4-2016

C4 Operations Optimization

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C4 Operations Optimization

Abstract
The primary objective of the project chronicled in this report was to design a model that optimizes C4 operations. This model will optimize the options for processing both "crude C4" and "Cat BB" streams, taking the feed stream makeup, market pricings, and capacity constraints into account. Crude C4 streams contain butanes, butenes, and butadienes, while "Cat BB" streams are similar in makeup but do not include butadienes.

It is assumed that the equipment for all unit operations is readily available. In addition, the plant will already have a baseload of feedstock that does not fully utilize all the equipment in the plant, which allows for the purchase of feedstock that could potentially be profitable.

Available unit operations include Butadiene extraction, MTBE production, Metathesis, 1-Butene distillation, Skeletal Isomerization, Olefin Isomerization, and Alkylation. The model will be required to make choices about which unit operations to utilize based on the constraints input by the user. While the model will not directly produce revenue, it will allow the company to optimize processes within the plant, finding the most profitable situation. Thus, it will be possible to assess the program's value based on its accuracy.

Disciplines
Biochemical and Biomolecular Engineering | Chemical Engineering | Engineering

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April 12, 2016

Dear Professor Fabiano, Dr. Shieh, and Mr. Sawyer,

The following report contains our project, *C4 Operations Optimization*, which was recommended by Mr. Gary Sawyer. The optimization program uses Microsoft Excel to determine the optimal processing of a crude C4 stream, and utilizes unit operations at an existing petrochemical plant. Given feed stream makeup, market pricings, and capacity constraints, the optimization program we designed is able to determine the most profitable course of action for the petrochemical plant in question.

Our report contains detailed information on the program that was designed, as well as information on unit operations, market analysis, utility and capacity requirements, and customer requirements. A discussion of typical scenarios is also included, as well as a sensitivity analysis and an investment opportunity analysis. The program is user-friendly and can be modified to fit the specifications of the petrochemical plant in question, meeting the requirements laid out in the project statement. The group recommends that the company begin use of this program immediately because it can significantly increase company profits. Suggestions for improvements to the code of the project program are included in this report as well.

Sincerely,

_______________ _______________ _______________ _______________

Michael Moroney   Evan Smith   Marissa Thompson   Fernando Torres

Optimization Model for a Crude C4 Refinery

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Primary Industry Consultant:
Mr. Gary Sawyer

April 12th, 2016

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Introduction

Crude C4s and Cat BBs are products of the steam cracking process designed to produce petrochemicals. These streams contain a mix of butanes, butenes and butadienes. Often, chemical refinery plants opt to process and sell these products, which calls for the use of an optimization program to determine the most profitable pathway. Both butadiene, which can be recovered through extractive distillation, and 1-butene, which can be recovered through conventional distillation, are valuable monomers if high in purity. In addition, isobutylene can be profitable as a monomer, but is often converted to methyl-tertiary butyl ether (MTBE), a high octane fuel additive that is typically more profitable. Furthermore, there are multiple options for the processing of cis- and trans-2-butene. These options include alkylation, skeletal isomerization, metathesis, and olefin isomerization. Alkylation requires isobutane and produces alkylate, a motor fuel. Skeletal isomerization allows for an equilibrium mixture of butene and isobutylene to be recycled back to the MTBE reaction unit to increase profit. Metathesis requires ethylene and produces propylene, a chemical typically more valuable than ethylene. Olefin isomerization, also commonly known as butene isomerization or positional isomerization, allows for the production and recuperation of 1-butene, which can then be sold. Hydrogenation of 2-butene to n-butane is an additional, albeit less desirable, option, where the n-butane is sold as feedstock.

The focus of this project was to create a program that made decisions based on feedstock composition, market prices of products, and capacity constraints of unit operations in the plant in order to maximize profit. The program was to also explore the opportunity of buying additional feedstock in the event that the base load did not fully utilize equipment capacity. This required research on utility costs, capacity information, and the petrochemical market, as well as the characterization of typical crude C4 and cat BB streams. These factors are discussed in the report. The majority of the project involved using Microsoft Excel to build a user-friendly model that could optimize refinery plant operations. Additional calculations included material balances and profit analysis.

