

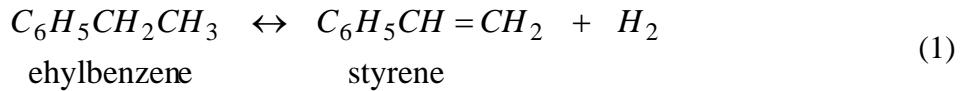
# **Fluid Mechanics, Heat Transfer, Thermodynamics Design Project**

## **Production of Styrene**

The feasibility of constructing a new, grass-roots, 100,000 tonne/y, styrene plant is being investigated. As part of the feasibility study, some of the details of the proposed plant must be analyzed.

### **Styrene Production Reaction**

For this analysis, it may be assumed that the only reaction is given in Equation 1.



For the purposes of this preliminary evaluation, it is assumed that the reaction occurs in an adiabatic packed bed of catalyst particles. Equilibrium limitations and equipment limitations make the maximum possible conversion 40%.

### **Feed and Reaction Sections**

The PFD for the feed and reaction sections is given in Figure 1. The feed to the process is liquid ethylbenzene. The pressure drop at all mixing points is 10 kPa.

The reaction is endothermic, and the reactor is adiabatic. The only constraint is a maximum temperature of 600°C. Following the reactor, the reaction products are cooled to the three-phase flash conditions. In the three-phase flash, hydrogen and wastewater are separated from the organics. Ethylbenzene and styrene are separated in a distillation column, which may be assumed to be a perfect separator for this semester's project only. The wastewater stream must be at 200 kPa and the hydrogen stream at 300 kPa for further treatment.

