,P,Q,W,Z,C,S1,S2 in the liquid
coating
% the crystals
moles_in_the_liquid_coating_the_crystals(2:9) =
(mole_fractions_in_liquid_after_removal_of_crystals(2:9)/mole_fractions
_in_liquid_after_removal_of_crystals(1))*moles_in_the_liquid_coating_th
e_crystals(1);
% Define a new vector,
% "Crystal_phase_Coating_Liquid_from_crystallizer(1:9)", that describes
the
% moles of A,B,P,Q,W,Z,C,S1,S2 in the liquid coating the crystals.
% "Crystal_phase_Coating_Liquid_from_crystallizer(1:9)" describes the
% composition of the liquid that leaves the crystallizer with the
crystals.
Crystal_phase_Coating_Liquid_from_crystallizer(1:9) =
moles_in_the_liquid_coating_the_crystals(1:9);
% Composition of the solid Crystal Product
Crystal_phase_from_crystallizer(3) = crystals_from_crystallizer;
Crystal_phase_from_crystallizer(1:2) = 0;
Crystal_phase_from_crystallizer(4:9) = 0;
% Composition of the liquid phase leaving the crystallizer
Liquid_phase_from_crystallizer(1:9) =
liquid_after_removal_of_crystals(1:9) -
Crystal_phase_Coating_Liquid_from_crystallizer(1:9);
% Energy Balance
heat_load_removed_during_liquid_cooling =
((Feed_to_crystallizer(3:8)*(Materials_Properties((3:8),1)/1000))*Mater
ials_Properties(8,3))*(Feed_to_crystallizer(10)-263); % Heat removed
during cooling to -10 C
heat_load_removed_during_crystallization =
(Feed_to_crystallizer(3)*Materials_Properties(3,1)/1000)*Materials_Prop
erties(3,5); % Heat of fusion of P removed during crystal formation, in
KJ
% Crystallization Period
load_for_cooling_and_crystallization =
heat_load_removed_during_liquid_cooling +
heat_load_removed_during_crystallization; % in KJ
Q = CrystallizerCool - CrystallizationStir; % in KW
CrystallizationTime = (load_for_cooling_and_crystallization/Q)/3600; %
in hours
%
heat_load_removed_due_to_stirrer =
CrystallizationStir*(3600*CrystallizationTime); % Heat added by
stirrer, which must be removed during crystallization, in KJ
Total_heat_removed = load_for_cooling_and_crystallization +

```

```

heat_load_removed_due_to_stirrer;
%
Liquid_phase_from_crystallizer(10) = 263; % Setting temperature of
exiting stream at -10 C.
Crystal_phase_from_crystallizer(10) = 263; % Setting temperature of
exiting stream at -10 C.
Crystal_phase_Coating_Liquid_from_crystallizer(10) = 263; % Setting
temperature of exiting stream at -10 C.
%
% Materials Costs
Materials_Costs(4,(1:5)) = zeros(1,5);
% Utilities Costs
Utilities_Costs(4,(1:7)) = 0;
Utilities_Costs(4,2) =
CrystallizationStir*CrystallizationTime*Electricity_cost; % Cost of
electricity for stirring
Utilities_Costs(4,5) = Total_heat_removed*Refrigeration_cooling_cost; %
Refrigeration cooling cost
% Labor Cost
crystallizer_labor_cost = (CrystallizationTime +
CrystallizationTurn)*(Labor_unit_cost); % in $
Labor_Costs(4) = crystallizer_labor_cost;
% Equipment Rental Cost
crystallizer_rental_cost = (CrystallizationTime +
CrystallizationTurn)*(Crystallizer_rental_cost_per_hour); % in $
Vessel_Rental_Costs(4) = crystallizer_rental_cost;
% Materials Credits
Materials_Credits(4,(1:5)) = zeros(1,5);
Vessel_Occupancy(4) = CrystallizationTime + CrystallizationTurn; %
Total occupancy time of the distillation system per batch

