CHE654 – Plant Design Project #3
Semester 1, 2022

DESIGN OF A DRYING OIL PRODUCTION PROCESS

(Courtesy of the Department of Chemical Engineering at West Virginia University)

Introduction

Drying oils are additives to paints and varnishes to aid in the drying process when these products are applied to surfaces. It has been determined that the market for drying oil in Southeast Asia is expanding. Therefore, we are planning to construct a new facility to increase capacity in that region. Specifically, you are to design a new facility that produces 50,000 tonne/y of 99 wt % drying oil. The by-product acetic acid may be sold at a purity of 99.5 wt %. The facility is to manufacture drying oil (DO) from acetylated castor oil (ACO). Both of these compounds are mixtures. However, for simulation purposes, acetylated castor oil is modeled as palmitic (hexadecanoic) acid ($C_{15}H_{31}COOH$) and drying oil is modeled as 1-tetradecene ($C_{14}H_{28}$). In an undesired side reaction, a gum can be formed, which is modeled as 1-octacosene ($C_{28}H_{56}$).

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. Note that although you are to look for a "best" solution in your design, optimization is NOT required in this design project.

Reaction Kinetics

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 reactions and reaction kinetics are as follows:

$$\underset{\text{ACO}}{C_{15}H_{31}COOH(l)} \xrightarrow{k_1} \underset{\text{acetic acid}}{CH_3COOH(g)} + \underset{\text{DO}}{C_{14}H_{28}(l)} \qquad (1)$$

$$\underset{\text{DO}}{2C_{14}H_{28}(l)} \xrightarrow{k_2} \underset{\text{gum}}{C_{28}H_{56}(s)} \qquad (2)$$

where

$$-r_1 = k_1 C_{ACO} \quad (3)$$

$$-r_2 = k_2 C_{DO}^2 \quad (4)$$

and

$$k_1 = 5.538 \times 10^{13} \exp(-44{,}500 / RT) \quad (5)$$

$$k_2 = 1.55 \times 10^{26} \exp(-88{,}000 / RT) \quad (6)$$

The units of reaction rate, r_i, are kmol/m^{3}s, and the activation energy is in cal/mol (which is equivalent to kcal/kmol).

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.

