A PRACTICAL GUIDE TO CHEMICAL PROCESS OPTIMIZATION: ANALYSIS OF A STYRENE PLANT

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ABSTRACT

This report acts as a beginner's guide to chemical processes optimization. Performed universally, optimization merely entails improving an existing process, situation, device or system. For a chemical engineer, optimization typically aims to maximize potential economics of a chemical process by manipulating decision variables while staying within known constraints. In order to maximize the overall economics of a chemical process, individual equipment or stream conditions are examined. The chemical process is implemented in simulation software The optimization of individual components of the process may aim to maximize or minimize an outcome specific to that component, but still ultimately maximizes economic potential. An engineer must determine how each component of the process ultimately impacts the overall economic potential.

Upon initial analysis of a chemical process, optimization can seem overwhelming. This report first defines, explains and exemplifies all the nomenclature used to develop, solve and evaluate optimization. This is follow by identification and analysis of the two types of optimization. This knowledge allows for final development of a generalized approach to chemical process optimization, including a specific and complete optimization example. All included examples focus on a specific chemical process designed for styrene production.

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1. INTRODUCTION

Optimization simply means improving an existing process, situation, device or system, such as a chemical process. It is a complex, endless practice that employs creative investigation of a given design. When manipulating aspects of design, the impact of change must be clearly understood, which is no easy task. In a chemical process, finding true optimum values would require comparison of infinite possible designs, meaning it is unobtainable.

Ultimately, this paper serves as a beginner's guide to practical chemical process optimization. This guide assists any skill level by decomposing the very complicated practice of chemical process optimization into its fundamental concepts. These concepts are each clarified by an example specific to a styrene production process. These examples focus on a particular unit responsible for styrene production, Unit 500.

2. OPTIMIZATION NOMENCLATURE

Base Case

Base Case defines initial conditions from which to begin optimization. As stated earlier, optimization means improving something already existing. Without a base case's defined process, there would be nothing to optimize. The base case can take many forms: a simple flowsheet, a detailed design, an operating plant, etc. Essentially, the base case can be as extensive as an entire chemical process or as simple as a single piece of equipment. The base case must include sufficient details to effectively and accurately optimize and evaluate the desired improvement. The scope of optimization is equivalent to the scope of the base case design. All chemical process optimization demands at least one product specification, such as product purity or production rates.

Unit 500 Base Case

Throughout this discussion, the base case design is the design for styrene production in Unit 500 from Richard Turton's *Analysis Synthesis and Design of Chemical Processes*. Unit 500 annually produces

100,000 metric tons of 99.5 weight% styrene from the dehydrogenation of ethylbenzene from a neighboring unit. This unit is part of larger plant that manufactures benzene, ethylbenzene, styrene, and polystyrene. Benzene is a product of the dealkylation of toluene, which is obtained as a byproduct of gasoline manufacture. The reaction of benzene and ethylene produces ethylbenzene, which can be used to produce styrene and eventually polystyrene.

In the base case design, the reactor section consists of two adiabatic packed bed reactors with interheating. Since the conversion of ethylbenzene to styrene is an endothermic reaction, interheating is included to provide energy necessary for the reaction. Ethylbenzene converts to benzene and ethylene or toluene and methane in competing reactions. Fresh ethylbenzene combines with a recycle of ethylbenzen and steam to form the gas phase reactor feed. An effluent cooling section and a separation section follows the reactor section. In Appendix 1, a process flow diagram (PFD) taken from *Analysis, Synthesis and Design of Chemical Processes* can be found. Please refer to this text for corresponding stream and equipment tables.

The reactions for production of styrene with the available catalyst are as follows:

$$\underset{\textit{ethylbenzene}}{C_6H_5C_2H_5} \leftrightarrow \underset{\textit{styrene}}{C_6H_5C_2H_3} + \underset{\textit{hydrogen}}{H_2} \quad (1)$$

$$\underset{\textit{ethylbenzene}}{C_6H_5C_2H_5} \rightarrow \underset{\textit{benzene}}{C_6H_6} + \underset{\textit{ethylene}}{C_2H_4} \quad (2)$$

$$\underset{\textit{ethylbenzene}}{C_6H_5C_2H_5} + \underset{\textit{hydrogen}}{H_2} \rightarrow \underset{\textit{toluene}}{C_6H_5CH_3} + \underset{\textit{methane}}{CH_4} \quad (3)$$

Objective Function

An *objective Function* is a mathematical function intending to maximize or minimize a restrained global characteristic of the process. This function defines a scalar quantitative performance measure. The scope of an objective function depends on the optimization goal. After choosing an objective function, potential improvement can be quantified by exploiting restricted available degrees of freedom. The same

global characteristic can be maximized or minimized in two very different chemical process optimizations, such as improving a design concept or expanding an existing plant.

Chemical process optimization usually aims to maximize profit or minimize costs, meaning the objective function generally has a unit of dollars. However, the chemical product very much dictates process design goals. Optimizing production of a specialty chemical might focus on increasing product purity and overall quality rather than reducing operating costs. This will largely depend on the market demand. For economic optimization, profit is often measured by calculating net present value (NPV), while cost is often measured by equivalent annual operating cost (EAOC).

Base Case Analysis

Unless previously defined, an objective function is identified through base case analysis. Without a well-chosen and precise objective function, the optimization results are worthless. Because the objective function is contingent to the base case, insufficient base case information will render useless optimization results. Therefore, it is essential that the base case analysis yields an objective function effected by all important decision variables. The initial analysis can neglect some decision variables if justified.

By first investigating a process under ideal conditions, the idealized value for the objective function provides a framework for assessing optimization results. This examination at the highest level ensures an overall process feasibility. The idealized process assumes equilibrium conversion, no equipment costs, no utility costs and perfect separations. Under these assumptions, initial base case cost analysis provides the economic potential for the process. The initial base case analysis sets optimization target and illuminates the next steps in the optimization process.

Unit 500 Base Case Analysis

The overall objective function of Unit 500 optimization is to maximize the net present value of the plant. To begin, conducting an economic potential analysis of the plant then determined its potential profitability, thereby providing an absolute maximum NPV. With an operating year defined at 8000 hours,

and assuming ideal separation, the economic potential of Unit 500 is equal to about $67 million per year. The process concept diagram for the economic potential analysis can be seen in Figure 1 below.