end

```

```

function Dryer
%
% 10.10 Project. Spring 2011.
% Prepared by: Kristie Stoneman, 04/08/2011
% Updated by: Kristie Stoneman, 04/27/2011
% Updated by: Jennifer Hsu, 04/28/2011
%
% This function simulates the performance of the Dryer and computes its
% associated economics. It is called by the function, "Simulator.m"
%
% INPUT Global Variables
global Crystal_phase Coating_Liquid_from_crystallizer
Crystal_phase_from_crystallizer Liquid_phase_from_crystallizer
global Dryer_heating_cost Dryer_rental_cost_per_hour DryerTurn
DryerHeatingPower
global Labor_unit_cost
global Materials_Properties
% OUTPUT Global Variables
global Materials_Costs Utilities_Costs Vessel_Rental_Costs Labor_Costs
Materials_Credits
global Vapor_stream_from_dryer Crystal_stream_from_dryer
%
% Mass Balances
%
Vapor_stream_from_dryer =
Crystal_phase Coating_Liquid_from_crystallizer; % Equal to the
composition
% of the Crystal_phase Coating_Liquid_from_crystallizer
Crystal_stream_from_dryer = Crystal_phase_from_crystallizer; % Equal to
the composition
% of the Crystal_phase_from_crystallizer
%
% Energy Balances
%
% Sensible heat absorbed by the components of the liquid coating the
% crystals; from 263 K to their temperature of vaporization
amount_of_each_liquid_component =
(Vapor_stream_from_dryer(1:9)).*(Materials_Properties((1:9),1)/1000));
% in Kgs
sensible_heat_absorbed_by_each_component =
amount_of_each_liquid_component(1:9).*(Materials_Properties((1:9),3).*(M
aterials_Properties((1:9),6)-263); % in KJ
temperature = max(Materials_Properties((1:9),6)) + 30; % The
temperature in the dryer is 30 degrees higher than the highest boiling
point.
sensible_heat_absorbed_by_crystal =
Crystal_stream_from_dryer(3)*(0.125)*(temperature-
Crystal_stream_from_dryer(10)); % in KJ
total_sensible_heat =
sum(sensible_heat_absorbed_by_each_component(1:9));
Vapor_stream_from_dryer(10) = temperature;
Crystal_stream_from_dryer(10) = temperature;
% Latent heat absorbed by the components of the liquid coating the
% crystals
latent_heat_absorbed_by_each_component =
Vapor_stream_from_dryer(1:9).*(Materials_Properties((1:9),4); % in kJ
total_latent_heat = sum(latent_heat_absorbed_by_each_component(1:9));
total_heat_absorbed_in_dryer = total_sensible_heat + total_latent_heat

```

```

+ sensible_heat_absorbed_by_crystal;
% Drying Period
drying_period = (total_heat_absorbed_in_dryer/DryerHeatingPower)/3600;
% in hours
% Economics
dryer_heating_cost = total_heat_absorbed_in_dryer*Dryer_heating_cost; %
in $
% Labor Cost
dryer_labor_cost = (drying_period + DryerTurn)*(Labor_unit_cost); % in
$
dryer_rental_cost = (drying_period +
DryerTurn)*(Dryer_rental_cost_per_hour); % in $
%
% SUMMARY OF DRYER ECONOMICS
%
Materials_Costs(5,(1:5)) = 0;
Utilities_Costs(5,(1:7)) = 0;
Utilities_Costs(5,6) = dryer_heating_cost;
Vessel_Rental_Costs(5) = dryer_rental_cost;
Labor_Costs(5) = dryer_labor_cost;
Materials_Credits(1,(1:5)) = zeros(1,5);
Vessel_Occupancy(5) = drying_period + DryerTurn; % Total occupance time
of the reactor vessel, per batch
%
end

```

```

function Waste_Treatment
%
% 10.10 Project. Spring 2011.
% Prepared by: Kristie Stoneman, 04/08/2011
% Updated by: Kristie Stoneman, 04/27/2011
%
% This function simulates the performance of the Batch Crystallizer and
% computes its associated economics. It is called by the function
% "Simulator.m"
%
global Vapor_stream_from_dryer
global Liquid_phase_from_crystallizer
global Liquid_waste_treatment_cost Vapor_waste_treatment_cost
global Utilities_Costs
global Materials_Costs Utilities_Costs Vessel_Rental_Costs Labor_Costs
Materials_Credits
global Materials_Properties
%
% Define feed streams to the Waste treatment Unit
Liquid_feed = Liquid_phase_from_crystallizer;
Vapor_feed = Vapor_stream_from_dryer;
%
% Cost of treating liquid wastes
liquid_amount = Liquid_feed(1:9)*Materials_Properties((1:9),1)/1000; %
in Kilograms
liquid_wastes_treatment_cost =
liquid_amount*Liquid_waste_treatment_cost; % in $
% Cost of treating vapor wastes
vapor_amount = Vapor_feed(1:9)*Materials_Properties((1:9),1)/1000; % in
Kilograms
vapor_wastes_treatment_cost = vapor_amount*Vapor_waste_treatment_cost;
% in $
%
Materials_Costs(6,(1:5)) = 0;
Utilities_Costs(6,(1:6)) = 0;
Utilities_Costs(6,7) =
liquid_wastes_treatment_cost+vapor_wastes_treatment_cost;
Labor_Costs(6) = 0;
Vessel_Rental_Costs(6) = 0;
end

```



