Fluid Mechanics, Heat Transfer, and Thermodynamics
Fall 2003

Design Project

Production of Drying Oil

Introduction

Drying oils are additives to paints and varnishes to aid in the drying process when these products are applied to surfaces. A facility is to be designed to manufacture 25,000 metric tons/yr of 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 ($C_{28}H_{56}$). The reactions that take place (at the reactor temperature and pressure) are given below in Equations (1) and (2).

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

$$\underset{\text{DO}}{2C_{14}H_{28}(l)} \xrightarrow{k2} \underset{\text{gum}}{C_{28}H_{56}(l)} \tag{2}$$

Process Description

The process flow diagram is shown in Figure 1. ACO is fed from a holding tank, V-501, where fresh feed, Stream 1, has been mixed with recycled ACO, Stream 14. The combined ACO, Stream 2, is pumped to reaction pressure of 300 kPa and then heated to reaction temperature in a fired heater, H-501. The reaction does not require a catalyst since it is initiated at high temperatures. Typical reaction temperatures are in the range of 300 to 380°C. At temperatures higher than 380°C, some of the trace components in the drying oil degrade and give rise to an undesirable color change in the product. The reactor, R-501, is simply a vessel with inert packing to promote radial mixing. At the temperatures used here, the reaction may be assumed to go to equilibrium. The simulation of the reactor in the flowsheet should be done using Chemcad and selecting the SRK enthalpy option with the Gibbs reactor in adiabatic mode. The reaction effluent, Stream 5, contains vapor that must be separated in V-502, and sent to the Separation Equipment Block. The liquid leaving V-502 is quenched in E-501.