The model in Microsoft Excel will be used by a large petrochemicals company. It will be designed to fit the specific needs of the company, and will be assessed based on ease of use and on accuracy. It is assumed that the company in question already possesses all of the necessary equipment for the unit operations, thus it will not be necessary to purchase additional units.

Project Charter

Name: C4 Operations Optimization

Project Students: Michael Moroney, Evan Smith, Marissa Thompson, and Fernando Torres

Project Advisors: Mr. Leonard Fabiano, Dr. Wen K. Shieh, and Mr. Gary Sawyer

Specific Goals: The development of an optimization program to be used for C4 optimization.

Scope: ***[In Scope]***

Capacity and utility costs of unit operations

Typical market pricing of products

Economic Analysis

Programming and coding to design optimizations program in Microsoft Excel

Mass and energy balances

[Out of Scope]

Reactor Design

Lab work and experimental procedures

Deliverables:

Fully functional optimization program that allows customizable user inputs

Economic and market analysis

Mass and energy balances (Incorporated into model)

Timeline: Completion of design project within the 3 month semester.

Market and Competitive Analyses

Market Analysis for Compounds

Volatility in oil prices globally factors into the petrochemical industry. With recent historically low oil prices, many petrochemical companies, especially those in Europe, have benefited from an increase in their margins.

Effect of decrease in oil prices on crackers in Europe

Crackers in Europe (companies who take feedstock and break it down to make olefins) have benefited most since their main feedstock is naphtha (C5-C8), a direct product from crude. Their energy costs have also gone down, since they use oil to fuel their cracking operations, as opposed to the United States, which uses shale gas (and has usually enjoyed much greater competitiveness thanks to its price). The drop in oil prices then comes as a relief to petrochemicals companies, considering as how feedstock and energy costs account for close to 85% of the operating cost.

However, their customers have not enjoyed the effects of this price drop. Many of these companies, under the financial strain they usually face, failed to make adequate investments that have now cost them in the form of unprecedented shutdowns. These have led to a decrease in the supply of their products (ethylene, propylene, byproducts, and derivatives), resulting in an increase in price. [16]

Ethylene

Supply for ethylene was tight in 2015, and looks to remain tight in 2016 as well. Prices have dropped in general, although the margin for the producer has increased because of the low oil price and the tight supply. The US is expecting to begin at least 7 large-scale projects to increase the production capacity of ethylene by 50% over the next few years. It can be expected that the increase of ethylene production capacity may result in a greater quantity of crude C4. [10, 16]

Propylene

Propylene supply is not expected to be tight in 2016. Demand for it has fallen relative to that of ethylene, as its derivatives' markets do not have as positive/steady outlooks. The margin gap between ethylene and propylene continues to broaden. [16, 20]

1-Butene

Linear low-density polyethylene (LLDPE) is currently the fastest growing application for alpha olefins such as 1-butene, driven by the increasing demand for high-quality plastics. As such, the demand for alpha olefins is expected to grow globally. Pricing, however, is inherently dependent on the volatile prices of the raw materials required for production.

Methanol

While methanol pricing should be independent of oil prices, because of Methanol to Olefins (MTO) and Methanol to Propylene (MTP) processes that are operational in China, the price of Methanol has been impacted. MTO and MTP processes that produce ethylene and propylene compete with the more traditional approach that uses naphtha as a feedstock. Since the costs of this traditional approach went down because of the drop in crude prices, in order to compete, the price of methanol also decreased. In 2015, capacity in the US for methanol production increased by more than 75%. 2016 is expected to be stable. Pricing was very volatile due to the uncertainty in supply, although current prices are at a 6-year low. [3, 21]