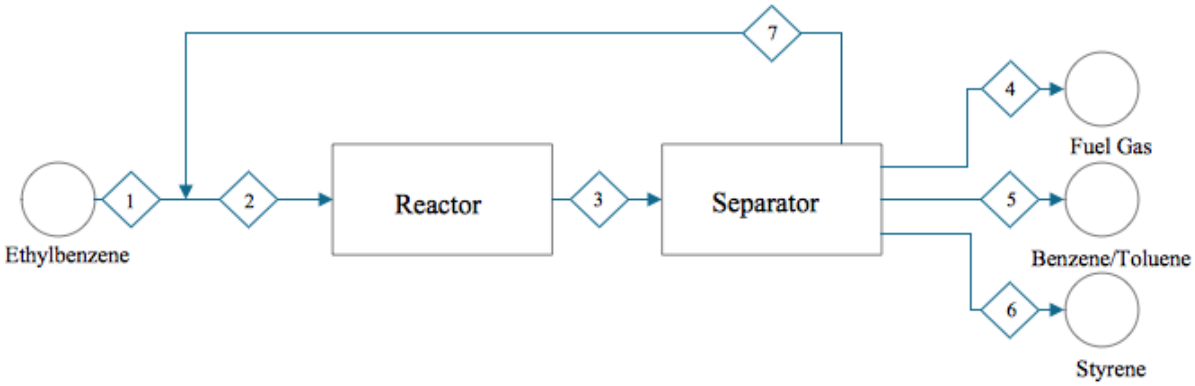


Figure 1. Process Concept Diagram for Unit 500.

Using the provided equipment descriptions, the base case styrene production process was simulated in PRO/II. Based on simulation results and heuristics, initial calculation of equipment sizes and pricing enabled calculation of the fixed cost investment. These simulation results and heuristics further permitted calculation of the cost of manufacturing. The heuristics were taken from *Analysis, Synthesis and Design of Chemical Processes*. Subsequent formation of a cash flow statement included these calculated costs, along with the economic factors described in the given base case. Based on the resulting annual cash flow statement, the base case final NPV equaled -$613 million, with a revenue of $170 million per year, a raw material cost of $117 million per year and a fixed capital investment of $251 million.

All calculations necessary for determining NPV were completed in Microsoft Excel. A well designed spreadsheet increased efficiency in evaluating optimization results. As previously discussed, the overall objective function decision variables often have their own functions, which can also contain variables with their own function. For any calculation that relies on a previously calculated value, the formula should never include the calculated value, but reference the cell of that value. This is essential for efficient optimization. For example, inputting an updated inlet process temperature change for a heat

exchanger will automatically update required equipment size, which will then update utility costs, equipment cost, the fixed capital investment and ultimately NPV.

As base case analysis demonstrates economic feasibility, a NPV of -$613 does not appear to warrant further optimization or design of Unit 500. Recalling the initial explanation that Unit 500 belongs to a larger plant that ultimately produces polystyrene, Unit 500 essentially produces a raw material. As the plant ultimately operates to produce polystyrene, expected NPV of the polystyrene producing unit should be significant larger than any other unit within the plant. In the polystyrene production unit, the raw material is styrene produced in Unit 500. Although Unit 500 might not be profitable, the savings by producing styrene rather than purchasing from an independent supplier can significantly reduce raw material cost for polystyrene production. Therefore, a negative NPV of Unit 500 can be acceptable.

Assumptions

The objective function should be formed based on assumptions. Assumptions simplify calculations and are necessary in forming an objective function. As optimization can only begin upon defining an objective function, process optimization often requires assumptions. However, they must be carefully chosen and their validity later confirmed. In addition, the objective function can be further simplified by assuming, which may mean neglecting, values of decision variables based on sensitivity analysis.

Assumptions can take many forms. For example, gross profit margin of a chemical process can be simplified by assuming equilibrium conversion, no equipment costs, no utility costs and perfect separations. Some other assumptions might be the value of raw material cost, the cheapest raw material supplier, no by-product reactions, etc.

Unit 500 Assumptions

The following list contains the economic and operating assumptions regarding Unit 500 that both allow and simplify NPV calculations:

- The cost of operating labor is $59,580 per operator per year

- The buildings will cost $3,000,000, will depreciate over 39 years, and will be worth $1,000,000 at the end of the project
- The land will cost $2,500,000 and will sell for $11,000,000 at the end of the project
- Plant construction will begin in June 2015, take 1 ½ years to build, and will last 12 years after startup
- The building will be bought in February and sold in December, in the appropriate years
- 1/3 of equipment cost will be allocated to the first year, and 2/3 will be allocated to the second
- Land cost will be allocated to the first year, and building cost to the second
- Working capital will cover a 1-month supply of raw materials and 3 months of personnel costs
- The corporate tax rate is 35%
- Inflation will increase labor and energy costs at the rate of 3% per year
- The salvage value of the equipment is 11% of the fixed capital investment
- The Minimum Acceptable Rate of Return (MARR) is 12%
- Equipment will depreciate using a 7 years Modified Accelerated Cost Recovery System (MACRS)
- The on-site ethylbenzene plant will provide the ethylbenzene feedstock at a cost of $0.90/kg. The cost for utilities and other chemicals used in the process are from *Analysis, Synthesis, and Design of Chemical Processes*[1].

Decision Variables

Decision Variables, also called *Design Variables*, are the independent variables that can be controlled or changed by the engineer. However, there are limits to the extent to which they can be changed. These variables can be continuous or discrete, the former meaning any value over a continuous range while the latter meaning specific values.

Optimization does not begin until decision variables are identified and prioritized. Forming the objective function requires a feasible starting value for every decision variable. An engineer must prioritize the decision variables in the initial stages of optimization based on their impact on the objective function. Prioritization of decision variables reduces computational time and effort, thus is essential for an efficient optimization process.

An engineer can easily identify the decision variables with the greatest impact on the objective function through a sensitivity analysis. Essentially, the objective function is evaluated by varying a specific decision variable within its limits, with all others are held constant. The objective function can also be evaluated at different percent changes of a single variable, keeping all other variables equal. Then the process is repeated for all variables susceptible to design change. By graphing percent change of variable versus objective function value, with each variable represented by a separate line, the decision variables with the greatest impact on the objective function can easily be identified.

Optimization often requires many variables within the overall objective function to have their own objective function. For example, the global objective function might measure profit, which is impacted by equipment cost, while a reactor included in that cost might have an independent objective function maximizing conversion. The true art in optimization lies in a thorough understanding of how changes in a decision variable's value impact both the other decision variables' values and the objective function. The infinite combinations of decision variables accounts for the endless nature of optimization.

An overall chemical process converts raw materials into desired products. Still, this simple goal process requires many steps accomplishing separation, mixing, heating, cooling, reaction, etc., depending on the specific process. In chemical process economic evaluation, sensitivity analysis often identifies raw material cost as having the largest impact, which is expected as this cost accounts for the majority of reoccurring costs. The majority of chemical processes utilize a recycle loop in order to recover unused

reactants, which effectively minimizes raw material costs. A recycle loop severely complicates optimization because a single change in an operating condition within the loop impacts all equipment and streams included in the recycle loop. This contrasts with an operating condition change in equipment outside a recycle loop impacting only the following, or downstream, equipment. Although raw material costs can be lowered through optimization, sufficient raw material must be purchased to meet the final product production rates. The minimum of raw materials needed occurs with 100% conversion of raw materials, no side reactions and no loss of raw materials throughout the process. This exemplifies the complex relationship between decision variables. Identifying raw material as the most significant, but highly constrained, variable actually indicates that reactor design plays a highly significant role in potential profitability. Without understanding the impact of the reactor on raw material costs, the importance of reactor design would be overlooked. This further validates the necessity of understanding decision variables and their role on the value of both the objective function and the other decision variables.