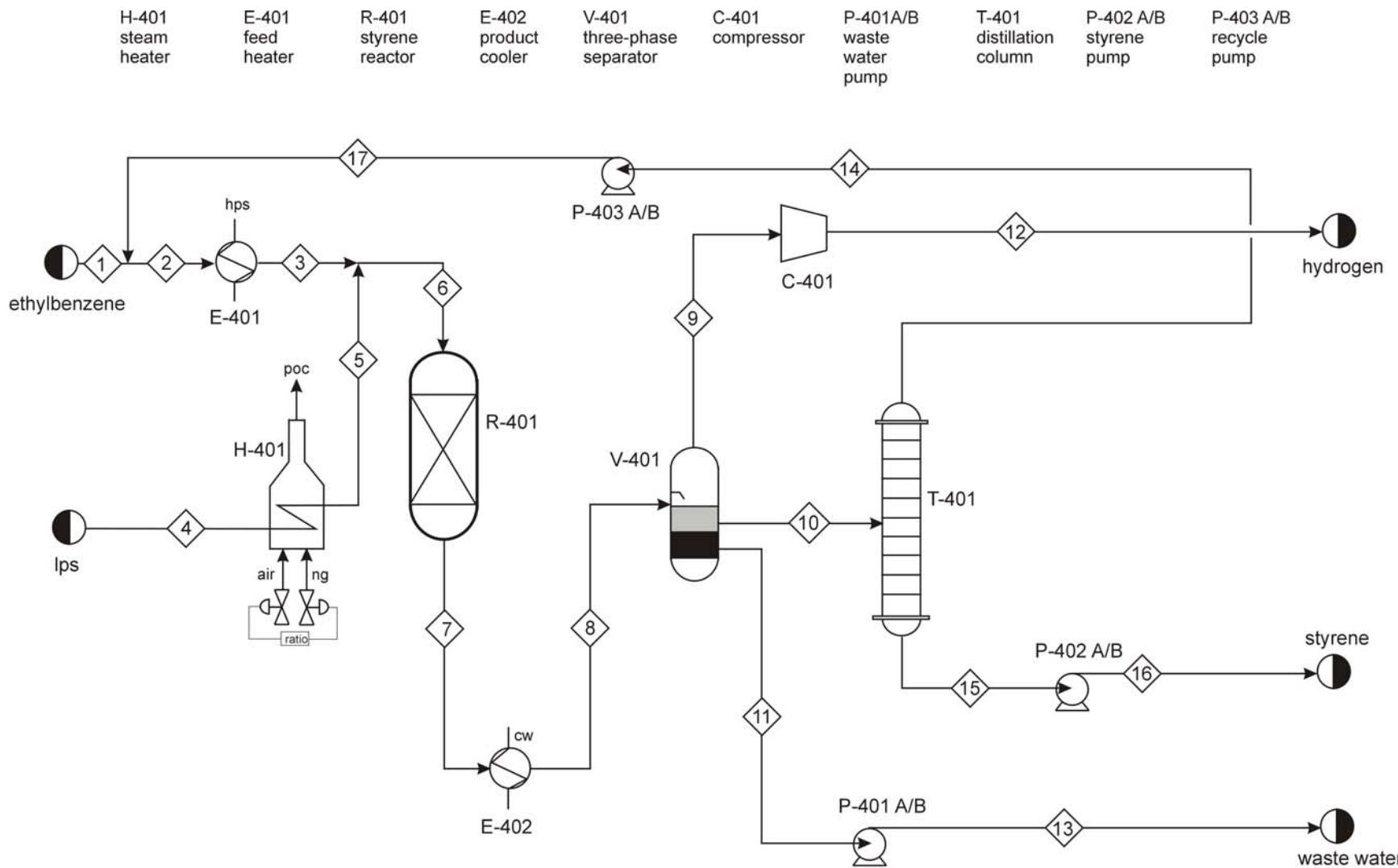


Figure 1: Unit 400: Production of Styrene from Ethylbenzene

## Process Details

### Feed Streams

- Stream 1: ethylbenzene liquid at 210 kPa, 136°C
- Stream 4: low-pressure steam at 3000 kmol/h
- Stream 17: recycle ethylbenzene, at 210 kPa – temperature is that of saturated liquid at pressure of distillation column, which is 60 kPa

### Effluent Streams

- Stream 12: Hydrogen by-product – must be at 300 kPa – purification and sale should not be considered – it can be burned for credit at its LHV
- Stream 13: Wastewater stream to treatment – must be at 200 kPa
- Stream 16: Styrene product – must be at 200 kPa

### Equipment Summary

- H-401: Fired Heater – a furnace that can heat to temperatures above high-pressure steam using an open flame – outlet temperature to be determined
- E-401: Heat Exchanger – to preheat and vaporize ethylbenzene feed to 240°C
- R-401: Reactor – adiabatic – inlet temperature must be 550°C and the inlet pressure must be 155 kPa – assume to have a pressure drop of 45 kPa
- E-402: Product cooler – cools reactor outlet stream to 65°C – assume to have a pressure drop of 35 kPa
- V-401: Three-phase separator operating at 75 kPa – produces an oil-water-gas three-phase mixture that is assumed to separate easily into three distinct streams – can be simulated on Chemcad using a perfect component separator
- C-401: Compressor – to compress hydrogen to the required pressure – the compressor has an isentropic efficiency of 75% and a maximum operating temperature of 200°C
- P-401: Pump – to pump waste water to required pressure – A/B means two in parallel with only one operating
- P-402: Pump – to pump styrene product to required pressure – A/B means two in parallel with only one operating

- P-403: Pump – to pump ethylbenzene recycle to required pressure – A/B means two in parallel with only one operating
- T-401: Distillation column – to produce styrene product and ethylbenzene for recycle – the component separator in Chemcad should be used – a perfect separator may be assumed (which is physically impossible) for this semester only, *i.e.*, all ethylbenzene to the recycle and all styrene to the product

## Assignment

The first task is to obtain base-case stream flows for the process using Chemcad.

The remainder of the assignment consists of five “mini-designs.”