Table 1: Chemical and Utility Prices

Material	MED	LOW	HIGH	CUSTOM	Source	Month	Year
Ethylene	$0.18	$0.15	$0.20	$0.18	Platt	January	2016
Propylene	$0.30	$0.26	$0.34	$0.30	Platt	January	2016
1-Butene	$0.67	$0.64	$0.69	$0.67	Argus	August	2015
Methanol	$0.41	$0.34	$0.29	$0.41	Platt	January	2016
MTBE	$0.23	$0.20	$0.26	$0.23	Platt	January	2016
Butadiene	$0.42	$0.36	$0.47	$0.42	Argus	August	2015
n-Butane	$0.51	$0.51	$0.51	$0.51	Argus	August	2015
i-Butane	$0.51	$0.51	$0.51	$0.51	Argus	August	2015
Crude C4	$0.01	$1.26	$1.51	$0.01	Argus	August	2015
isobutylene	$0.58	$0.55	$0.60	$0.58	Argus	August	2015
Alkylate	$0.20	$0.20	$0.27	$0.20	OPIS	February	2016
Hydrogen	$8.00	$8.00	$8.00	$8.00			
Electricity	$0.06			$0.06	"Cost Sheet Outline" on page 604 of Dr. Warren Seider's *Product and Process Design Principles*.	NA	2016
Steam (150 psig)	$10.50			$10.50			
Cooling water	$0.02			$0.02			
Process water	$0.20			$0.20			
boiler feed water	$0.50			$0.50			
Natural Gas	$3.20			$3.20			
Chilled Water	$4.00			$4.00			
Steam (50 psig)	$6.60			$6.60			

MTBE

The majority of MTBE (95%) is used to oxygenate gasoline and boost its octanes. Although the supply of MTBE is expected to decrease in Europe next year (2016), it is expected to grow in other emerging economies. As China and India impose stricter environmental rules, the demand for MTBE is expected to increase. Throughout 2015 prices were fairly volatile. [7]

Butadiene

Most Butadiene is obtained by extracting it from the crude C4 which results from naphtha cracking to make olefins. In the US, roughly 75% of butadiene is used to produce styrene butadiene rubber (SBR), which is used in the production of tires. Of this about 80% is used in the replacement tire market, which has suffered a drop in demand. The remaining Butadiene produced in the US is used to make acrylonitrile-butadiene-styrene (ABS), which is used to make plastics for cars, amongst other things. For most of 2015, supply remained ample with a steady but mediocre demand. In general, the price of Butadiene fell with the price of oil, although for periods in 2015 the price increased, most probably due to supply constraints. Another development has been in the technologies used to make Butadiene. While the traditional method employs a naphtha feedstock, new methods explore using lighter feedstocks like ethane, while others explore the dehydrogenation of n-butane. Overall, the view of the Butadiene market from participants is pessimistic. The markets of Butadiene customers are expected to decrease, and demand is expected to further slow. [6]

N-Butane and i-Butane

About two-thirds of the butane produced globally is used in liquefied petroleum gas (LPG). Demand for LPG as a domestic fuel has surged in both commercial and residential sectors, leading to the growth of the butane market. The tight supply of ethylene has also contributed to the growth of the butane market, since butanes are used in the production of ethylene. Exceptional growth, however, has been held back by the volatile crude oil market and environmental concerns. Overall, the market is expected to increase modestly. [16]

Competitive Analysis for Model

Although similar models exist at competitor plants, because this model is designed specifically for the plant in question, there is no direct competitor. Since the model has been created from scratch in Microsoft Excel, there are no concerns about patent infringement. The company must have a license for Microsoft Excel to run the model, but there are no other royalties or fees to outside parties that the company needs to pay. However, it is essential that the model fits all standards set by the company so that the plant is able to earn more profits and compete against other petroleum plants.

Customer Requirements

Our group has been hired by the Operations Planning department of a petrochemical company. As previously stated, the project is to design an optimization model that will determine profitable opportunities to buy feedstock. This program must be user-friendly, and must be demonstrated at the final presentations in April of 2016. The customer has required that the model find optimal process configurations given capacity information, pricing information, and the feed composition. Typical utility information is also required for the model to function correctly. All of these customer requirements are classified as fitness-to-standard (FTS). Ease of use could potentially be categorized as new-unique-difficult (NUD), as could other variables such as warnings about unrealistic pricing inputs, or infeasible capacity restraint inputs.

