Energy Balances and Numerical Methods

Design Project

Production of a Drying Oil

Drying oils are additives to products like paint and varnish to aid the drying process when these products are coated on a surface.

The purpose of this project is to do a preliminary analysis to determine the feasibility of constructing a chemical plant to manufacture 50,000 tonne/y drying oil.

A suggested process flow diagram is attached. You should use this as a starting point. Your primary task is to recommend operating conditions for the reactor and a reactor choice that maximizes the gross profit (defined later). However, any change that you can justify that does not violate the laws of nature is allowed. Your assignment is to develop a "best" case, where "best" is dependent upon economic considerations.

Chemical Reaction

The raw material is acetylated castor oil (ACO), which we will model as palmitic acid ($C_{15}H_{31}COOH$). The primary reaction is one in which the acetylated castor oil is thermally cracked to the drying oil (DO, which we will model as tetradecene, $C_{14}H_{28}$) and acetic acid (AA) (CH_3COOH). There is an undesired reaction in which the drying oil dimerizes to form a gum, which we will model as $C_{28}H_{56}$.

The chemical reactions are as follows:

$$C_{16}H_{32}O_2(l) \rightarrow CH_3COOH(g) + C_{14}H_{28}(l) \tag{1}$$

$$2C_{14}H_{28}(l) \rightarrow C_{28}H_{56}(s) \tag{2}$$

Process Description

The process is illustrated in Figure 1. The acetylated castor oil (ACO) feed is mixed with recycled ACO and passed through a vessel that helps maintain constant flow downstream of the mixing point. The ACO stream is then heated to the required reactor temperature in a fired heater (furnace), H-501. The hot ACO stream is fed to the reactor (R-501), where the reaction proceeds. In the reactor, reactions in Eqs. (1) and (2) occur. The reactor effluent is quenched to 180°C in E-501, using cooling water. In F-501, the gum is filtered out, and the filtrate is fed to a distillation column, T-501, where the unreacted ACO is recycled. The top product of T-501 is fed to a second distillation column, which purifies the AA and DO. More details on distillation columns and the associated heat exchangers are presented later.

V-501	H-501	R-501	E-501	F-501	T-501	E-502	E-503	T-502	E-504	E-505
Recycle Mixing Vessel	Fired Heater	Reactor	Reactor Quench Exchanger	Gum Filter	ACO Recycle Column	ACO Column Reboiler	ACO Column Condenser	DO Purification Column	DO Column Reboiler	DO Column Condenser