### 1. Fluid Mechanics (ChE 310) – Optimization of the Feed Section and Wastewater Pump.

Pump P-401 A/B should be sized. The optimum pipe size for Streams 11 and 13 should be determined. The objective function for the optimization is the Equivalent Annual Operating Cost (EAOC) of the pipe in Streams 11 and 13 and of P-401 A/B (\$/y). The EAOC is defined as:

$$EAOC = CAP \left( \frac{A}{P}, i, n \right) + \text{annual operating costs for P - 401 A/B} \quad (2)$$

where  $CAP$  = the installed cost of P-401 A/B and the pipe in Streams 11 and 13, and

$$\left( \frac{A}{P}, i, n \right) = \frac{i(1+i)^n}{[(1+i)^n - 1]} \quad (3)$$

where  $i = 0.15$  (15% rate of return) and  $n = 10$  (ten-year plant life).

Raw-material costs or wastewater-treatment costs should not be included, so  $CAP$  only includes the installed cost of pipes and pumps, and operating costs include the electricity to run the pump. The liquid level to be maintained in V-401 to avoid cavitation of P-401 A/B should be specified. Pump P-401 A/B is 5 m horizontally distant from the V-401 draw, the tank bottom is 3 m above the pump suction line, and this piping contains two 90° elbows. Stream 13 has an equivalent length of 100 m. There is a supply of centrifugal pumps used in other plants. Their pump curves and their NPSH curves are attached (Figures 2 and 3). The data for these figures are shown in Table 1. The design should include flexibility for 30% scale-up in the future.