As raw conversion the purpose of a chemical process, the process design begins with the reactor design; thus the reactor should be optimized first. Reactor design not only determines raw material requirements, but it determines the overall quantity and composition of inerts and reactants fed to the reactor in order to meet product demand. Inerts are unreactive material that help control reactions and processes, typically separated as a waste stream. The resulting reactor effluent contains the amount of desired products, unwanted by-products, waste and unreacted feed. Any remaining reactants will almost always be recycled because of high material costs. Separation requirements of a process typically involve purifying the remaining reactant for recycle and purifying the desired products for sale. The demands on the separation section design entirely hinge on the quantity and composition of the reactor effluent. Therefore, separation design entirely depends on the optimized reactor. As the reactor defines separation

demands, and the reactor and separation define heating and cooling duties, the reactor design truly defines process requirements. Hence, optimization of a chemical process will almost always begin and rely on the reactor design. After designing a heat integration network for heating and cooling of process streams, any remaining heating and cooling duties call for utilities. Utilities can often be a substantial reoccurring cost. Carefully design and optimize the heat integration network, as minimizing utilities can significantly impact an economic objective function. Finally, optimize waste treatment. The chemical process waste output depends on all the previously mentioned designs. Figure 2 depicts the optimization hierarchy, with the reactor appropriately in the center.

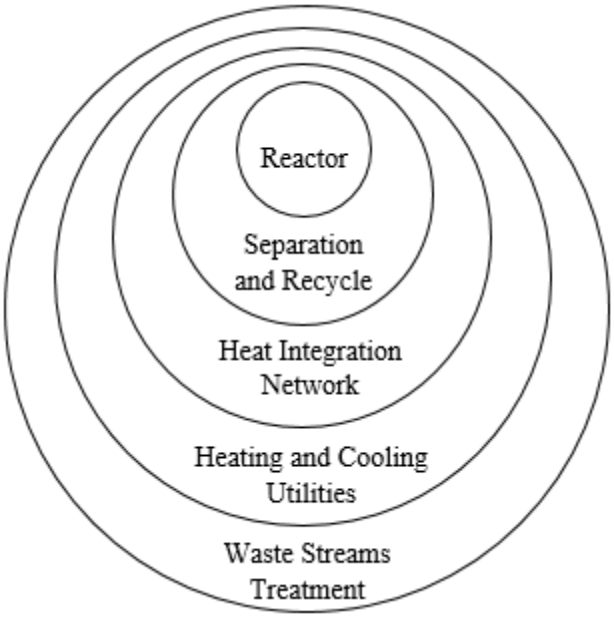


Figure 2. Hierarchy of Chemical Process Optimization. Adapted from *Chemical Process Design and Integration*.

On the following page, some of the important decision variables in optimizing chemical processes are listed. A specific process might have other key decision variables not discussed, but most chemical process optimizations will include investigation of the following:

1. Reactor Operating Conditions— such as reactant component concentrations, temperature and pressure. The constraints to these operating conditions are typically inherent to reactor design like a catalyst's maximum allowable temperature.
2. Reactor Single-Pass Conversion— desired product selectivity is a function of single pass conversion, which is a function of reactor operating conditions
3. Unused Reactant Recovery
4. Purge Ratios for Recycle Streams Containing Inerts
5. Product Purity
6. Reflux Ratio and Component Recovery in Distillation Columns
7. Mass Separating Agents Flow to Equipment (i.e. absorbers, strippers, etc.)
8. Operating Pressure in Separating Equipment

Unit 500 Decision Variables

In calculating NPV of Unit 500, the yearly net cash flow accounted for the fixed capital investment, cost of labor, cost of utilities, raw material cost, waste treatment costs, revenue, depreciation of buildings, depreciation of equipment, depreciation of machines, and income taxes. These described factors are all potential decision variables. Based on the assumptions and process definition, the decision variables consist of cost of equipment included in fixed capital investment, cost of utilities, cost of raw materials and cost of waste treatment. All other variables included in the NPV calculations cannot be controlled.

A sensitivity analysis on the net present value was performed in order to prioritize the important decision variables of Unit 500, as shown in Figure 3. From this analysis, revenue, cost of raw materials, cost of utilities, and cost of equipment had the greatest effect on NPV. Thus, optimization should concentrate on decreasing raw materials, utilities, pieces of equipment, and equipment size. Although revenue is not a decision variable since the styrene sales price and production rate is fixed, the inclusion hopes to exemplify revenue's major impact on NPV.

As typical in the optimization process, further analysis provides insight into how the costs are related, such as determining annual equipment costs. Calculating the equivalent annual operating cost (EAOC) and the associated utility cost for each piece of equipment fosters a deeper understanding of process variables' relationship to NPV. This cost analysis for Unit 500 can be seen in Figure 4, where, for example, "Fired Heater" is the sum of the EAOC of H-501 and the annual cost of natural gas.