```

function [F] = Overall_Process_Economic_Objective(X)
%
% 10.10 Project. Spring 2003.
% Prepared by George Stephanopoulos.
%
% This function directs the computation of the "Net Operating Cost",
% which is the economic metric that we use to optimize the operation
% of the overall process.
% In addition, it computes the values of other economic parameters,
which
% are used to inform the chemical engineer of the distribution of
costs
% in the process.
%
% INPUT Variables
% X---- is the vector of values of the three optimization
variables:
% X(1) = The power output of the heater used in the reactor
(KW)
% X(2) = The period of heating of the reacting mixture
(seconds)
% X(3) = The amount of of Solvent, S2, used in the extractor
(m3)
% INPUT Global Variables
global Overhead Annual_operating_period
global Materials_Costs Utilities_Costs Labor_Costs
Vessel_Rental_Costs Materials_Prices Materials_Credits
global Materials_Properties
global Crystal_phase_from_crystallizer
global Vessel_Occupancy
% OUTPUT Global Variables. They are used by the function
% "Results_Displayer" for printing purposes
global Total_Materials_Cost Total_Utilities_Cost Total_Labor_Cost
Total_Rental_Costs Total_Materials_Credits
global Total_Operating_Cost Net_Operating_Cost
Cost_per_Kilogram_of_Product Profit_per_Kilogram_of_Product
global Number_of_batches_per_year Annual_Materials_Cost
Annual_Utilities_Cost Annual_Labor_Cost Annual_Rental_Cost
global Annual_Net_Operating_Cost Annual_Production Annual_Income
Annual_Profit
%
ReactorHeater = X(1);
ReactionHeatingPeriod = X(2);
AmountSolvent_S2 = X(3);
%
% Use the following conditions to prevent the violation of certain
% constraints
if ReactionHeatingPeriod<= 0 | ReactorHeater<=0 | AmountSolvent_S2<=0
% Physical constraints;
% These quantities cannot be negative.
% Set the value of the objective artificially high, in order to
% prevent the optimizer from violating the above constraints.
F = 1e25;
return
end
if AmountSolvent_S2 > 4
% Set the value of the objective artificially high, in order to
% prevent the optimizer from violating the above constraints.

```

```

    F = 1e25;
    return
end
if ReactorHeater > 500 % The reactor heater has a maximum output of
500 KW
    % Set the value of the objective artificially high, in order to
    % prevent the optimizer from violating the above constraints.
    F = 1e25;
    return
end
%
% EVALUATION OF THE OVERALL PROCESS ECONOMICS, PER BATCH
%
Total_Materials_Cost = sum(Materials_Costs(1,(1:5))) +
sum(Materials_Costs(2,(1:5)));
%
% Materials_Costs(i,j) is a matrix. The first index, i, indicates
the
% processing unit, and the second index, j, indicates one of the
% materials used in the process:
% Index, i:
% i = 1. Batch Reactor
% i = 2. Batch Extractor
% i = 3. Batch Distillation.
% i = 4. Batch Crystallizer
% i = 5. Dryer
% i = 6. Waste Treatment unit.
% Index, j:
% j = 1. Reagent, A
% j = 2. Reagent, B
% j = 3. Catalyst, C.
% j = 4. Solvent, S1.
% j = 5. Solvent, S2.
% So, Materials_Costs(1,1) = cost of reagent, A, used in the
Batch Reactor, and
% Materials_Costs(2,5) = cost of Solvent, S2, used in the
Batch Extractor.
%
a =
sum(Utilities_Costs((1:6),1))+sum(Utilities_Costs((1:6),2))+sum(Utiliti
es_Costs((1:6),3));
b =
sum(Utilities_Costs((1:6),4))+sum(Utilities_Costs((1:6),5))+sum(Utiliti
es_Costs((1:6),6))+sum(Utilities_Costs((1:6),7)));
Total_Uilities_Cost = a + b;
%
% The matrix, Utilities_Costs(i,j) indicates the cost of the j-th
type of
% utility used in the i-th processing unit.
% Index, i: See above.
% Index, j:
% j = 1. Electricity used for heating.
% j = 2. Electricity used for stirring.
% j = 3. Water cooling.
% j = 4. Steam heating.
% j = 5. Refrigeration cooling.
% j = 6. Fuel-based heating. Used in the dryer.
% j = 7. Treatment of wastes.

```