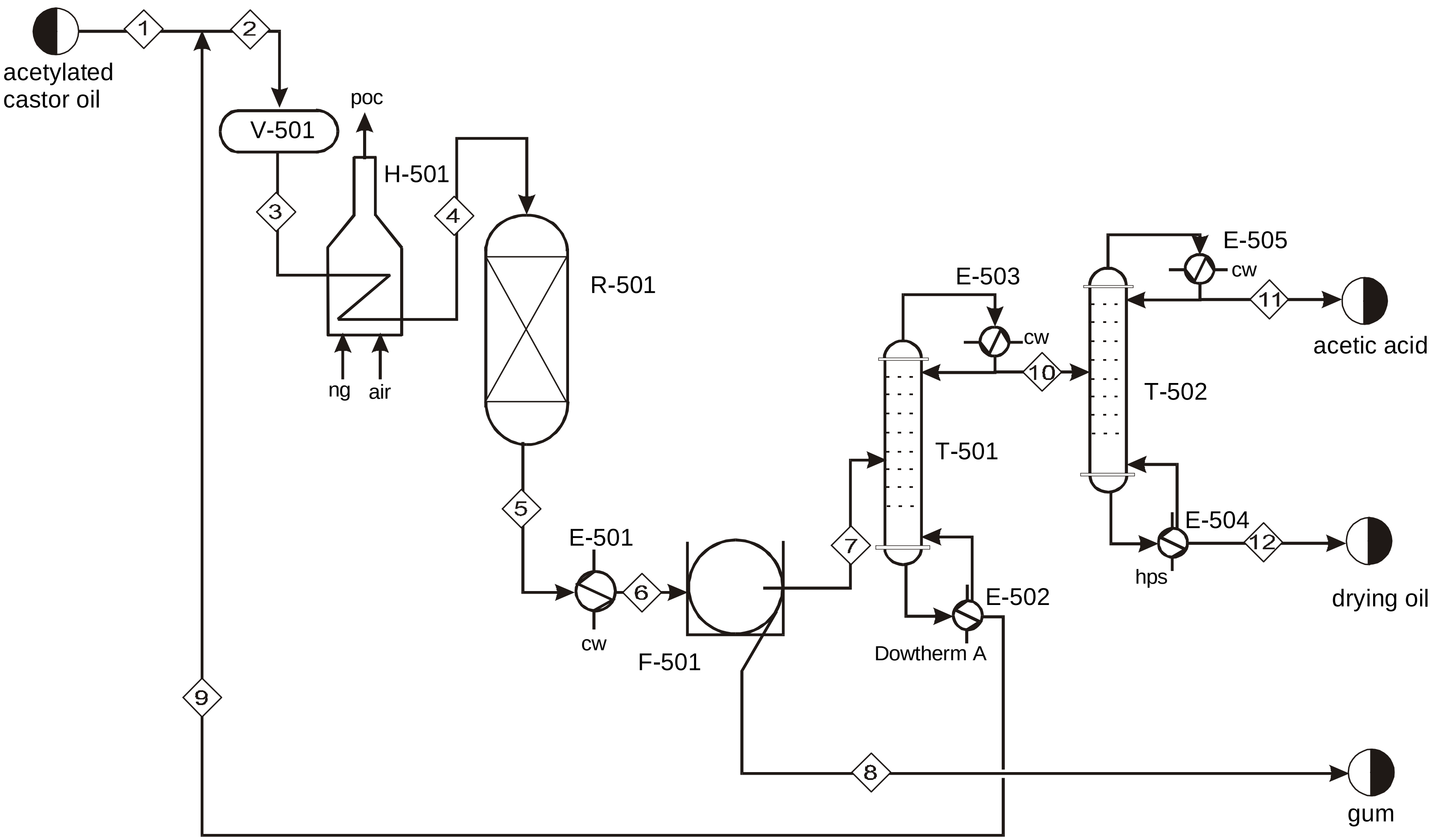

Figure 1: Preliminary Process Flowsheet for Drying Oil Production

Process Details

Feed Stream and Effluent Streams

Stream 1: ACO – $0.59/kg – Stream at 25°C

Stream 8: Gum waste – no value

Stream 11: Acetic acid by-product – $0.99/kg

Stream 12: DO – $1.19/kg

Equipment

Vessel (V-501)

This is the location where feed and recycle streams mix.

Fired Heater (H-501)

The fired heater heats feed to the reaction temperature. Energy is provided by burning natural gas (CH_4). The lower heating value should be used to determine the cost of the required natural gas. Additional natural gas is needed to provide energy to reheat Dowtherm used in E-502.

Reactor (R-501)

This is where the reactions in Eqs. (1) and (2) occur. More details on the reactor are presented later.

Filter (F-501)

In the filter, all gum is removed in Stream 8, all AA, ACO, and DO go to Stream 7.

Distillation Column (T-501)

In T-501, all AA in Stream 7 goes to Stream 10, all ACO in Stream 7 goes to Stream 9, 99.5% of DO in Stream 7 goes to Stream 10. The column pressure is determined by the constraint that the bottom of the column may not exceed 300°C, to avoid additional reaction at the bottom of the column that may form gum.

Heat Exchanger (E-503):

In this heat exchanger, the contents of the top of T-501 are condensed from saturated vapor to saturated liquid at the column pressure at a rate three times the flow of Stream 10. One-third of the condensate becomes Stream 10, and the remainder is returned to the column. There is a cost for the amount of cooling water needed to remove the necessary energy. The cooling water must always be at a lower temperature than the stream being condensed. It may be assumed that the stream being condensed condenses at the dew point temperature of the mixture at the column pressure.

Heat Exchanger (E-502):

In this heat exchanger, you may assume that the stream being vaporized has the same flowrate as Stream 9. The stream is vaporized from saturated liquid to saturated vapor at a column pressure, determined by the temperature constraint at the bottom of he column, and is returned to the column. The pressure of the stream being vaporized is the vapor pressure of ACO at the bottom temperature constraint. There is a cost for the amount of Dowtherm needed to supply the necessary heat, as stated in the description for H-501. The Dowtherm enters at 380°C and leaves at 360°C. It must be reheated to 380°C in the fired heater. The Dowtherm temperature must be above the temperature of the vaporizing stream.

Distillation Column (T-502)

Here, 99.5% of AA in Stream 10 goes to Stream 11, and 99.5% of DO in Stream 10 goes to Stream 12. This column operates at atmospheric pressure.

Heat Exchanger (E-505):

In this heat exchanger, the contents of the top of T-502 (pure AA) are condensed from saturated vapor to saturated liquid at the column pressure at a rate three times the flow of Stream 11. One-third of the condensate becomes Stream 11, and the remainder is returned to the column. There is a cost for the amount of cooling water needed to remove the necessary energy. The cooling water must always be at a lower temperature than the stream being condensed.