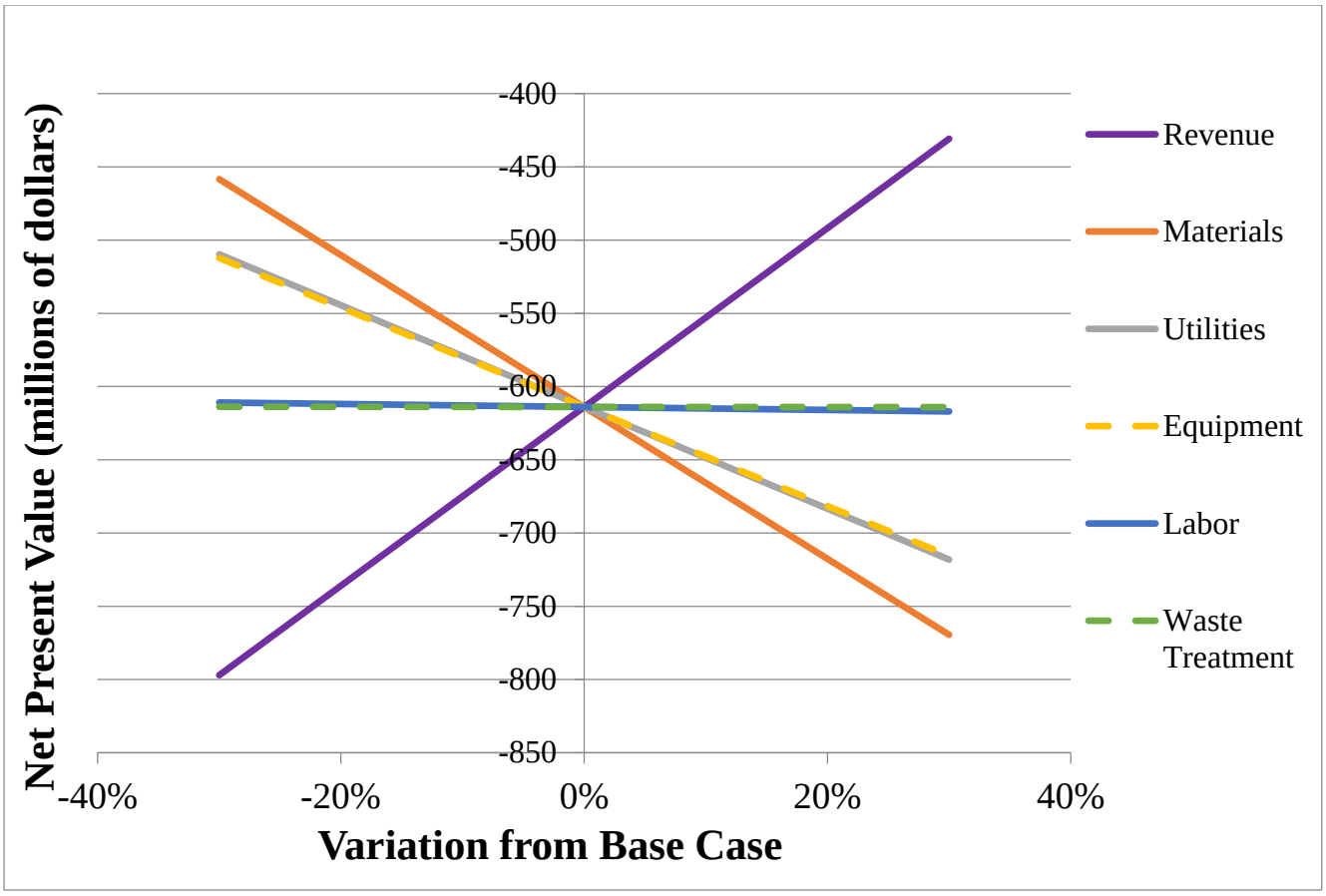


Figure 3. Sensitivity Analysis of the Base Case.

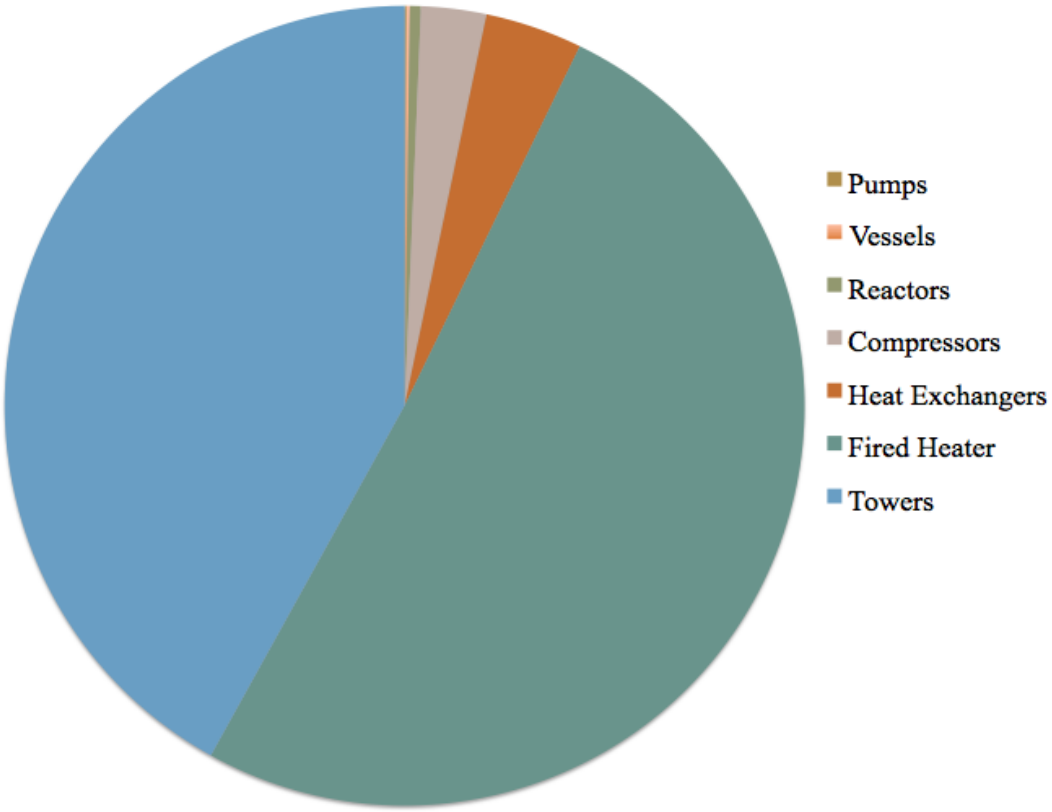


Figure 4. Base Case Equipment Contribution to Annual Operating Cost of Unit 500.

From this analysis, most of the yearly cost came from the fired heater and towers. For this reason, I wanted to efficiently optimize Unit 500 by focusing efforts on reducing the costs associated with these units. However, a thorough Unit 500 optimization, including these units, is outside the scope of this report. This merely demonstrates that in-depth economic analysis is an extremely useful tool when beginning optimization for acquiring a familiarity of a decision variables relationship between other decision variables and NPV.

Constraints

Constraints are the limits, maximum and minimum, of a decision variable's values. These limitations on one variable often depend on the value of at least one other decision variable and are therefore sometimes susceptible to change throughout the optimization process. Constraints arise from assumptions previously made, the nature of the process, consumer preferences, ethical concerns, environmental regulations, industry standards or a combination of these and other factors.

There are two types of constraints: equality constraint and inequality constraint. The former reduces the number of decision variables included in an objective function, while the latter reduces the range of values a variable can take. *Equality Constraint* is an equality concerning two or more decision variables, such as specific inerts concentration in feed. The mole balance on the inerts in the reactor feed would be an equality constraint. *Inequality Constraint* is an inequality concerning one or more decision variables. An example of this constraint is an endothermic reaction occurring above and below specified temperature and pressure, respectively. Equality constraints effectively decreases the number of truly independent decision variables, known as reducing dimensionality of an optimization problem. Inequality constraints reduce, and also typically bound, the range of possible values a decision variable can assume. As evident, both equality and inequality constraints reduce the possible combinations of decision variable values, which simplifies the optimization process.