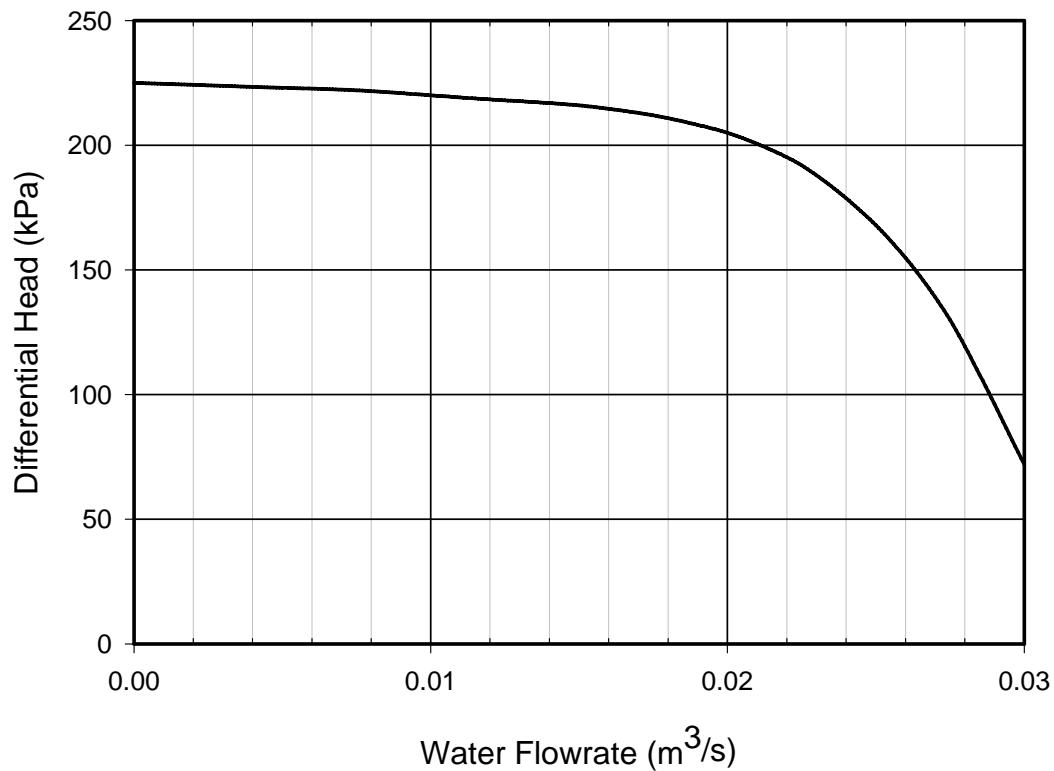


Figure 2: Pump Curve for P-401 A/B

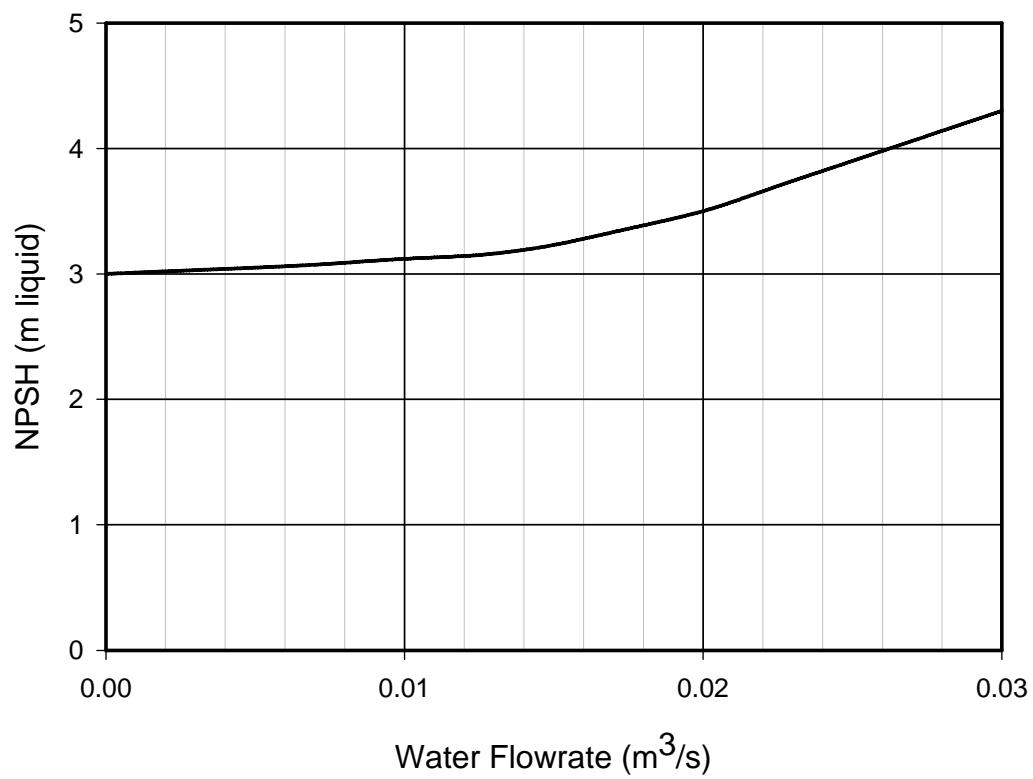


Figure 3: NPSH Curve for P-401 A/B

**Table 1: Data for Figures 2 and 3**

<b>water flowrate (m<sup>3</sup>/s)</b>	<b>differential head (kPa)</b>	<b>NPSH (m liquid)</b>
0.0000	225	3.000
0.0025	224	3.025
0.0050	223	3.050
0.0075	222	3.080
0.0100	220	3.120
0.0125	218	3.150
0.0150	216	3.230
0.0175	212	3.360
0.0200	205	3.500
0.0225	192	3.700
0.0250	168	3.900
0.0275	130	4.100
0.0300	72	4.300

The pressure drop from V-401 to the compressor inlet is 10 kPa, which is applicable to the thermodynamics design section.

## 2. Heat Transfer (ChE 311) – Design of E-401.

The heat exchanger, E-401, must be designed in detail for the base case. Assume the inlet pressure is the same as Stream 1. The outlet pressure must be as specified based on the heat-exchanger design and the required inlet pressure to the reactor. It should be assumed that utilities are available at the conditions specified in the Appendix of this problem statement. For this heat exchanger design, the following information should be provided:

- Diameter of shell
- Thickness of shell wall
- Number of tube and shell passes (where applicable)
- Number of tubes per pass
- Tube pitch and arrangement (triangular/square/..)
- Number of shell-side baffles, if any, and their arrangement (spacing, pitch, type)
- Tue diameter, tube-wall thickness, and length of tubes
- Calculation of both shell- and tube-side film heat transfer coefficients
- Calculation of overall heat transfer coefficient (you may assume that there is no fouling on either side of the exchanger)
- Heat transfer area of the exchanger
- Shell-side and tube-side pressure drops (calculated, not estimated)
- Materials of construction for the shell and the tubes
- Approximate cost of the exchanger

The maximum heat exchanger length is 20 ft., and the shell diameter should be the minimum required for the stated duty. A detailed sketch of the exchanger should be included along with a set of comprehensive calculations in an appendix to the mini-design.