Because this product is to be designed for a specific company, it does not have to compete with those at other companies. However, it must be efficient and accurate. It must outperform whatever previous models the company has been using, potentially giving them a competitive edge and allowing them to increase profits through the most efficient use of unused capacity.

Product Concepts

Several different programming tools were available for the product design. These tools included Microsoft Excel, Matlab, and potentially ASPEN Plus. Microsoft Excel features an add-in called

Solver that serves as an optimization tool. Matlab can also be used to create extensive operations optimization. Finally, ASPEN Plus is an additional option, however it requires different inputs than the Microsoft Excel and Matlab options.

Superior Concept

The programming tool selected for this product design was Microsoft Excel and the Solver add-in. This allows for the design of an optimization model using multiple spreadsheets for each of the mass balances. In addition, a user-friendly "landing page" can be created that allows the user to input the necessary constraints and prices. Furthermore, Solver blocks can be easily troubleshooted and the file itself easily shared. The Excel format requires certain assumptions, namely utilities that scale linearly with process throughput in order for the model to provide a suggested C4 purchase amount in a timely manner. While the assumption of proportional utilities introduces some error in the cost calculations, particularly in the 1-butene distillation and any process unit running at very low throughput, the model can be easily updated with utility requirements observed by process operators.

Matlab and ASPEN were decided against because they did not easily allow for the same accessibility and visual output that an Excel model could possess. Matlab would have required the user to keep track of a very large workspace of variables that could cause confusion and error if the user did not take extreme care when changing multiple process parameters. More of the coding for graphical analysis would have been left for the user to input, restricting the potential users to those in the company with proficient Matlab skills.

Assumptions

Several assumptions were necessary in order to create a working optimization model. First, it was assumed that utilities scale linearly with throughput. This allowed the model to quickly provide a purchase amount using the information available to the group. It is also assumed that all unit operations exist at the given petrochemicals plant, and that these unit operations are readily available. The reactors in these processes were assumed to operate under the same conditions regardless of throughput. Any additional reactants, i.e. hydrogen, were added in stoichiometric proportion. By doing this, the group is assuming that there is already excess reactant that is being recycled in the process, requiring only stoichiometric makeup of the reactant for the process to operate. Varying reactor conditions was not considered as an optimization parameter. For the program to function, it was necessary to assume that the unit operations were already heat integrated and no further heat integration was necessary. For the investment page of the program, it was assumed that the interest rate was constant, the prices and utility costs were constant, and that there was no inflation.

Description of Model

The optimization model must make a series of choices regarding the possible processes that can be carried out in the plant. Both butadiene and 1-butene can be sold as monomers, and are quite profitable when sold in pure form. Isobutylene can also be sold as a monomer, but it is often used in the reaction to form MTBE. 2-butene is not as valuable as a monomer, but there are several processes that can serve as profitable options for 2-butene. These options include: Alkylation, which creates a motor fuel known as "alkylate"; skeletal isomerization to form isobutylene and butenes, which in turn can be converted to MTBE; Metathesis, which creates propylene that can be sold for profit; and olefin isomerization, which creates an equilibrium mix of both 1- and 2-butenes, where the 1-butene can be recovered and sold. The model optimizes the plant by varying the split fractions of the Raffinate 2 stream leaving the MTBE unit, the split fractions of the Raffinate 3 stream leaving the 1-butene distillation, and the amount of additional crude C4 purchased.

Spreadsheet Layout

The model comes preset with capacity, utility, and chemical price values as cited in the following sections of the report. However, the user is free to change these parameters, denoted by blue cell shading, to whatever values the user sees fit. This allows the user to update the model to reflect changes in prices in the chemical marketplace and/or changes in the operating characteristics of the plant brought on by maintenance, fouling, etc.