Unit 500 Constraints

As with any chemical process, production of styrene faces many limitations due to process demands and safety concerns. Endothermic processes fundamentally constrain design by necessitating addition of heat, manifested in Unit 500 by interheating, as previously discussed. The following list includes Unit 500 design constraints that arise from the chemical process or design specifications:

- Reactor temperature cannot exceed 1000 K with a maximum 50 K variation in temperature over the length of the reactor
- Pressure must be between 0.75 bar and 2.5 bar
- The benzene/toluene mole fraction must be 0.9 or higher in order to sell the stream for 50% of the pure component values
- Total molar flow rate for styrene must be 120 kmol per hour
- The maximum return temperature for cooling water is 313 K
- One operating year is 8000 hours

Heuristics

Heuristics are experience-based shortcut calculation methods and guidelines used to estimate equipment size and performance, estimate process unit costs, determine initial process simulator inputs and confirm validity of computer simulated results. As true chemical processes are uncertain, heuristics are a useful tool for adapting optimized values of decision variables, thereby adding contingency. Heuristics provide general rules for adjusting final decision variable values to account for the normal chemical process errors without overestimation.

Consider the optimization of a distillation column. The final number of calculated trays will adequately separate the idealized process stream, not accounting for any process errors. As no actual process will be ideal, t1he idealized separation design will ineffectively meet purity requirements in an actual operation. Adding too many additional trays to the calculated number not only can threaten operation, but will make the equipment unnecessarily expensive. A heuristic allows the appropriate number of trays to be calculated, to ensure separation without significant cost or process. Specifically, the Fenske-Underwood equation is the recommended heuristic for calculating minimum number of trays as shown in the following equation

$$N_{min} = \frac{\ln\left[\frac{\left(\frac{X}{1-X}\right)_{ovhd}}{\left(\frac{X}{1-X}\right)_{btms}}\right]}{\ln[\alpha]} \qquad (2)$$

Where N_{min} is the minimum number of trays

X_{ovhd} is the more volatile component's mole fraction in the overhead distillate

X_{btms} is the more volatile component's mole fraction in the bottoms

α is the relative volatility of the more volatile to the less volatile component

As helpful as heuristics can be, they can also be flawed and seem unjustifiable in final optimization result analysis. Use of heuristics does not always indicate a solution will be found. Sometimes, heuristics

contradict each other and thus cannot always be followed. Overall, they are a very useful, time-saving tool in process evaluation and optimization, but understanding their limits defines the validity of optimization results.

3. TYPES OF OPTIMIZATION

Topological Optimization

Topological Optimization is optimizing topology or process equipment arrangement. In other words, the physical nature of the design. Topological optimization should occur before parametric, whether improving a new process unit design or upgrading an existing unit. Topological optimization not only has a more significant impact on overall profitability, but topological optimization further constrains and reduces the possible operating conditions– the focus of parametric optimization. Thus topological optimization not only eases the process of parametric optimization, but implements realistic and significant constraints on the process. The extent to which topology optimization constrains parametric optimization depends largely on the stage of the design process. When optimizing a conceptual flow sheet, topology can easily be changed, unlike in an existing plant where topology changes have substantial associated costs.

According to *Analysis, Synthesis and Design of Chemical Processes,* an engineer must ask the following four questions in this order when designing process topology:

1. Can unwanted by-products be eliminated?
2. Can equipment be eliminated or rearranged?
3. Can alternative separation methods or reaction configurations be employed?
4. To what extent can heat integration be improved?

Can unwanted by-products be eliminated?

Raw materials typically account for the majority of reoccurring costs, as previously discussed. Therefore, eliminating the by-products of competing reactions is a priority in optimizing chemical

processes. Minimizing raw material costs requires careful choice of reaction mechanisms, reactor operation and reactor catalyst. A design aims to reach 100% reactant conversion and 100% desired product selectivity, although this is impossible in reality.

Since side reactions cannot be completely prevented, unwanted by-products and waste streams will be produced. While optimizing, investigate potential unwanted by-products, which are distinct from waste streams as they can be sold, and the consequences of any hazardous waste product. Unwanted by-products intrinsically will not be sold for an overall profit, otherwise they wouldn't be unwanted, making this additional revenue serve as a partial economic credit. Minimize production of waste and unwanted by-products with the appropriate catalyst and operating conditions.

There are different design choices that might eliminate or reduce side reactions, but often have unforeseen costs that ultimately lower profitability. Confirm that any new step design implemented in the process has the desired overall effect on the objective function. Side reactions can be suppressed by reducing the per-pass conversion of the limiting reactant or choosing a different catalyst. The former reduces the concentration of products that react to form by-products. Diminishing per-pass conversion requires a change in feed ratio or combining a reactor effluent recycle with fresh, raw materials to feed into the reactor. Both recycle and feed ratio design aim at lowering the concentration of desired products that react to form side products.

Can equipment be eliminated or rearranged?

It is assumed that the base case does not include any redundant equipment. Therefore, any further elimination of equipment will result from parametric changes. Besides obvious changes, such as compressing a gas rather than a liquid, equipment rearrangement typically results from an in-depth analysis of the separation section and heat integration within a process. Determining the best separation sequence requires extensive parametric optimization for the possible topologies.

Can alternative reaction configurations or separation methods be employed?

Alternative reaction configurations depend on the specific process and the reactor configuration previously designed to specifically eliminate unwanted by-products. Using the most cost effective separation method can dramatically increase the economic potential. Today, separation of chemical components can be accomplished using a wide range of equipment and technologies. Liquid-gas processes typically separate using distillation, gas absorption with liquid stripping and liquid-liquid extraction. Despite the many separation techniques, 90 to 95% of separations, product recovery, and purifications rely on distillation of some form, according to *Analysis, Synthesis and Design of Chemical Processes*. Determining the best separation sequence requires extensive parametric optimization for the possible topologies.

To what extent can heat integration be improved?

Implementing heat integration can drastically reduce the recurring utility costs. Heat integration aims at heating and cooling process streams to their desired temperature with other process steams rather than utilities. Begin by identifying process streams to be cooled or heated. Then, determine whether heat integration can be implemented by investigating initial temperature and desired final temperature and whether a process steam can supply or absorb heat. There can be no violation of the minimum approach temperature. Often, utilities can only be partially eliminated. Heat integration can often have unforeseen consequences making it impractical. Successful heat integration requires further knowledge of minimum number of heat exchanger calculations. HENSAD, which stands for Heat-Exchanger-Network-Synthesis-Analysis-Design, is a useful computer software tool for validating heat integration design.

Parametric Optimization

Parametric Optimization means optimizing the operating variables of a specific process or piece of equipment. As discussed in topological optimization, parametric optimization is much more efficient when the topology is fixed. Parametric optimization first requires determining the overall objective

function's decision variables that are subject to operating condition design change or further optimization. Proceed by developing a unique objective function based on operating conditions for those decision variables. As the efficiency of the optimization process is contingent on allocating time for the key variables, the approach to parametric optimization must be well thought out and justified.