```

%
Total_Labor_Cost = sum(Labor_Costs(1:6));
Total_Rental_Costs = sum(Vessel_Rental_Costs(1:6));
%
%   Labor_Costs(i) and Vessel_Rental_Costs(i) are two vectors
indicating
%   the labor cost and vessel-rental cost of the processing unit, i.
The
%   index, i, has the same values as indicated above.
%
Total_Operating_Cost = (Total_Materials_Cost + Total_Uilities_Cost +
Total_Labor_Cost + Total_Rental_Costs);
Total_Materials_Credits = sum(Materials_Credits(3,(1:5)));
%
%   The matrix, Materials_Credits(i,j), indicates the credit given to
unit,
%   i, for the recovery of material, j. The values of indices, i and
j, have the same
%   meaning as for the matrix, Materials_Costs(i,j), see above.
%
Net_Operating_Cost = (1/Overhead)*(Total_Operating_Cost -
Total_Materials_Credits);
Cost_per_Kilogram_of_Product =
Net_Operating_Cost/(Crystal_phase_from_crystallizer(3)*Materials_Properties(3,1)/1000);
Profit_per_Kilogram_of_Product = Materials_Prices(3) -
Cost_per_Kilogram_of_Product;
%
%   EVALUATION OF THE OVERALL PROCESS ECONOMICS, ANNUAL BASIS
%
%   Estimate the number of batches per year, by dividing the
%   Annual_operating_period by the maximum vessel occupancy period by a
unit
%   in the process. This unit with the maximum occupancy period
determines
%   the critical time-period for a complete batch.
time = max(Vessel_Occupancy(1:4));           % Determine the critical
occupancy period.
Number_of_batches_per_year = Annual_operating_period/time;
%
%   Compute the various Cost Components on an annual basis
Annual_Materials_Cost = (Total_Materials_Cost -
Total_Materials_Credits)* Number_of_batches_per_year;
Annual_Uilities_Cost = Total_Uilities_Cost *
Number_of_batches_per_year;
Annual_Labor_Cost = Total_Labor_Cost *
Number_of_batches_per_year;
Annual_Rental_Cost = Total_Rental_Costs *
Number_of_batches_per_year;
Annual_Net_Operating_Cost = Net_Operating_Cost *
Number_of_batches_per_year;
Annual_Production =
((Crystal_phase_from_crystallizer(3)*Materials_Properties(3,1))/1000) *
Number_of_batches_per_year;
Annual_Income = Annual_Production * Materials_Prices(3);
Annual_Profit = Profit_per_Kilogram_of_Product *
Annual_Production;
%

```

```
F = - Annual_Profit;    % The Annual_Profit is our economic objective  
to maximized (or, its negative minimized)  
%  
end
```

```

function Results_Displayer
%
%
% 10.10 Project. Spring 2011.
% Prepared by George Stephanopolous.
% Transcribed by Kristie Stoneman.
% Updated by: Jennifer Hsu, 04/28/2011
%
% This function organizes the display of the simulation and economic
% results for the whole process.
%
% INPUT Global Variables
global FigureNumber
global ReactorHeater ReactionHeatingPeriod AmountSolvent_S2
global Reactor_feed Reactor_effluent
global ReactorTimeVector Reactor_dynamics Reactor_effluent
global Solvent_S2 Extractor_Phase_1_exit_stream
Extractor_Phase_2_exit_stream
global Materials_Costs Utilities_Costs Vessel_Rental_Costs Labor_Costs
Materials_Credits
global Materials_Prices Materials_Properties
global Crystal_phase_Coating_Liquid_from_crystallizer
Crystal_phase_from_crystallizer Liquid_phase_from_crystallizer
global Distillation_overhead_product Distillation_bottoms_product
global Vessel_Occupancy
global Total_Materials_Cost Total_Utilities_Cost Total_Labor_Cost
Total_Rental_Costs Total_Operating_Cost
global Total_Materials_Credits Net_Operating_Cost
Cost_per_Kilogram_of_Product Profit_per_Kilogram_of_Product
global Vapor_stream_from_dryer Crystal_stream_from_dryer
global Number_of_batches_per_year Annual_Materials_Cost
Annual_Utilities_Cost Annual_Labor_Cost Annual_Rental_Cost
global Annual_Net_Operating_Cost Annual_Production Annual_Income
Annual_Profit
%
disp(' ');
disp(' ');
disp(' ');
%
% STEP-3(A): DISPLAY THE VALUES OF THE OPTIMIZATION VARIABLE
%
disp('VALUES OF THE OPTIMIZATION VARIABLES');
fprintf(' Reactor Heater Output (KW/hr) = %f\n',
ReactorHeater);
fprintf(' Reactor Heating period (seconds) = %f\n',
ReactionHeatingPeriod);
fprintf(' Amount of Extraction Solvent, S1 (m3) = %f\n\n\n',
AmountSolvent_S2);
% STEP-3(B): DISPLAY THE PROCESS INFORMATION FOR A SINGLE BATCH OF
% PRODUCTION.
%
disp('TABLE OF PROCESS STREAMS PER BATCH OF PRODUCTION');
disp(' ');
disp(['Process Stream Moles, A Moles, B Moles, P
Moles, Q Moles, W Moles, Z Moles, C Moles, S1
Moles, S2 Temperature']);
disp('-----
-----

```