The Landing Page

Opening the model displays the Landing Page (Figure 1), which contains a detailed summary of the plant operations at the process level with the throughput, throughput constraints, capacity, product, and profit of each unit displayed in the "Process Information" table. In the top left of the Landing Page is the "Feed Information" table, which allows the user to manually input: the amount of crude C4 incoming from the upstream processes, as well as the composition of the C4 feeds. The amount of External Feed is determined by the model and is not a user input. Composition inputs are changed using drop down menus, which reference preset standard compositions and user selected compositions located in the Feed Information sheet (the 6th sheet listed). To the right of the "Feed Information" table, the "Price Scenario" table provides the user with dropdown menus for each of the relevant reactants/products in the plant. These prices reference the Pricing Information sheet, which contains the most up-to-date prices the team could find. As prices can vary geographically and will vary over time, a custom price input is available for each chemical. The "Reset Price" button will automatically reset the price of all chemicals to the "Mid" value as listed in the Pricing Information sheet. To the right of the "Price Scenario" table is the "Utility Information" table, which has utility costs for the relevant utilities in the units specified in the table. The table values are preset according to the "Cost Sheet Outline" on page 604 of Dr. Warren Seider's *Product and Process Design Principles*.[18] Like chemical pricing, utility costs can vary by region and will vary over time, so the model allows the user to input updated utility values in the 'Pricing Information' Sheet, automatically updating those in the Landing Page. The column to the right of the aforementioned tables contains the button that the user clicks to run the optimization simulation with the selected inputs. Displayed below the button is the total profit for the plant for a week of operation. The opportunity cost listed below the total profit is the amount of money the company could expect to make from selling a week's worth of upstream crude C4 production at market price instead of running it through the plant. The table directly below the opportunity cost is a summary of the profit breakdown by product. It should be noted that the profit breakdown for the products reflects the difference between the product revenue and the total cost of operation for the unit which directly produces that product. To make the sum of the profits equal to the total profit, the profit of MTBE includes the utilities of the skeletal isomerization unit, and the 1-butene profit includes the utilities of the olefin isomerization unit. A more accurate representation of the profit from producing each chemical would be given by spreading the utility costs of upstream processes like butadiene extraction to downstream products like propylene and alkylate, which need these upstream processes in order to be produced. Putting a price on the intermediate streams could also be used to obtain more accurate profit margins for the chemicals. The team would make this improvement in the next version of the model by distributing utility costs, as pricing intermediate streams accurately would require market data from the user, which is expensive and may not be directly available. Finally, the two tables at the bottom of the right column display the split fractions of the