As described in *Analysis, Synthesis and Design of Chemical* Processes, the following operating conditions should be considered in optimizing chemical processes:

1. **Reactor:** reaction kinetics, reaction thermodynamics, reactor volume, space time, configuration, heat transfer in reactor, catalysts, selectivity, and yield
2. Perform the easiest separation first—that is, the one least demanding of trays and reflux—and leave the most difficult to last
3. When neither relative volatility nor feed composition varies widely, remove components one by one as overhead products
4. When the adjacent ordered components in the feed vary widely in relative volatility, sequence the splits in order of decreasing volatility
5. When the concentrations in the feed vary widely but the relative volatilities do not, remove the components in order of decreasing concentration

4. APPROACHES TO OPTIMIZATION

The overall optimization process is summarized in the following steps:

1. Define an optimization problem
2. Quantify the optimization value assuming an ideal process
3. Identify the design conditions, assumptions and constraints
4. Strategize how to implement design changes
5. Evaluate the result of the optimization

Optimization requires looking alternatively at the big picture or the fine details, essentially alternating between a top-down and bottom-up strategy. By examining the big picture, process configuration or decision variable values can be significantly altered, but these changes have no meaning without confirming whether the changes are improvements. This confirmation usually involves investigation of the details. Although recommended earlier, topology optimization cannot be entirely finished before parametric optimization. Many of the topological design of a chemical process rely on the parametric design, hence a successful optimization will often require optimizing topology multiple times based on parametric optimization. Alternating between topology and parametric optimization is equivalent to alternating between a top-down and bottom-up strategy.

The key to successful optimization is justification. The overall objective function, a decision variable's objective function, key decision variables, and the final chosen values of decision variables must be well reasoned and explained. Sensitivity analysis provides a basis for prioritizing decision variables, but it cannot be the sole source. A thoughtful, creative, and logical approach must also be employed. A recycle loop containing the decision variables complicates objective function evaluation and can only be correctly optimized with a thorough understanding of the process.

Most chemical process optimizations will require an objective function based on both simulations of the process and mathematical functions. The benefits or consequences in a possible topology change is typically measured by a mathematical function, unlike evaluating parametric changes in process simulation.

Chemical Process Simulation is a computer software's mathematical model of a defined chemical process. Synthesizing a chemical process in any modern process simulator software first involves selecting individual steps in the process and then interconnecting these steps. It is recommended to run the process with every added step. If the simulation is invalid after addition of a step, the problem in the process is

easily identified. Inputting and connecting the entire process steps before simulation makes for difficult problem identification of an invalid process. The feed components should be the only input process stream. The simulation model calculates all other stream conditions, flowrates and compositions based on the feed and all equipment inputs. These calculations include approximations and assumptions, meaning they are not 100% reliable. This explains why heuristics calculations are used to confirm the process simulation results.

When employing chemical process simulation, the software can perform case studies. The user defines process conditions to be changed and defines an output to evaluate. Essentially, the dependent variable or "output" is what the objective function desires to maximize or minimize and the input includes the independent or decision variables capable of change. Therefore, a case study generated in chemical process simulation requires sequentially choosing:

1. Initial set of decision variables
2. Decision variable search range and direction. For original case study end points, typically use maximum/minimum process constraints or begin at the initial value and investigate in the direction known to improve the objective function.
3. *Step Size*: A variable's magnitude of change on any one step in cycle matrix. The total number of simulation runs increases by a factor equivalent to the amount of step sizes required to examine the previously determined decision variable range

The input case study matrix variables, range, and step sizes must take into account total cycle time. Running a case study with a single variable changed can be a highly useful step in creating a case study matrix. This clearly demonstrates whether a variable impacts the objective function and to what degree. This allows simplification of variable range. By narrowing the range, the step size can be decreased and this in turn decreases the process simulation time. An effective case study matrix necessitates simplifying

decision variables, their range and step sizes, while collecting sufficient information. By including too narrow of a range or too large of a step size, the designed case study can act as a filter. Oversimplification will produce case study results that do not capture the actual relationship between a decision variable and an objective function, thus invalidating optimization results.

Case studies are not often an applicable tool for the overall objective function, but can be highly useful in optimizing the decision variables within that overall objective function. For example, chemical process simulation can run case studies on reactors so as to maximize conversion, even if the objective function intends to maximize profitability. As maximizing conversion decreases the costs associated with raw materials, recycling, separation, equipment, and much more, a case study only on a reactor can clearly have an overall impact on profitability.

There is no set way to best optimize a chemical process. Chemical process simulation can be an extremely useful tool, case studies can provide helpful insight to defining decision variables, but this software only provide estimations and can often waste time. Optimization is a skill of understanding and finding the best balance and synergy of variables.

5. OPTIMIZATION OF UNIT 500 REACTOR

A complete optimization of Unit 500 is not included. However, a previous, but incompletely optimized Unit 500 PFD can be found in Appendix 2. This inclusion merely intends to demonstrate the difference between a base case design an optimized design.

The following optimization of reactor design serves as a concrete example of why, how and where to first optimize and implement change. Through process simulation and case studies, the single piece of equipment optimized in this discussion should be the first focus of maximizing Unit 500's NPV.

In defining and prioritizing decision variables, the optimization of Unit 500 should focus on minimizing the cost of raw materials, cost of utilities and cost of equipment, as earlier recommended.

From the sensitivity analysis, we also recommended to disregard NPV's sensitivity to revenue since it is fixed. An optimized reactor design would lower all the prioritized costs and should always be the focus of initial optimization. Designing a reactor to maximize yield not only lowers cost of raw material, but the improved conversion reduces the required recycle flow rate. A reduced recycle flow rate subsequently lowers utility costs related to pre-heating of feed, cooling reactant effluent and separating reactor effluent as less mass needs to be cooled, heated and separated.

It is desired to use a fluidized bed reactor instead of the current packed bed reactor design, including two reactors in series with interheating. It is to be noted that the included optimized Unit 500 design never investigated this type of reactor. A fluidized bed reactor is simulated in Pro/II using an isothermal plug flow reactor. An estimate of 10% of feed bypasses the catalyst due to the bubbling nature of a fluidized bed, meaning the maximum single-pass conversion is 90% of the equilibrium conversion, even in an infinitely large reactor. To account for this, the simulation includes a 10% reactor feed bypass.

The objective function of yield for the reactor design is defined in the following equations and is unit-less

$$yield = \frac{mols\ of\ styrene\ formed}{mols\ of\ ethylbenzene\ consumed} \tag{3}$$

$$yield = \frac{mols\ of\ styrene\ in\ product - mols\ of\ styrene\ in\ feed}{mols\ of\ ethylbenzene\ in\ feed - mols\ of\ ethylbenzene\ in\ product} \tag{4}$$

The optimum value, accounting for bypass, of the objective function is equivalent to 90%, which would entail 90% conversion of the ethylbenzene fed to the reactor with no side reactions.