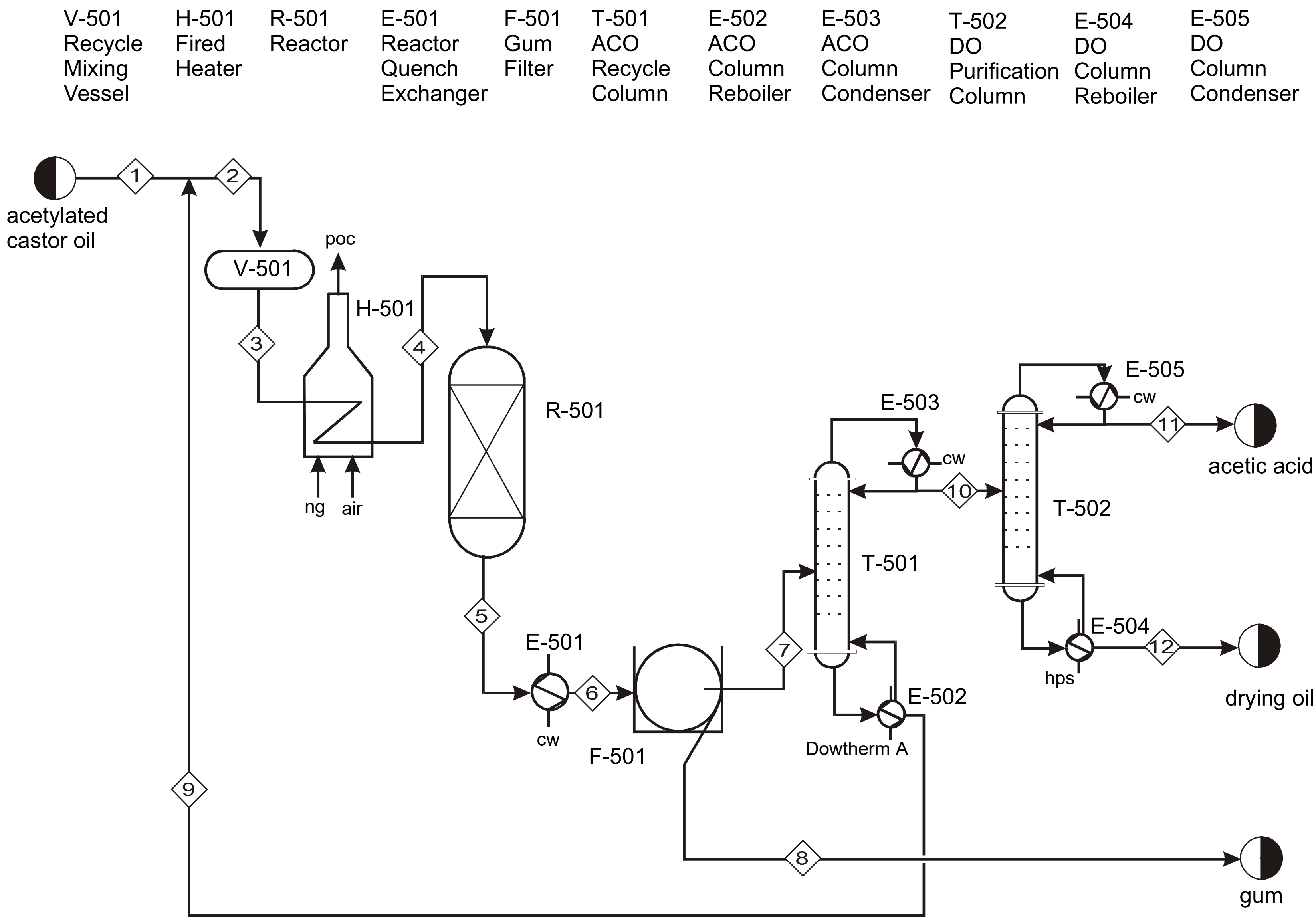

Figure 1: Preliminary Process Flowsheet for Drying Oil Production

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.

Note that the data given in this section may or may not be needed because reaction kinetics are available. Whether you will need these data depends on your assumptions so you must exercise your engineering judgments.

Design of Heat Exchanger E-501

You should perform a detailed design of the exchanger E-501 (after the reactor). You should assume that either cooling water or boiler feed water may be used to cool the stream and these are available at the conditions specified in the appendix of this problem statement. For this heat exchanger design, you should report the following information:

- Materials of construction
- Diameter of shell
- Number of tube and shell passes
- Number of tubes per pass
- Tube pitch and arrangement (triangular/square/..)
- Number of shell-side baffles and their arrangement (spacing and type)
- Diameter, thickness, and length of tubes
- Calculation of both shell- and tube-side film heat transfer coefficients.
- Calculation of overall heat transfer coefficient

- Heat transfer area of the exchanger
- Shell-side and tube-side pressure drops (note that the process-side pressure drop is used for the fluids mini-project)
- Estimated cost of exchanger

A detailed sketch of the exchanger should be included along with a set of comprehensive calculations in an appendix for the design of the heat exchangers. You should use ASPEN Exchanger Design & Rating (EDR) in the ASPEN Plus simulator to carry out the detailed design.

You should bear in mind that there could be some gum formation on the heat transfer surfaces in this exchanger. Thus your design should account for the effects of gum formation in the short-term (at start-up) and during the long-term operation of the exchanger. In addition, the exchanger may need to be taken out of service periodically for cleaning. Remember to design the unit so that easy cleaning is possible.

Economic Analysis

When evaluating alternative cases, you should carry out an economic evaluation and profitability analysis based on a number of economic criteria such as payback period, internal rate of return, and cash flow analysis. In addition, the following objective function should be used. It is the equivalent annual operating cost (EAOC), and is defined as

EAOC = −(product value – feed cost – other operating costs – capital cost annuity)

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

Utility costs are those for steam, cooling water, boiler-feed water, natural gas, and electricity.

The capital cost annuity is an ***annual*** cost (like a car payment) associated with the ***one-time***, fixed capital cost of plant construction and installation. A list of fixed capital costs on an installed basis (“installed cost”) for all pieces of equipment will be provided by mid-March.

The capital cost annuity is defined as follows:

$$\textit{capital cost annuity} = FCI\frac{i(1+i)^n}{(1+i)^n-1} \qquad (12)$$

where *FCI* is the installed cost of all equipment; *i* is the interest rate; and *n* is the plant life, in [y]. For accounting purposes, take $i = 0.15$ and $n = 10$.

For detailed sizing, costing, and economic evaluation including profitability analysis, you may use the Aspen Process Economic Analyzer (formerly Aspen Icarus Process Evaluator) in Aspen Plus. However, it is also a good idea to independently verify the final numbers based on other sources such as cost data given below.

Other Information

You should assume that a year equals 8,000 hours. This is about 330 days, which allows for periodic shut-down and maintenance.