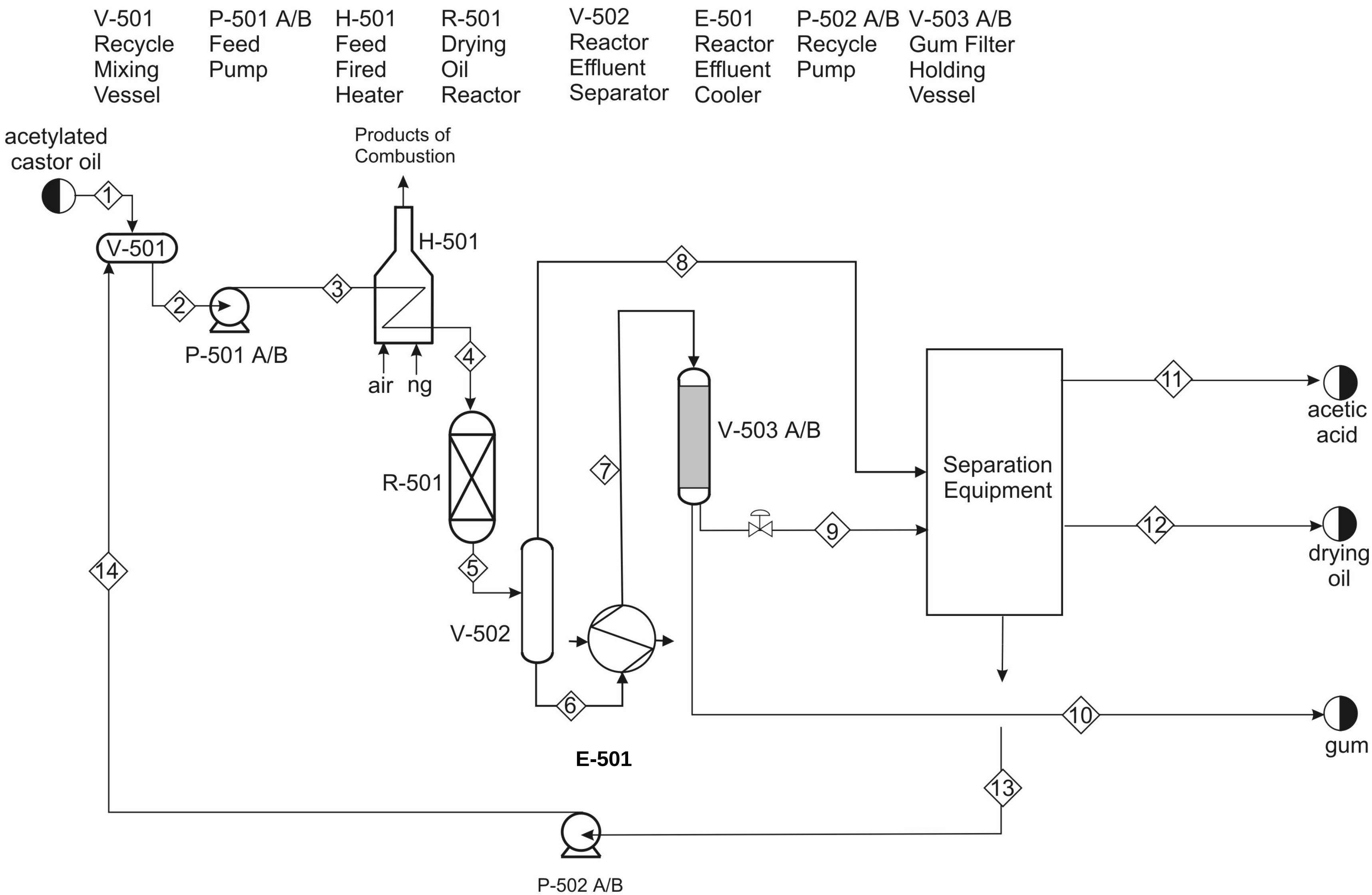


Figure 1: Preliminary Process Flow Diagram for Drying Oil Production Process

The rate of gum formation is a strong function of the maximum temperature in the reactor and correlations using past operating data have shown that the fraction of drying oil that is converted to gum is given by the following equation:

$$\text{Fraction of DO converted to Gum} = 0.04\frac{(T-300)}{(380-300)} \tag{3}$$

where *T* is the maximum (inlet) temperature in the reactor in degrees Centigrade.

Any gum that has been formed is removed by filtration in one of two packed beds, V-503A/B, containing a proprietary sorbent. These filtration vessels can only process liquid feeds at temperatures below 180°C and thus Stream 7, leaving E-501, must be a liquid at this temperature. The gum adheres preferentially to the sorbent while the other products pass through unchanged. There are two filtration vessels, V-503 A/B, one of which is used to filter the reaction products while the other one is emptied of the gum, which is subsequently sent for waste disposal. This allows a continuous flow of material, Stream 9, into the separation equipment. It should be noted that the gum contains some trace amounts of carcinogens and is to be treated as a hazardous waste.

The separation unit, which is shown as a single block in Figure 1, is comprised of many pieces of equipment. The net effect of this block is to separate the acetic acid and drying oil from the unreacted ACO, Stream 13, which is recycled back to the mixing vessel, V-501, at the front end of the process. The temperatures of acetic acid (Stream 11), DO (Stream 12), and recycled ACO (Stream 13) leaving the separation equipment block are, 120, 250, and 300°C, respectively. Streams 11 and 12 are cooled (in exchangers not shown in Figure 1) prior to being sent to storage. The purities of the three streams are 99.8 mol% acetic acid (remainder is DO), 99 mol% DO (remainder is equal mole amounts of acetic acid and ACO), and 99.8 mol% ACO (remainder is DO). In order to complete an energy balance for the separation unit, you should assume that both the heating load and cooling load for the separation unit are equal to four (4) times the net energy difference between the inlets, Streams 8 and 9, and the outlets, Streams 11 – 13. The cooling load is supplied using cooling water and the heating load is supplied with natural gas.