Heat Exchanger (E-504):

In this heat exchanger, you may assume that the stream being vaporized has the same flowrate as Stream 12. The stream is vaporized from saturated liquid to saturated vapor at the column pressure and is returned to the column. The temperature of the stream being vaporized is the boiling point of DO at the column pressure. There is a cost for the amount of steam needed to supply the necessary heat. The steam temperature must be above the temperature of the vaporizing stream.

Other Equipment:

For two or more streams to mix, they must be at identical pressures. Pressure reduction may be accomplished by adding a valve. All of these valves are not necessarily shown on the attached flowsheet, and it may be assumed that additional valves can be added as needed at no cost. Flow occurs from higher pressure to lower pressure. Pumps are used to increase the pressure of a liquid stream. If pumps are needed, they are not shown on the PFD.

Reactor Information

The reaction conditions are limited to temperatures between 310°C and 400°C. Table 1 gives conversion and selectivity information for the reactor for one reactor size. You should recommend the optimum reactor temperature and space time. The smaller the space time, the smaller the reactor.

Table 1: Reactor Conversions and Selectivities

***T* (°C)**	***X*** **conversion to AA space time 10 min**	**selectivity moles DO/moles gum space time 10 min**
310	0.130	6.43×10^{7}
320	0.184	4.97×10^{6}
330	0.245	9.18×10^{5}
340	0.314	2.38×10^{5}
350	0.375	7.08×10^{4}
360	0.444	2.29×10^{4}
370	0.513	8.55×10^{3}
380	0.559	3.38×10^{3}
390	0.597	1.43×10^{3}
400	0.635	5.58×10^{2}

It may be assumed that the conversion obeys the following function of space time, τ:

$$X = 1 - e^{-a\tau} \tag{3}$$

and that the selectivity obeys the following function of space time

$$S = e^{b/\tau} \tag{4}$$

Any space time is possible, and the corresponding selectivity and conversion can be obtained by determining the parameters in Equations 3 and 4 from the data in Table 1.

Economic Analysis

When evaluating alternative cases, the following objective function should be used. It is the equivalent annual operating cost (EAOC), and is defined as

EAOC = – (product value – feed cost – utility costs – cost of gum removal – capital cost annuity)

A negative EAOC means there is a profit. It is desirable to minimize the EAOC; *i.e.*, a large negative EAOC is very desirable.

Other operating costs are utilities, such as steam, cooling water, natural gas, and electricity.

There is a cost associated with removing the gum, which can be ignored (and F-501 removed) if the gum level is below 1 ppm (mass basis) in Stream 6. This cost is function is

$$\text{cost of gum removal (\$/kg DO leaving reactor)} = 10^{-3}[(\text{ppm gum in Stream 6}) - 1] \qquad (5)$$

If the cost of gum removal in Eq. (5) is less than zero, the cost is zero.

The capital cost annuity is an ***annual*** cost (like a car payment) associated with the ***one-time***, fixed cost of plant construction. A list of capital costs for all pieces of equipment will be provided in early to mid March.

The capital cost annuity is defined as follows:

$$\textit{capital cost annuity} = FCI\,\frac{i(1+i)^n}{(1+i)^n - 1}$$

where *FCI* is the installed cost of all equipment; i is the interest rate, $i = 0.15$; and n is the plant life for accounting purposes, $n = 10$.

Optimization

We will learn optimization methods in ChE 230. The objective function (EAOC) is defined above. It is your responsibility to define appropriate decision variables. If there are too many decision variables to do a reasonable optimization, it is your responsibility to determine, with appropriate justification, which ones most significantly affect the objective function and focus on only those decision variables.

Utility Costs

Low-Pressure Steam (618 kPa, saturated, cost or credit)	\$7.78/1000 kg
Medium-Pressure Steam (1135 kPa, saturated, cost or credit)	\$8.22/1000 kg
High-Pressure Steam (4237 kPa, saturated, cost or credit)	\$9.83/1000 kg
Natural Gas or Fuel Gas (446 kPa, 25°C)	
cost	\$6.00/GJ
credit	\$5.00/GJ

Electricity $0.06/kWh

Boiler Feed Water (at 549 kPa, 90°C) $2.45/1000 kg

(There is only a cost for boiler feed water if the steam produced enters process streams. If it is made into steam and subsequently condensed, it can be made into steam again, so there is no net cost for boiler feed water.)