Final Comments

As with any open-ended problem; i.e., a problem with no single correct answer, the problem statement above is deliberately vague. You may need to fill in some missing data by doing a literature search, Internets search, or making assumptions. The possibility exists that as you work on this problem, your questions will require revisions and/or clarifications of the problem statement. You should be aware that these revisions/clarifications may be forthcoming.

Moreover, in some areas (e.g. sizing/costing) you are given more data and information than what is needed. You must exercise engineering judgment and decide what data to use. Also you should also seek additional data from the literature or Internet to verify some of the data, e.g. the prices of products and raw materials.

Appendix

Equipment Cost and Design Data

Additional Property Data

The following data are provided (but may not be needed because ASPEN Plus is used). 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

Raw Materials

ACO – $0.59/kg

Product

Acetic acid – $0.99/kg

DO – $1.19/kg

Waste Disposal Cost

Gum – $1.00/kg to dispose of gum as a hazardous waste

Utility Costs

Low-Pressure Steam (618 kPa saturated) *	$6.62/1000 kg
Medium-Pressure Steam (1135 kPa saturated) *	$7.31/1000 kg
High-Pressure Steam (4237 kPa saturated) *	$8.65/1000 kg
Natural Gas (446 kPa, 25°C)	$3.00/GJ
Fuel Gas (not available for this project)	$2.75/GJ
Electricity	$0.06/kW h
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 — $0.35/GJ
available at inlet conditions of 516 kPa and 30°C
return pressure ≥ 308 kPa
return temperature <45°C

Deionized Water — $1.00/1000 kg
available at 5 bar and 30°C

Wastewater Treatment — $50/1000 m^3

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 available at 300 kPa and 25°C	$0.067/1000 kg
Waste Water Treatment	$56/1000 m^3

*You may assume that credit will be given for any and all steam produced in your process. When accounting for this credit, use the cost of the natural gas saved in any steam generating exchanger, do not use the value of the cost of the steam shown in the table above.

Equipment Costs (Purchased)

Note that not all this information is required to do this project

Piping	straight pipe	\$/m = 5.0 (nominal pipe diameter, in)(1+sch #/20)$^{0.25}$ sch = schedule number for pipe use the same sch number same for fittings and valves
	fittings (except valves)	\$/fitting = 50.0 (nominal pipe diameter, in)(1+sch #/20)$^{0.25}$
Valves	for gate (isolation) valves	\$100 (nominal pipe diameter, in)$^{0.8}$ (1+sch #/20)$^{0.25}$
	for globe valves	\$300 (nominal pipe diameter, in)$^{0.8}$ (1+sch #/20)$^{0.25}$
	for control valve use	\$1000 (nominal pipe diameter, in)$^{0.8}$(1+sch #/20)$^{0.25}$
Pumps		\$630 (power, kW)$^{0.4}$
Heat Exchangers		\$1030 (area, m^2)$^{0.6}$ add 50% additional for boilers or evaporators
Compressors		\$770 (power, kW)$^{0.96}$ + \$400 (power, kW)$^{0.6}$ assume 70% efficiency
Turbine		\$2.18×10^5 (power output, MW)$^{0.6}$ assume 65% efficiency
Fired Heater		\$635 (duty, kW)$^{0.8}$ assume 80% thermal efficiency
Vessels		$\$[1.67(0.959 + 0.041P - 8.3\times10^{-6}P^2)]\times10^z$ $z = (3.17 + 0.2D + 0.5 \log_{10}L + 0.21 \log_{10}L^2)$ D = diameter, m 0.3 m < D < 4.0 m L = height, m 3 < L/D < 20 P = absolute pressure, bar
Reactor		assume cost to be 10 times that of a vessel
Tanks		$\$1000V^{0.6}$ V = volume, m^3

Equipment Cost Factors

Pressure Factors

Pressure (absolute)	< 10 atm, 0.0	does not apply to turbines, compressors, vessels, packing, trays, or catalyst, since their cost equations include pressure effects
	10 - 20 atm, 0.6	
	20 - 40 atm, 3.0	
	40 - 50 atm, 5.0	
	50 - 100 atm, 10	

Material Factors

Carbon Steel	0.0
Stainless Steel	4.0

Total Installed Cost = Purchased Cost (4 + material factor + pressure factor)

Heat Exchangers

For heat exchangers that do not have to be designed in detail, use the following approximations for heat transfer coefficients to allow you to determine the heat transfer area and heat exchanger cost.

situation	h (W/m^2 °C)
condensing steam	6,000
condensing organic	1,000
boiling water	7,500
boiling organic	1,000
flowing liquid (hc/oils) cooling water	1,000 3,000
flowing gas	60

MEMORANDUM

TO: ChEPS Class-18 Students

FROM: Dr. Hong-ming Ku

DATE: July 13, 2022

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