```

-----');
fprintf('Reactor \n');
fprintf('      Feed      %8.4f      %8.4f      %8.4f
%8.4f      %8.4f      %8.4f      %8.4f      %8.4f      %8.4f      %6.2f
\n', Reactor_feed(1:10));
fprintf('      Effluent      %8.4f      %8.4f      %8.4f
%8.4f      %8.4f      %8.4f      %8.4f      %8.4f      %8.4f      %6.2f
\n', Reactor_effluent(1:10));
fprintf('Extractor \n');
fprintf('      Fresh Solvent, S2      %8.4f      %8.4f      %8.4f
%8.4f      %8.4f      %8.4f      %8.4f      %8.4f      %8.4f      %6.2f
\n', Solvent_S2(1:10));
fprintf('      Solvent, S1-Phase      %8.4f      %8.4f      %8.4f
%8.4f      %8.4f      %8.4f      %8.4f      %8.4f      %8.4f      %6.2f
\n', Extractor_Phase_1_exit_stream(1:10));
fprintf('      Solvent, S2-Phase      %8.4f      %8.4f      %8.4f
%8.4f      %8.4f      %8.4f      %8.4f      %8.4f      %8.4f      %6.2f
\n', Extractor_Phase_2_exit_stream(1:10));
fprintf('Distillation \n');
fprintf('      Overhead      %8.4f      %8.4f      %8.4f
%8.4f      %8.4f      %8.4f      %8.4f      %8.4f      %8.4f
%6.2f \n', Distillation_overhead_product(1:10));
fprintf('      Bottoms      %8.4f      %8.4f      %8.4f
%8.4f      %8.4f      %8.4f      %8.4f      %8.4f      %8.4f      %6.2f
\n', Distillation_bottoms_product(1:10));
fprintf('Crystallizer \n');
fprintf('      Crystal-Phase, Solid %8.4f      %8.4f      %8.4f
%8.4f      %8.4f      %8.4f      %8.4f      %8.4f      %8.4f
%6.2f \n', Crystal_phase_from_crystallizer(1:10));
fprintf('      Crystal-Phase, Liquid%8.4f      %8.4f      %8.4f
%8.4f      %8.4f      %8.4f      %8.4f      %8.4f      %8.4f
%6.2f \n', Crystal_phase_Coating_Liquid_from_crystallizer(1:10));
fprintf('      Liquid-Phase      %8.4f      %8.4f      %8.4f
%8.4f      %8.4f      %8.4f      %8.4f      %8.4f      %8.4f      %6.2f
\n', Liquid_phase_from_crystallizer(1:10));
fprintf('Dryer \n');
fprintf('      Crystal-Phase(pure) %8.4f      %8.4f      %8.4f
%8.4f      %8.4f      %8.4f      %8.4f      %8.4f      %8.4f
%6.2f \n', Crystal_stream_from_dryer(1:10));
fprintf('      Vapor-Phase      %8.4f      %8.4f      %8.4f
%8.4f      %8.4f      %8.4f      %8.4f      %8.4f      %8.4f
%6.2f \n', Vapor_stream_from_dryer(1:10));
%
disp('      ');
disp('NET UTILIZATION OF MATERIALS PER BATCH (Fresh Materials -
Reclaimed Materials) ');
disp('      ');
fprintf(' Reagent, A (Kgs) = %7.2f\n', (Reactor_feed(1)-
Distillation_overhead_product(1))*Materials_Properties(1,1)/1000 );
fprintf(' Reagent, B (Kgs) = %7.2f\n', (Reactor_feed(2)-
Distillation_overhead_product(2))*Materials_Properties(2,1)/1000 );
fprintf(' Catalyst, C (Kgs) = %7.2f\n',
Reactor_feed(7)*Materials_Properties(7,1)/1000 );
fprintf(' Solvent, S1 (Kgs) = %7.2f\n',
Reactor_feed(8)*Materials_Properties(8,1)/1000 );
fprintf(' Solvent, S2 (Kgs) = %7.2f\n\n', ((Solvent_S2(9)-
Distillation_bottoms_product(9))*Materials_Properties(9,1))/1000); %
added "(" before Solvent_S2(9)

```