Specific Objectives of this Project

The main objective of this project is to optimize the drying oil production process. In order to do this, you will need to establish the flows and temperatures of all streams (Streams 1 –14) in Figure 1. You should use the Chemcad process simulator to do this task using the SRK thermodynamics package. The objective function that you should optimize (minimize) is the equivalent annual operating cost, *EAOC*, which is given below:

$$\begin{aligned} EAOC\ (\$/yr) = &\{\textstyle\sum \text{Installed Cost of Equipment}(\$)\}\{A/P,i,n\} + \text{Utility Costs}(\$/\text{yr}) \\ &+ \text{Raw Material Costs } (\$/\text{yr}) + \text{Waste Disposal Costs } (\$/\text{yr}) - \text{Product Revenue}(\$/\text{yr}) \end{aligned} \tag{4}$$

where, i is the interest rate (8% per year), n is the life of the project (assume 10 years), and the amortization factor is given by:

$$(A/P,i,n) = \frac{i(1+i)^n}{(1+i)^n - 1}$$

It should be noted that since we want to make a profit, it is desirable to have the most negative *EAOC* possible. Equipment, utility, raw materials, and product costs are given in the appendix.

Once flows and temperatures are set, you should complete the mini-projects that relate to ChE 310, and 311. The thermodynamics project should be completed at the base conditions described in the following section.

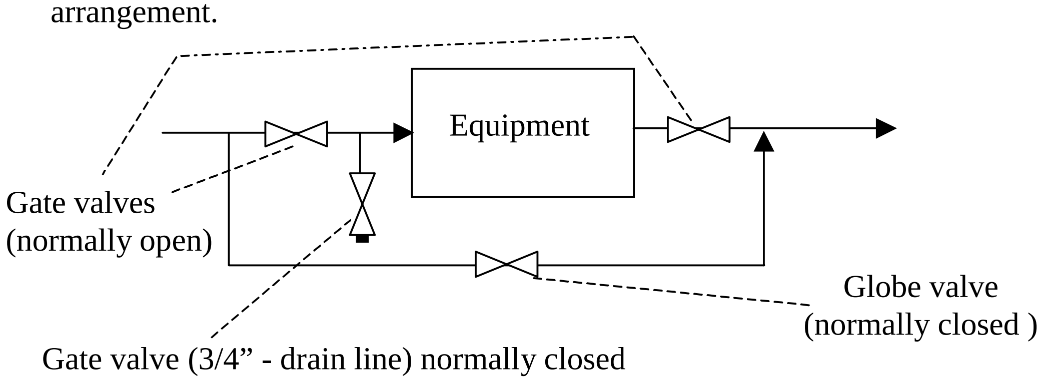
Thermodynamics (ChE 320) Mini-Project

You are to evaluate various calculation methods for the flash calculation in V-502. You should assume equilibrium conversion from the reactor for inlet conditions of 600 K and 300kPa and using the SRK k-value model as the base case. You should compare the results for liquid and vapor-phase concentrations, at these same conditions, using the Peng-Robinson, UNIFAC, and ideal vapor pressure k-value models for the flash by using the CHEMCAD software. You should make the same calculations using the VLMU software provided with your textbook, and by hand, assuming ideal solutions. Your report should compare and discuss these results.

Fluid Flow (ChE310) Mini-Project

You are required to find the optimum pipe sizes and make the pressure drop calculations for the major process lines that include all piping, pipe fittings, heat exchangers, fired heaters, reactors, and separators in the loop comprising of Streams 2 through 9.

- For any heat exchanger for which a detailed design is not performed (see the Heat Transfer section), a pressure drop of 3 psi should be used, for the process-side. For any heat exchanger for which a detailed design is required, the pressure drop must be calculated from the information in the detailed design.
- For each piece of equipment in the loop (heat exchangers, fired heaters, reactor, exchanger, and filters), isolation gate valves and a bypass line should be provided to allow for use in the event of unscheduled maintenance. The sketch below illustrates this arrangement.