### **3. Thermodynamics (ChE 320) – Design of the hydrogen compression system**

The equivalent annual operating cost, *EAOC*, for the hydrogen compression section of the process should be minimized with the following in mind:

- The hydrogen effluent should be compressed to the required effluent conditions (300 kPa). According to the compressor manufacturer, the maximum compressor operating temperature for operation with hydrogen should be 200°C. Therefore, the compressor section must be optimized within these constraints.

The optimization for this mini-project should include the cost of the compressor(s), the cost of any heat exchangers required, the cost of cooling water, and the cost of electricity. Raw material costs should not be included, so *CAP* (the capital investment for equipment used in the equation for *EAOC* given in Equation 2) includes only the installed cost of compressor stages and heat exchangers, and annual operating costs include the electricity to run the compressor stages and the cost of cooling water in the intercoolers, if used. Note that there is no revenue term for this mini-design.

The objective function for the optimization is the Equivalent Annual Operating Cost (*EAOC* \$/y) of the hydrogen compression system including the compressor. The *EAOC* was defined in Equations 2 and 3.

### **4. 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 as well as the impact of any extreme process conditions. The purpose of the safety analysis report is to make management aware of risks to personnel due to extreme operating conditions as well as 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 discussion of the major concerns for each chemical should be given as a separate section of the report. This discussion should include general concerns and concerns that are specific to the operating conditions in this process. In addition, a brief discussion of possible safety hazards for each piece of equipment in your process should be provided. Finally, an aspect of your process design that addresses one of these safety concerns should be explained.

### **5. Chemcad/Process Improvements**

A Chemcad simulation of the base case of the process shown in Figure 1 should be provided. Process improvements that do not violate the laws of physics may be suggested. An explanation of the rationale for such process improvements should be

provided, including an economic analysis, if possible. For a process improvement involving additional equipment, use Equation 2, where  $CAP$ , is the cost of additional equipment and “annual operating costs” are the savings realized (hence a negative number). This is called an “incremental” analysis, and the  $EAOC$  for a good process modification should be negative, *i.e.*, profitable.

## Other Information

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

## Suggested Plan of Attack

The safety analysis can begin as soon as the project is distributed. A good place to find MSDS sheets is <http://siri.org>. The Chemcad simulation can also be done immediately. Once the Chemcad simulation is done, the fluid mechanics optimization, the heat exchanger design, and the compressor optimization can be completed.

## Deliverables

### Written Reports

Each team must deliver a report written using a word processor. Three identical copies should be submitted, one for each instructor, unless an electronic copy is requested by the instructor after this document is distributed. The written project reports for all teams, regardless of presentation date, are due by 11:00 a.m. Wednesday, November 30, 2011. Late projects will receive a minimum of a one letter grade deduction.

The report should be clear and concise. Guidelines are in 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 (example will be provided). The preferred software for preparing PFDs is Corel Draw. A PFD from Chemcad is unacceptable; however, it should be included in the appendix along with a Consolidated Chemcad Report for the base case. The Consolidated Chemcad Report should contain stream compositions, **but not stream properties**. 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-design.” 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. In either case, the calculations should be clear and all assumptions made should be explained and justified. 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, which summarizes the results of your work, emphasizing what you found, not what you did. There should also be an introduction that orients the reader to the all the mini-designs. Then, there should be a results section followed by a discussion section for each “mini-design.” A general conclusion and recommendation section

should follow. At a minimum, there should be one appendix for each of the “mini-designs,” with detailed calculations that are clearly written and easy to follow.