In order to perform the optimization, I assumed no changes in reactor feed flow rate or composition. The catalyst is assumed to have a density of 2000 kg/m^3 and contain near-spherical particles with a diameter of 5 mm. At minimum fluidizing conditions, the spherical particle voidage is assumed to be 0.45. Finally, the reactor length is assumed to be 20 ft and contains a 10% bypass.

The decision variables, determined by any operating condition that can be controlled, comprise of feed temperature, feed pressure and reactor diameter. Constraints for the reactor include a maximum temperature of 1000 K and an entering and exiting pressure of at least 0.75 bar no and greater than 2.5 bar, as with the previous reactor design. The fluidized bed pressure drop calculation used the following equation

$$\Delta P = g(1-\varepsilon)(\rho_c - \rho)L \quad (4)$$

Where P is the pressure drop

g is the acceleration due to gravity

ε voidage of spherical particles

ρ is the process stream density

ρ_c is the catalyst density

L is the reactor length

The fluidized bed's final operating conditions should yield a superficial gas velocity 3-10 times larger than the minimum fluidizing velocity, u_{mf}, implementing a further constraint. Calculating this velocity requires manipulation of the following two equations

$$Ar = \frac{d_p^3(\rho_c - \rho)\rho g}{\mu^2} \quad (5)$$

$$Re_{p,mf} = \frac{u_{mf} d_p \rho}{\mu} = (1135.69 + 0.0408Ar)^{0.5} - 33.7 \quad (6)$$

Where $Re_{p,mf}$ is the Reynolds number

Ar is the Archimedes number

d_p is the particle diameter

μ is the process stream viscosity

Optimizing the new decision variables does not require development of process equations, but merely simulation in Pro/II. For determining whether NPV increased with the optimized reactor, the new reactor must be simulated in the overall process. However, investigation of the simulation reactor should only include the feed, a separator to bypass 10% of reactants, the reactor and a mixer to combine the bypass with the reactor product. The case study input included the identified decision variables and then output not only the objective of yield, but the superficial velocity as this determined validity of a case study results.

In order to perform the case studies, I first had to decide on the decision variable range to be implemented in the case study matrix. This range had to be sufficiently large, ensuring the data captured changes in yield caused by changes in a single variable. Typically, this should always be completed before running a complete case study matrix. Deeper understanding of the variable's impact on the objective function reduces the required range and step sizes for an effective case study matrix, thus reducing simulation time. For example, if yield levels off and sees little increase past a certain temperature, this should replace the range maximum of 1000 K previously chosen based on design constraints. Higher temperatures raise utility costs and can only be justified by increased styrene yield. Again the importance in understanding the relationship and tradeoffs between decision variables are emphasized.

Unfortunately, this reactor has a distinctive relationship between reactor diameter, pressure and temperature. For any decision variable value, the reactor will only operate at certain values of the other two variables. This is clearly demonstrated in Figure 5, where only one variable is varied. The other two variables are held constant at the values dictated on the top of graph. The step size was 10 K, 0.01 bar, or 100 mm for temperature, pressure, or reactor diameter, respectively, with the examined range equivalent to the axis values. As shown, production of styrene is largely unsuccessful with change in a single variable value. However, a variables impact on velocity follows a distinct trend, which can implement restrictions

on variable range upon calculating absolute maximum process velocities. Running an initial case study matrix, with a vast range and large step sizes to reduce computational time, later reduced the range by identifying results outside the velocity constraints. This is not ideal, but is required for this specific piece of equipment.

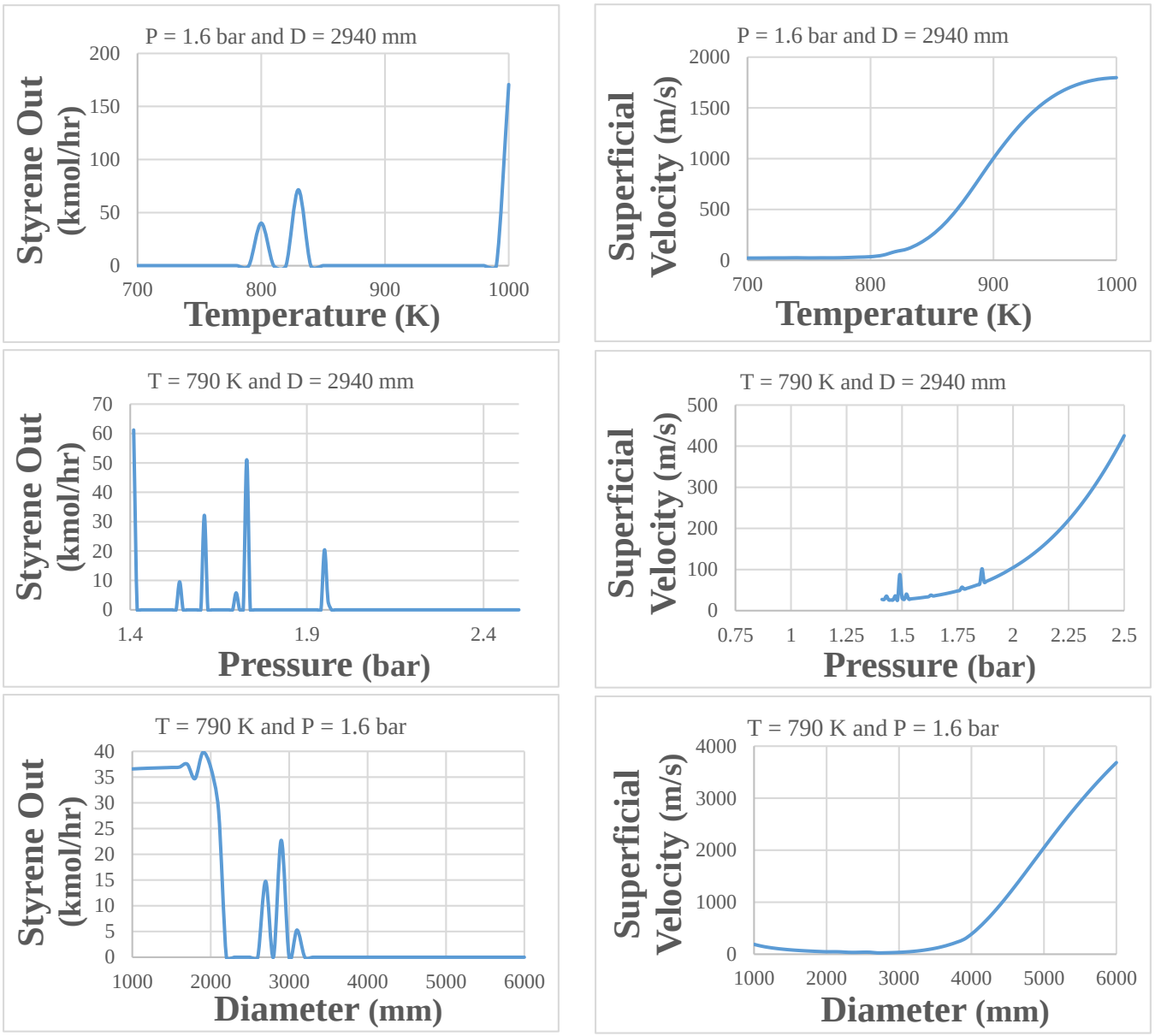


Figure 5. Initial Case Study Results of Fluidized Bed Reactor.