```

disp('AMOUNT OF PRODUCT');
disp(' ');
fprintf(' P, (Kilograms per Batch) = %5.2f \n\n\n\n ',
Crystal_phase_from_crystallizer(3)*Materials_Properties(3,1)/1000);
%
% STEP-3(C): DISPLAY THE RESULTS OF PROCESS ECONOMICS PER BATCH.
%
disp('TABLE OF PROCESS ECONOMICS PER BATCH')
disp(' ');
disp(' ');
disp([' Reactor Extractor Distillation
Crystallization Dryer Waste Treatment']);
disp('-----');
fprintf('MATERIALS COSTS PER BATCH ( $ ) \n');
fprintf(' Reagent, A %7.2f %7.2f %6.2f
%6.2f %6.2f %6.5f\n', Materials_Costs(1,1), 0, 0, 0,
0, 0);
fprintf(' Reagent, B %7.2f %7.2f %6.2f
%6.2f %6.2f %6.5f\n', Materials_Costs(1,2), 0, 0, 0,
0, 0);
fprintf(' Catalyst, C %7.2f %7.2f %6.2f
%6.2f %6.2f %6.5f\n', Materials_Costs(1,3), 0, 0, 0,
0, 0);
fprintf(' Solvent, S1 %7.2f %7.2f %6.2f
%6.2f %6.2f %6.5f\n', Materials_Costs(1,4), 0, 0, 0,
0, 0);
fprintf(' Solvent, S2 %7.2f %7.2f %6.2f
%6.2f %6.2f %6.5f\n', 0, Materials_Costs(2,5), 0, 0,
0, 0);
disp('-----');
fprintf('Total Materials Cost ( $ per batch) = %7.2f \n',
Total_Materials_Cost);
disp(' ');
disp(' ');
fprintf('UTILITIES COSTS PER BATCH ( $ ) \n');
fprintf(' Electricity-Heat %7.2f %7.2f %6.2f
%6.2f %6.2f %6.5f\n',Utilities_Costs((1:6),1));
fprintf(' Electricity-Stir %7.2f %7.2f %6.2f
%6.2f %6.2f %6.5f\n',Utilities_Costs((1:6),2));
fprintf(' Water Cooling %7.2f %7.2f %6.2f
%6.2f %6.2f %6.5f\n',Utilities_Costs((1:6),3));
fprintf(' Steam Heating %7.2f %7.2f %6.2f
%6.2f %6.2f %6.5f\n',Utilities_Costs((1:6),4));
fprintf(' Refrigerant Cooling %7.2f %7.2f %6.2f
%6.2f %6.2f %6.5f\n',Utilities_Costs((1:6),5));
fprintf(' Fuel Heating-Dryer %7.2f %7.2f %6.2f
%6.2f %6.2f %6.5f\n',Utilities_Costs((1:6),6));
fprintf(' Waste Treatment %7.2f %7.2f %6.2f
%6.2f %6.2f %6.5f\n\n\n',Utilities_Costs((1:6),7));
disp('-----');
fprintf('Total Utilities Cost ( $ per batch) =
%7.2f\n',Total_Uilities_Cost);
disp(' ');
disp(' ');
fprintf('LABOR COSTS PER BATCH ( $ ) \n');

```

```

fprintf('    Unit Labor Cost      %7.2f      %7.2f      %6.2f
%6.2f      %6.2f      %6.5\n', Labor_Costs(1:6));
disp(' ');
disp('-----');
disp(' ');
fprintf('Total Labor Cost ( $ per batch) = %7.2f\n', Total_Labor_Cost);
disp(' ');
disp(' ');
fprintf('EQUIPMENT RENTAL COSTS PER BATCH ( $ ) \n');
fprintf(' Vessel Rental Cost    %7.2f      %7.2f      %6.2f
%6.2f      %6.2f%6.5\n', Vessel_Rental_Costs(1:6));
disp(' ');
disp('-----');
disp(' ');
fprintf('Total Rental Costs ( $ per batch) = %7.2f\n\n\n',
Total_Rental_Costs );
fprintf('TOTAL OPERATING COST PER BATCH ( $ ) = %7.2f\n',
Total_Operating_Cost);
disp('-----');
disp(' ');
disp('-----');
disp(' ');
fprintf('MATERIALS CREDITS PER BATCH ( $ ) \n');
fprintf(' Recovered, A      %7.2f      %7.2f      %6.2f
%6.2f      %6.2f      %6.5f\n', 0, 0, Materials_Credits(3,1), 0,
0, 0);
fprintf(' Recovered, B      %7.2f      %7.2f      %6.2f
%6.2f      %6.2f      %6.5f\n', 0, 0, Materials_Credits(3,2), 0,
0, 0);
fprintf(' Recovered, S2      %7.2f      %7.2f      %6.2f
%6.2f      %6.2f      %6.5f\n', 0, 0, Materials_Credits(3,5), 0,
0, 0);
disp('-----');
disp(' ');
fprintf('TOTAL MATERIALS CREDITS PER BATCH ( $ ) = %7.2f \n\n\n',
Total_Materials_Credits);
fprintf('NET OPERATING COST PER BATCH ( $ )      = %7.2f \n\n',
Net_Operating_Cost);
fprintf('COST PER KILOGRAM, P ( $/Kg)      = %7.2f \n\n',
Cost_per_Kilogram_of_Product);
fprintf('PROFIT PER KILOGRAM, P ( $/Kg)      = %7.2f \n\n',
Profit_per_Kilogram_of_Product);
%
% STEP-3(D): DISPLAY A SUMMARY OF ECONOMICS ON AN ANNUAL BASIS
%
disp(' ');
disp('-----');
disp(' ');
disp('SUMMARY OF PROCESS ECONOMICS ON AN ANNUAL BASIS (In $ for a 4,000
hours Annual Operation)');
disp(' ');
disp(' ');
fprintf('    NUMBER OF BATCHES PER YEAR      = %4.2f \n\n',
Number_of_batches_per_year);
fprintf('    ANNUAL PRODUCTION OF P, Kgs      = %9.2f \n\n',
Annual_Production);
fprintf('    MATERIALS COST (Net), $          = %9.2f \n\n',
Annual_Materials_Cost);

```