- Each piece of equipment will be separated by at least 10 ft and you should estimate the amount of piping required to allow for maintenance. You should draw a rough equipment layout and determine the pipe lengths needed for each part of the piping loop based on this sketch.
- The height of liquid in V-501 may be assumed to be 3m. You should assume that the L/D = 3.0 and that when full the vessel could hold the equivalent of 30 minutes of liquid feed. The pressure in the feed vessel should be set at 101 kPa.
- The pressure drop for the fired heater should be based on liquid velocity of 2 m/s in 1”-18 BWG diameter tubes. The tubes have an equivalent length of 100 ft.
- The reactor should be sized such that the L/D = 10.0 and the exit velocity of 2 m/s. This is a vertical vessel with the feed from the top. The pressure drop across the reactor is estimated as 20 kPa at the design conditions.
- The flash vessel (V-502) should be sized such that the L/D = 3.0 and the diameter is calculated so that the upward vapor velocity is 1 m/s.
- The pressure drop through the filter, V-503, should be based on a maximum superficial velocity of 0.5 m/s with the filter packed with ¼” diameter spheres, a minimum residence time of 10 seconds, and L/D ratio of 4:1. You should use the standard equations for packed bed flow.
- The piping between the Gum Filters, V-503A/B, Stream 9, and the Separation Equipment block, should consist of 50 ft of straight pipe, 6 - 90° standard elbows, a gate valve, an orifice meter with a full scale reading of 100 inches of water pressure drop (the design flow should be 70% of full scale), the orifice meter should have two isolation gate valves and a bypass (similar to the arrangement for equipment shown in the sketch above). The inlet pressure to the separation equipment is regulated by a control valve and must be at 125 kPa. You should assume that the entrance to the separation block is at an elevation of 5m above ground level.
- For equipment with one feed and two product lines, do not include bypass lines just place a gate valve on each line.

The optimization of the piping arrangement should be done by calculating an EAOC for the piping loop. This must take into account the pumping costs and the capital costs of the pump, piping, and pipe fittings. The EAOC, defined in Equation (4), using relevant costs for the piping, pump, etc, should be used as the objective function.

It is also desired that the piping and pumping system be designed so that the process flows may be scaled-up from the base case design. You should assume that the pump you purchase (P-301 A/B) has a maximum pressure 110% of the design pressure and that the maximum volume that can be pumped is 40% greater than the design. The dimensionless form of this pump curve is given below:

$$\frac{P}{P_{design}} = 1.1 - 0.1\left[\frac{\dot{V}}{\dot{V}_{design}}\right]^{7.1265} \qquad (5)$$

where P_{design} is the pressure rise across the pump at the design volumetric flowrate of $V_{design.}$, and $\dot{V}$ is the volumetric flowrate at any pressure rise, P, across the pump.

Calculations for the optimum pipe size and maximum scale-up should be included in an appendix for this mini-project.

Heat Transfer (ChE 311) Mini-Project

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 to the mini-project.

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.

Deliverables

Written Reports

Each group must deliver a report written using a word processor. Three identical copies should be submitted, one for each instructor. The written project reports are due by 1:00 p.m. Friday, November 21, 2003. Late projects will receive a minimum of a one letter grade deduction.

The report should be clear and concise. For the correct formatting information, refer to the document entitled *Written Design Reports*. The report must contain a labeled process flow diagram (PFD) and a stream table, each in the appropriate format. The PFDs from CHEMCAD are generally unsuitable unless you modify them significantly. Figure 1 should be used as a template for your PFD. When presenting results for different cases, graphs are superior to tables. For the optimal case, the report appendix should contain details of calculations that are easy to follow. There should be separate appendices for each “mini-project.” These may be hand written if done neatly, alternatively, excel spreadsheets may be included, **but** these must be well documented so that the reader can interpret the results. Calculations that cannot be easily followed and that are not explained will lose credit.

Since this project involves “mini-designs,” it is suggested that the report be organized as follows. There should be a general abstract and introduction. Then, there should be a results section followed by a discussion section for each “mini-design.” General conclusion and recommendation sections should follow. At a minimum, there should be one appendix for each of the “mini-designs.” With this organization, there is no need for a separate section of the report for each class, as suggested in the document entitled *Written Design Reports*.

In order to evaluate each group members writing skills, the results and discussion sections for each mini-design should be written by a different group member. The authorship of each of these mini-reports should be clearly specified in the report. For groups with four members, the member not authoring a mini-report should author the safety analysis report, which is described below. The remainder of the report, namely the general abstract, general introduction, general conclusions, and general recommendations sections should be a group effort. For the group with 5 members, the 5^{th} group member must write an executive summary for the report. This executive summary should be between 3 and 5 pages long and should clearly summarize the major findings of the report. The executive summary is a standalone document and after reading it, the reader should have a clear picture of the accomplishments of the group’s work. No executive summary is required for the groups with four members.