In order to evaluate each team member’s writing skills, the results and discussion sections for each mini-design should be written by a different team member. The authorship of each of these mini-reports should be clearly specified in the report. Although the individual written portions of the reports must be authored by a single team member, it is the intent of the instructors that team members should help each other in writing different sections. To this end, it is recommended that input be sought from your team members, including items such as proofreading and critiques.

The reports will be evaluated as follows:

- course-specific technical content – 50%
- oral presentation – 20%
- written report – 20%
- technical quality of general sections (safety, simulation, etc.) – 10%

For a more detailed set of evaluation criteria that we will use, see the following web site (design project assessment, oral report assessment, written report assessment):

<http://www.che.cemr.wvu.edu/ugrad/outcomes/rubrics/index.php>

Each report will be assessed separately by each of the three instructors. A historical account of what each team did is neither required nor desired. Results and explanations should be those needed to justify your choices, not a litany of everything that was tried. Each mini-report should be limited to 4-5 double space pages plus figures and tables.

## Oral Reports

Each team 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 team member must speak. Each team member should speak only once. A 5-10 minute question-and-answer session will follow, and all members must participate. Guidelines are in the document entitled *Oral Reports*. The oral presentations will be Wednesday, November 30, from 11:00 a.m. to 1:00 p.m.; Thursday, December 1, 2011, from 11:00 a.m. to 2:00 p.m.; and on Friday, December 2, 2011, from 11:00 a.m. to 1:00 p.m. 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 failing to present with his or her team is subject to a minimum one-letter-grade deduction from the project grade.***

## Project Review

There will be a project review at 11:00 a.m. on Friday, December 9, 2011. Attendance is expected.

## Teams

This project will be completed in teams of 3 or 4. More details of team formation will be discussed in class. There will also be peer evaluations of team members, one midway through the project and one after the project is submitted. These will be done on-line, and there will be a window of time when the evaluation must be submitted. **Anyone not completing either the interim or the final peer evaluation will lose one full letter grade in the design grade for all three classes for each evaluation not completed. The results of this evaluation may affect individual team members' grades, so that each team member may not receive the same grade for the project.**

## 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 the project proceeds, questions from the class will require revisions and/or clarifications. It is important to be aware that these revisions/clarifications may be forthcoming.

## Appendix

### Economic Data

#### Equipment Costs (Purchased)

Note: The numbers following the attribute are the minimum and maximum values for that attribute. For a piece of equipment with a lower attribute value than the minimum, the minimum attribute value should be used to compute the cost. For a piece of equipment with a larger attribute value, extrapolation is possible, but inaccurate. To err on the side of caution, the price for multiple, identical, smaller pieces of equipment should be used.

Pumps  $\log_{10}(\text{purchased cost}) = 3.4 + 0.05\log_{10}W + 0.15[\log_{10}W]^2$   
 $W = \text{power (kW, 1, 300)}$   
assume 80% efficiency

Heat Exchangers  $\log_{10}(\text{purchased cost}) = 4.6 - 0.8\log_{10}A + 0.3[\log_{10}A]^2$   
 $A = \text{heat exchange area (m}^2, 20, 1000)$

Compressors  $\log_{10}(\text{purchased cost}) = 2.3 + 1.4\log_{10}W - 0.1[\log_{10}W]^2$   
 $W = \text{power (kW, 450, no limit)}$   
assume 65% efficiency

Compressor Drive  $\log_{10}(\text{purchased cost}) = 2.5 + 1.4\log_{10}W - 0.18[\log_{10}W]^2$   
 $W = \text{power (kW, 75, 2600)}$

Turbine  $\log_{10}(\text{purchased cost}) = 2.5 + 1.45\log_{10}W - 0.17[\log_{10}W]^2$   
 $W = \text{power (kW, 100, 4000)}$   
assume 65% efficiency