Cooling Water $0.354/GJ

available at 516 kPa and 30°C
return pressure ≥ 308 kPa
return temperature should be no more than 15°C above the inlet temperature

Refrigerated Water $4.43/GJ

available at 516 kPa and 5°C
return pressure ≥ 308 kPa
return temperature is no higher than 15°C

Process Water $0.067/1000 kg

available at 300 kPa and 25°C

Waste Water Treatment $56/1000 m^3

Data

The following data are provided. Data are scarce for these chemicals, so it should be understood that not all of these data are exact, but they should be close enough to suffice in the solution of this project. Therefore, these data are to be used only for this project and not for any subsequent project.

Heat of Formation at 25°C (units of kJ/mol – all in gas phase except gum, which is solid phase)

acetic acid	ACO	DO	Gum
-432.25	-824.99	-332.05	-314.56

Heat of Vaporization at normal boiling point (kJ/mol)

acetic acid	ACO	DO
23.70	64.3	47.61

Vapor Phase Heat Capacity ($C_p/R = a+bT+cT^2+dT^3+eT^4$ – T in Kelvin, units of C_p are determined by value used for R)

	acetic acid	ACO	DO
a	4.375	39.947	18.375
$b\times10^3$	-2.37	-206.52	6.585
$c\times10^5$	6.757	114.814	32.307
$d\times10^8$	-8.764	155.548	-42.663
$e\times10^{11}$	3.478	67.534	16.59

Liquid Phase Heat Capacity (C_p/R) (Solid Phase for Gum – units of C_p are determined by value used for R)

acetic acid	ACO	DO	Gum
123.10	501.45	438.48	662.5

Antione's Equation Constants ($\log_{10}P^*$ (bar) = $A - B/(T(°C) + C)$)

	acetic acid	ACO	DO
A	4.454456	4.15357	4.1379
B	1555.12	1830.51	1740.88
C	224.65	154.45	167.72

Properties of Dowtherm A™ - Heat Transfer Fluid

Temperature Use Range Liquid 16°C - 400°C
Gas 257°C - 400°C
Above 400°C Dowtherm A™ starts to decompose thermally.

Liquid Properties for 350-400°C

Thermal Conductivity	0.0943	W/m.K
Specific Heat Capacity	2630	J/kg K
Viscosity	1.4×10^{-4}	kg/m s
Density	680	kg/m^3
Vapor Pressure (400°C)	10.5	bar

Other Information

You should assume that a year equals 8000 hours. This is about 330 days, which allows for periodic shut down and maintenance.

Deliverables

Each group must deliver a word-processed report. It should be clear and concise. The format is explained in a separate document. When presenting results for different cases, graphs are superior to tables. The body of the report should be short, emphasizing only the results and briefly summarizing computational strategies. The report appendix should contain details of calculations that are easy to follow. Calculations that cannot be followed easily will lose credit.

The project is due April 28, 2003, at 3:00 p.m. There will be oral presentations of project results on that day. If all presentations cannot be completed on that day, there will be additional presentations on April 30, 2003, at 3:00 p.m. There will be a project review on Thursday, May 1, 2003 (ChE 202 class). In addition, everyone must attend the senior design presentation at 2:30 p.m. on Tuesday, April 29, 2003. Furthermore, attendance is required of all students during their classmates' presentations (this means in the room, not in the hall or the computer room). Failure to attend any of the above-required sessions will result in a decrease in one letter grade (per occurrence) from your project grade in both ChE 202 and ChE 230.

Anyone not participating in this project will automatically receive an F for ChE 202 and ChE 230, regardless of other grades earned in these classes.

Groups

You will work on this project in groups of 3 or 4. More details of group formation and peer evaluation will be discussed in class.

Revisions

As with any open-ended problem; i.e., a problem with no single correct answer, the problem statement above is deliberately vague. The possibility exists that as you work on this problem, your questions will require revisions and/or clarifications. You should be aware that these revisions/clarifications may be forthcoming.

MEMORANDUM

TO: Sophomores in ChE 201 and ChE 230

FROM: R. K. Gupta
C. D. Stinespring

DATE: May 5, 2003

SUBJECT: Equipment Costs for Design Project

The equipment costs for the drying oil plant are given below. Each cost is for an individual piece of equipment, including installation.

Equipment	**Installed Cost in thousands of $**
Reactor	400
Distillation Columns, each (including peripheral heat exchangers)	200
Other Heat Exchangers shown on process flow diagram	250
Additional heat exchangers, each	50
Other equipment not shown on process flow diagram (such as pumps)	75

Fired Heater installed cost in dollars:

$$11 \times 10^{x}$$

where

$$x = 2.5 + 0.8 \log_{10} Q$$

where Q is the heat duty in kW