To reduce time spent on evaluating case study results, an estimated pressure drop and an estimated maximum fluidizing velocity for all process conditions were calculated. As the values that significantly change both pressure drop and minimum fluidizing velocity are constant, with only the process stream's density and viscosity susceptible to change, changes in decision variables did not change the calculated values. These process stream conditions had little impact on velocity calculations, even at extreme changes in the decision variables. Based on these calculations, all case studies examined a reactor with a 0.657 bar pressure drop and neglected a result with a superficial gas velocity over 28 m/s, which is greater than 10 times the calculated minimum fluidizing velocity.

Table 1 summarizes the final optimized reactor results that maximized yield while staying within constraints. Determination of final decision variable values involved running many case study matrices, with each subsequent simulation further reducing range based on the most recent case study results. When yield did not increase with any further narrowing of range, optimization was complete upon validating the velocity and pressure drop assumption.

Table 1. Fluidized Bed Reactor Optimization Results

Temperature	787 K
Inlet Pressure	1.74 bar
Reactor Diameter	2566 mm
Styrene Yield	99.95%
Conversion of Ethylbenzene	16.1%
Pressure Drop	0.657 bar
Maximum Superficial Velocity	25.093 m/s
Minimum Fluidizing Velocity	2.510 m/s
Velocity Ratio	9.996

6. SUMMARY

To truly justify the optimization results from the fluidized bed reactor example, all possible reactor arrangements should be optimized for maximum yield. Then, the new reactors should be simulated in the

base case to find a new value of NPV. Comparison of these NPV values would thoroughly justify the results. Higher yield rates with a specific reactor type might be less optimal due to unforeseen costs.

Hopefully, this discussion provided a clear-cut method for calculation and evaluation of chemical process optimization, although endless and complicated. The included optimization example demonstrates the complexity in a single step within an entire optimization process. This, along with previously discussed methods, can guide any beginner through improving a process design.

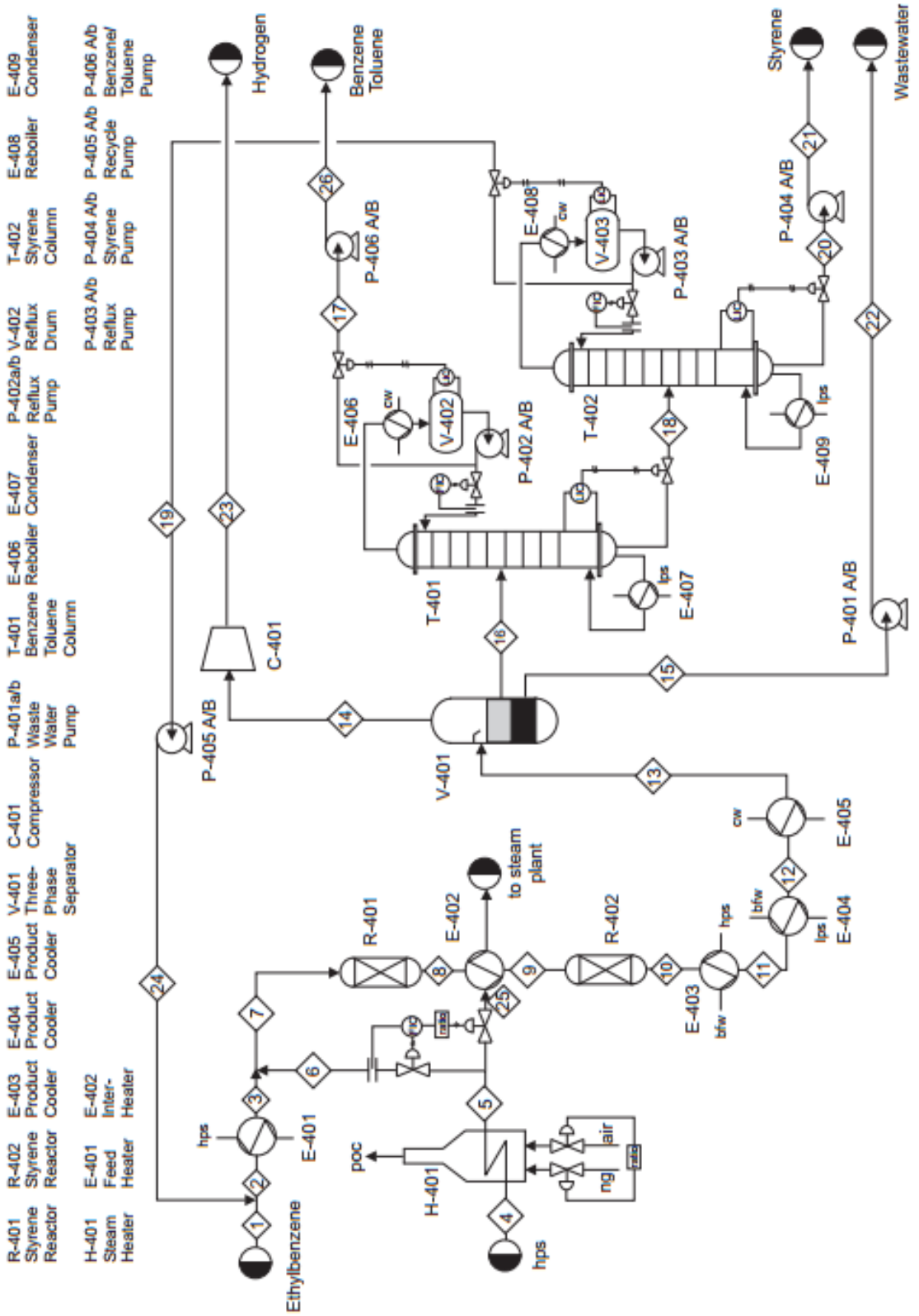
REFERENCES

Smith, Robin. *Chemical Process Design and Integration*. Chichester, West Sussex, England: Wiley, 2005. Print.

Turton, Richard et al. *Analysis, Synthesis, and Design of Chemical Processes*. 3rd ed. Upper Saddle River, NJ: Prentice-Hall, 2009. Print.

APPENDIX 1: Base Case PFD, Stream Tables and Equipment Tables

Taken Directly from *Analysis, Synthesis and Design of Chemical Processes*



APPENDIX 2: An Example of Previous Optimization Results