Fired Heater  $\log_{10}(\text{purchased cost}) = 3.0 + 0.66\log_{10}Q + 0.02[\log_{10}Q]^2$   
 $Q = \text{duty (kW, 3000, 100,000)}$   
assume 80% thermal efficiency  
assume can be designed to use any organic compound as a fuel

Vertical Vessel  $\log_{10}(\text{purchased cost}) = 3.5 + 0.45\log_{10}V + 0.11[\log_{10}V]^2$   
 $V = \text{volume of vessel (m}^3, 0.3, 520)$

Horizontal Vessel  $\log_{10}(\text{purchased cost}) = 3.5 + 0.38\log_{10}V + 0.09[\log_{10}V]^2$   
 $V = \text{volume of vessel (m}^3, 0.1, 628)$

Storage Tanks  $\log_{10}(\text{purchased cost}) = 4.85 - 0.397\log_{10}V + 0.145[\log_{10}V]^2$   
 $V = \text{volume of tank (m}^3, 90, 30000)$

## Additional Cost Information

Piping straight pipe:  $\$/m = 5.0 \text{ (nominal pipe diameter, in)}(1+(sch \#)/20)^{0.25}$   
sch = schedule number for pipe  
use the same schedule number for fittings and valves

Fittings (except valves)  $\$/fitting = 50.0 \text{ (nominal pipe diameter, in)}(1+(sch \#)/20)^{0.25}$

### Valves

for gate (isolation) valves  $\$100 \text{ (nominal pipe diameter, in)}^{0.8} (1+(sch \#)/20)^{0.25}$   
for control valve use  $\$1000 \text{ (nominal pipe diameter, in)}^{0.8} (1+(sch \#)/20)^{0.25}$

## Utility Costs

Low-Pressure Steam (618 kPa saturated)	\$13.28/GJ
Medium-Pressure Steam (1135 kPa saturated)	\$14.19/GJ
High-Pressure Steam (4237 kPa saturated)	\$17.70/GJ
Natural Gas (446 kPa, 25°C)	\$11.00/GJ
Fuel-gas/Off-gas Credit	at LHV
Electricity	\$0.06/kWh
Boiler Feed Water (at 549 kPa, 90°C)	\$2.45/1000 kg
Cooling Water	\$0.354/GJ
available at 516 kPa and 30°C	
return pressure $\geq 308 \text{ kPa}$	
return temperature is no more than 15°C above the inlet temperature	
Refrigerated Water	\$4.43/GJ
available at 516 kPa and 10°C	
return pressure $\geq 308 \text{ kPa}$	
return temperature is no higher than 20°C	
Deionized Water	\$1.00/1000 kg
available at 5 bar and 30°C	
Low-temperature Refrigerant	\$7.89/GJ
available at -20°C	

Very low-temperature Refrigerant  
available at -50°C \$13.11/GJ

Wastewater Treatment \$56/1000 m<sup>3</sup>

## Equipment Cost Factors

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

Pressure (absolute)	< 10 atm, PF = 0.0	does not apply to turbines, compressors, vessels, packing, trays, or catalyst, since their cost equations include pressure effects
10 - 20 atm, PF = 0.6		
20 - 40 atm, PF = 3.0		
40 - 50 atm, PR = 5.0		
50 - 100 atm, PF = 10		
100 - 200 atm, PF = 25		

Carbon Steel MF = 0.0

Stainless Steel MF = 4.0

## Heat Exchangers

For heat exchangers that do not have to be designed in detail, the following approximations should be used for heat transfer coefficients to calculate the heat transfer area and heat exchanger cost.

situation	<i>h</i> (W/m <sup>2</sup> °C)
condensing steam	6000
condensing organic	1000
boiling water	7500
boiling organic	2000
flowing liquid	600
flowing gas	60

## Raw Material Costs/Product Value

Raw Material or Product	price
ethylbenzene	see <a href="http://www.icis.com/StaticPages/a-e.htm">http://www.icis.com/StaticPages/a-e.htm</a>
styrene	see <a href="http://www.icis.com/StaticPages/a-e.htm">http://www.icis.com/StaticPages/a-e.htm</a>
hydrogen	\$1.00/kg