```

fprintf('    UTILITIES COST, $           = %9.2f \n\n',
Annual_Uilities_Cost);
fprintf('    LABOR COST, $             = %9.2f \n\n',
Annual_Labor_Cost);
fprintf('    EQUIPMENT "RENTAL" COST     = %9.2f \n\n',
Annual_Rental_Cost);
fprintf('    NET OPERATING COST, $         = %9.2f \n\n',
Annual_Net_Operating_Cost);
fprintf('    ANNUAL INCOME, $              = %9.2f \n\n',
Annual_Income);
fprintf('    OPERATING PROFIT, $            = %9.2f \n\n',
Annual_Profit);
%
%   STEP-3(E):  DISPLAY THE TIME_DEPENDENT RESPONSE OF THE BATCH
REACTOR
%
print_decision = input('Would you like to plot the Batch Reactor
dynamics? print y (yes) or n (no). So, y or n?.....', 's');
if print_decision == 'y'
    FigureNumber = FigureNumber + 1;
    TransientPlots(ReactorTimeVector, Reactor_dynamics);
end
%
end

```

```

function TransientPlots(tvec,Y)
%
% 10.10 Project. Spring 2011
% Prepared by Herb Sawin
% Updated by: Kristie Stoneman, 04/27/2011
% Updated by: Kristie Stoneman, 04/28/2011
%
% This function plots molar amounts of the six chemicals and
temperature,
% resulting from the simulation of the Batch reactor, as a function of
% time.
% It is called by the functions, "Results_Display", if and only if
the
% user has indicated so.
%
global FigureNumber
% Make a plot showing the species molar amounts and temperature with
time
% in the reactor.
figure(FigureNumber); % Open a new figure for each set of plots
subplot(4,2,1), plot(tvec,Y(:,1)), xlabel('time,
sec'),ylabel('Reactant, A')
subplot(4,2,2), plot(tvec,Y(:,2)), xlabel('time,
sec'),ylabel('Reactant, B')
subplot(4,2,3), plot(tvec,Y(:,3)), xlabel('time, sec'),ylabel('Product,
P')
subplot(4,2,4), plot(tvec,Y(:,4)), xlabel('time, sec'),ylabel('By-
Product, Q')
subplot(4,2,5), plot(tvec,Y(:,5)), xlabel('time, sec'),ylabel('Waste,
W')
subplot(4,2,6), plot(tvec,Y(:,6)), xlabel('time, sec'),ylabel('Waste,
Z')
subplot(4,2,7), plot(tvec,Y(:,10)-273), xlabel('time,
sec'),ylabel('Temperature, C')
FigureNumber = FigureNumber+1;
% Table of Moles, A versus time
disp(['   Time' '   Temperature']);
for k=1:length(tvec);
    fprintf(' %7.3f   %6.3f\n',tvec(k),Y(k,10));
end
end

```

```

function Results_To_Excel
%
%
% 10.10 Project. Spring 2011.
% Prepared by Jennifer Hsu
%
% This function prints results of the simulation and economic
% results for the whole process.
%
% INPUT Global Variables
global FigureNumber
global ReactorHeater ReactionHeatingPeriod AmountSolvent_S2
global Reactor_feed Reactor_effluent
global ReactorTimeVector Reactor_dynamics Reactor_effluent
global Solvent_S2 Extractor_Phase_1_exit_stream Extractor_Phase_2_exit_stream
global Materials_Costs Utilities_Costs Vessel_Rental_Costs Labor_Costs
Materials_Credits
global Materials_Prices Materials_Properties
global Crystal_phase_Coating_Liquid_from_crystallizer
Crystal_phase_from_crystallizer Liquid_phase_from_crystallizer
global Distillation_overhead_product Distillation_bottoms_product
global Vessel_Occupancy
global Total_Materials_Cost Total_Utilities_Cost Total_Labor_Cost
Total_Rental_Costs Total_Operating_Cost
global Total_Materials_Credits Net_Operating_Cost
Cost_per_Kilogram_of_Product Profit_per_Kilogram_of_Product
global Vapor_stream_from_dryer Crystal_stream_from_dryer
global Number_of_batches_per_year Annual_Materials_Cost Annual_Utilities_Cost
Annual_Labor_Cost Annual_Rental_Cost
global Annual_Net_Operating_Cost Annual_Production Annual_Income
Annual_Profit