Although the individual written portions of the reports must be authored by a single group member, it is the intent of the instructors that group members should help each other in writing different sections. To this end, we recommend that you seek input, such as proofreading and critiques, from other members of you group.

Safety Analysis Report

When designing a chemical process, it is important to know the properties of the chemicals being consumed and produced in the process. The reactivity and toxicity of the reactants and products will not only affect the design but will also affect the procedures that might be implemented during an unscheduled event such as an emergency shutdown. The purpose of the Safety Analysis Report is to make management aware of risks to personnel due to the flammability and toxicity of all chemicals consumed or produced in the process. As a minimum, the MSDS (material and safety data sheets) for all these chemicals should be provided in an appendix, and a brief description of the major concerns for each chemical should be given. Also briefly discuss possible safety hazards for each piece of equipment in your process. Finally, a feature of your process design that addresses one of these concerns should be explained.

Oral Reports

Each group will give an oral report in which the results of this project will be presented in a concise manner. The oral report should be between 15-20 minutes, and each group member must speak. Each group member should speak only once. A 5-10 minute question-and-answer session will follow, and all members must participate. Refer to the document entitled *Oral Reports* for instructions. The oral presentations will be Tuesday December 2, 2002, from 11:00 a.m. to 2:00 pm. 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 of one-letter grade (per occurrence) from your project grade in ChE 310, ChE 311, and ChE 320***.

Anyone not participating in this project will automatically receive an F for ChE 310, ChE 311, and ChE 320, regardless of other grades earned in these classes.

Groups

You will do this project in a group of four or five. You have already selected a partner, and groups of two have been paired up by the instructors. Since there are 25 students doing the project, there will be 5 groups of 4, and 1 group of 5.

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 of the problem statement. You should be aware that these revisions/clarifications may be forthcoming.

Appendix

Equipment Cost and Design Data

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)	\$2.54/1000 kg
Cooling Water available at inlet conditions of 516 kPa and 30°C return pressure ≥ 308 kPa return temperature <45°C	\$0.35/GJ
Deionized Water available at 5 bar and 30°C	\$1.00/1000 kg
Wastewater Treatment	\$50/1000 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)$(1+\text{sch }\#/20)^{0.25}$ 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)$(1+\text{sch }\#/20)^{0.25}$
Valves	for gate (isolation) valves	\$100 (nominal pipe diameter, in)$^{0.8}$ $(1+\text{sch }\#/20)^{0.25}$
	for globe valves	\$300 (nominal pipe diameter, in)$^{0.8}$ $(1+\text{sch }\#/20)^{0.25}$
	for control valve use	\$1000 (nominal pipe diameter, in)$^{0.8}$$(1+\text{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		$\$2.18\times10^5$ (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 $0.3 \text{ m} < D < 4.0 \text{ m}$ 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 10 - 20 atm, 0.6 20 - 40 atm, 3.0 40 - 50 atm, 5.0 50 - 100 atm, 10	does not apply to turbines, compressors, vessels, packing, trays, or catalyst, since their cost equations include pressure effects

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*** **($W/m^2\ ^\circ C$)**
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

Other Information

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

Unless specifically stated in class, the information in this document is valid for this project only. Any information in the sophomore projects not specifically stated in this document is not valid for this project.

Equipment Design and other Equipment Issues

You have not yet covered the theory to design some of the equipment for this project. The following information, along with the list of assumptions given in the fluids mini-project, are provided to help you design this equipment.

Storage Tanks: you should not consider the cost of (offsite) storage facilities for this project

Separation Equipment: the fixed capital investment (installed cost) for the separation equipment should not be considered in the current project.

Feed Pumps: the feed pumps must be capable of delivering the liquid feed to the reactor at the desired pressure and then the liquid must be delivered to the separation section of the plant at a pressure of 125 kPa and at a height of 5m above ground level.

Heat Exchanger: the heat exchanger after the flash vessel should be designed as per the instructions in the heat transfer mini-project.