filename = 'data.xls';

line = {ReactorHeater; ReactionHeatingPeriod; AmountSolvent_S2};
xlswrite(filename, line, 1, 'B2');

line = [Reactor_feed(1:10)];
xlswrite(filename, line, 1, 'B9');
line = [Reactor_effluent(1:10)];
xlswrite(filename, line, 1, 'B10');
line = Solvent_S2(1:10)';
xlswrite(filename, line, 1, 'B12');
line = [Extractor_Phase_1_exit_stream(1:10)];
xlswrite(filename, line, 1, 'B13');
line = [Extractor_Phase_2_exit_stream(1:10)];
xlswrite(filename, line, 1, 'B14');
line = [Distillation_overhead_product(1:10);
Distillation_bottoms_product(1:10)];
xlswrite(filename, line, 1, 'B16');
line = [Crystal_phase_from_crystallizer(1:10);
Crystal_phase_Coating_Liquid_from_crystallizer(1:10);
Liquid_phase_from_crystallizer(1:10)];
xlswrite(filename, line, 1, 'B19');
line = [Crystal_stream_from_dryer(1:10); Vapor_stream_from_dryer(1:10)];

```

```

xlswrite(filename, line, 1, 'B23');

line = [(Reactor_feed(1)-
Distillation_overhead_product(1))*Materials_Properties(1,1)/1000; ...
        (Reactor_feed(2)-
Distillation_overhead_product(2))*Materials_Properties(2,1)/1000; ...
        Reactor_feed(7)*Materials_Properties(7,1)/1000; ...
        Reactor_feed(8)*Materials_Properties(8,1)/1000; ...
        ((Solvent_S2(9)-
Distillation_bottoms_product(9))*Materials_Properties(9,1))/1000];
xlswrite(filename, line, 1, 'B27');

line = [Crystal_phase_from_crystallizer(3)*Materials_Properties(3,1)/1000];
xlswrite(filename, line, 1, 'B33');

line = Materials_Costs(1,1:4)';
xlswrite(filename, line, 1, 'B38');
line = zeros(4,5);
xlswrite(filename, line, 1, 'C38');
line = [Materials_Costs(2,5),0,0,0,0,0];
xlswrite(filename, line, 1, 'B42');
line = zeros(1,4);
xlswrite(filename, line, 1, 'C42');
line = [Total_Materials_Cost];
xlswrite(filename, line, 1, 'B43');

line = Utilities_Costs((1:6),(1:7))';
xlswrite(filename, line, 1, 'B46');
line = [Total_Uilities_Cost];
xlswrite(filename, line, 1, 'B53');

line = Labor_Costs(1:6);
xlswrite(filename, line, 1, 'B56');
line = [Total_Labor_Cost];
xlswrite(filename, line, 1, 'B57');

line = Vessel_Rental_Costs(1:6);
xlswrite(filename, line, 1, 'B60');
line = [Total_Rental_Costs];
xlswrite(filename, line, 1, 'B61');

line = [Total_Operating_Cost];
xlswrite(filename, line, 1, 'B63');

line = [0, 0, Materials_Credits(3,1), 0, 0, 0];
xlswrite(filename, line, 1, 'B66');
line = [0, 0, Materials_Credits(3,2), 0, 0, 0];
xlswrite(filename, line, 1, 'B67');
line = [0, 0, Materials_Credits(3,5), 0, 0, 0];
xlswrite(filename, line, 1, 'B68');

line = [Total_Materials_Credits];
xlswrite(filename, line, 1, 'B69');
line = [Net_Operating_Cost];
xlswrite(filename, line, 1, 'B71');

```

```

line = [Cost_per_Kilogram_of_Product];
xlswrite(filename, line, 1, 'B72');
line = [Profit_per_Kilogram_of_Product];
xlswrite(filename, line, 1, 'B73');

line = [Number_of_batches_per_year];
xlswrite(filename, line, 1, 'B76');
line = [Annual_Production];
xlswrite(filename, line, 1, 'B77');
line = [Annual_Materials_Cost];
xlswrite(filename, line, 1, 'B78');
line = [Annual_Utilities_Cost];
xlswrite(filename, line, 1, 'B79');
line = [Annual_Labor_Cost];
xlswrite(filename, line, 1, 'B80');
line = [Annual_Rental_Cost];
xlswrite(filename, line, 1, 'B81');
line = [Annual_Net_Operating_Cost];
xlswrite(filename, line, 1, 'B82');
line = [Annual_Income];
xlswrite(filename, line, 1, 'B83');
line = [Annual_Profit];
xlswrite(filename, line, 1, 'B84');

end

```