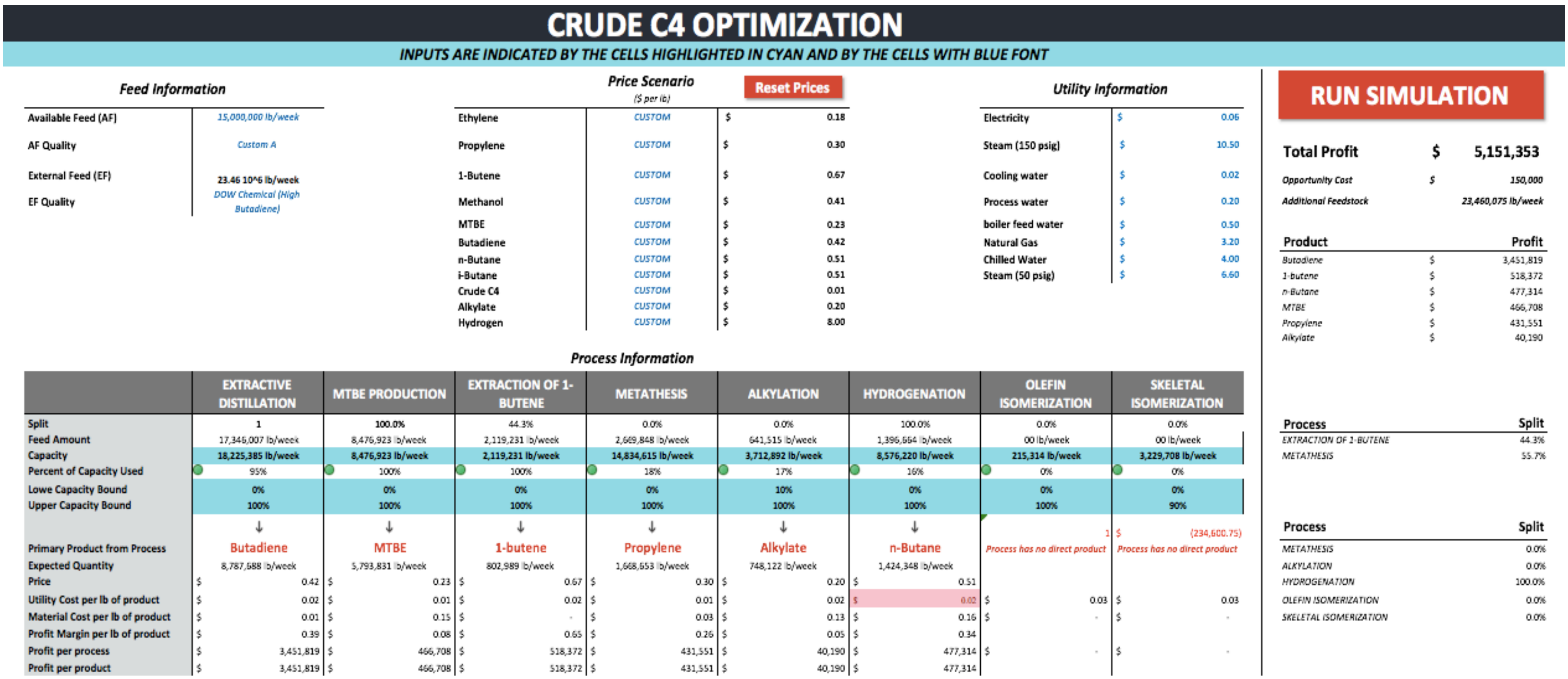


Figure 1: Landing Page

Raffinate 2 and Raffinate 3 streams, respectively. The Raffinate 2 is the product of the MTBE unit, and the Raffinate 3 is the bottoms product of the 1-butene distillation.

3D Sensitivity Analysis

The second sheet is the 3D Sensitivity Analysis. This sheet allows the user to quickly visualize the impact of price changes of two chemicals and/or utilities, selected by the user, on the total weekly profit of the plant. The user also selects the percent change in the selected material/utility prices. The model will apply this percent change to the average price of the material/utility, as given in the 'Price Information' sheet, in order to get eight data points. The "Run Analysis" button executes a macro which runs the optimization program varying the prices of the selected chemicals by the specified increments. The macro also plots the data automatically in a 3D surface plot. While the user can select any two prices to vary, the most interesting and important results arise from the varying of prices of two products that require Raffinate 2 or Raffinate 3 as inputs. This setup would allow the user to see which product holds more influence over the profitability of the plant and is therefore vital in deciding where the majority of the raffinate goes when the plant is running optimally. By varying the price of an input and product of one process, for example ethylene and propylene, the user will be able to observe how changes in profitability of one unit operation impacts overall plant profitability. This analysis could be used in conjunction with econometric forecasting of chemical prices to produce a range of forecasted profits for the plant. The optimal split fractions for the units could also be forecasted and preparations could be made to scale units up or down depending on the analysis results.

Investment Analysis

The third sheet, Investment Analysis, provides the user with a way to quickly examine the cost/benefit analysis of expanding the capacity of a bottlenecked process. The user decides by what percentage to increase capacity and how much it will cost on a per pound basis. The user also selects the interest rate used to evaluate the net present value of the investment as well as the number of years that the investment will last. The process to be expanded is chosen by the user, but it is recommended that the user choose a process that is operating at 100% capacity.

Based on these inputs, the sheet will calculate the new capacity of the selected process and the cost of process expansion.

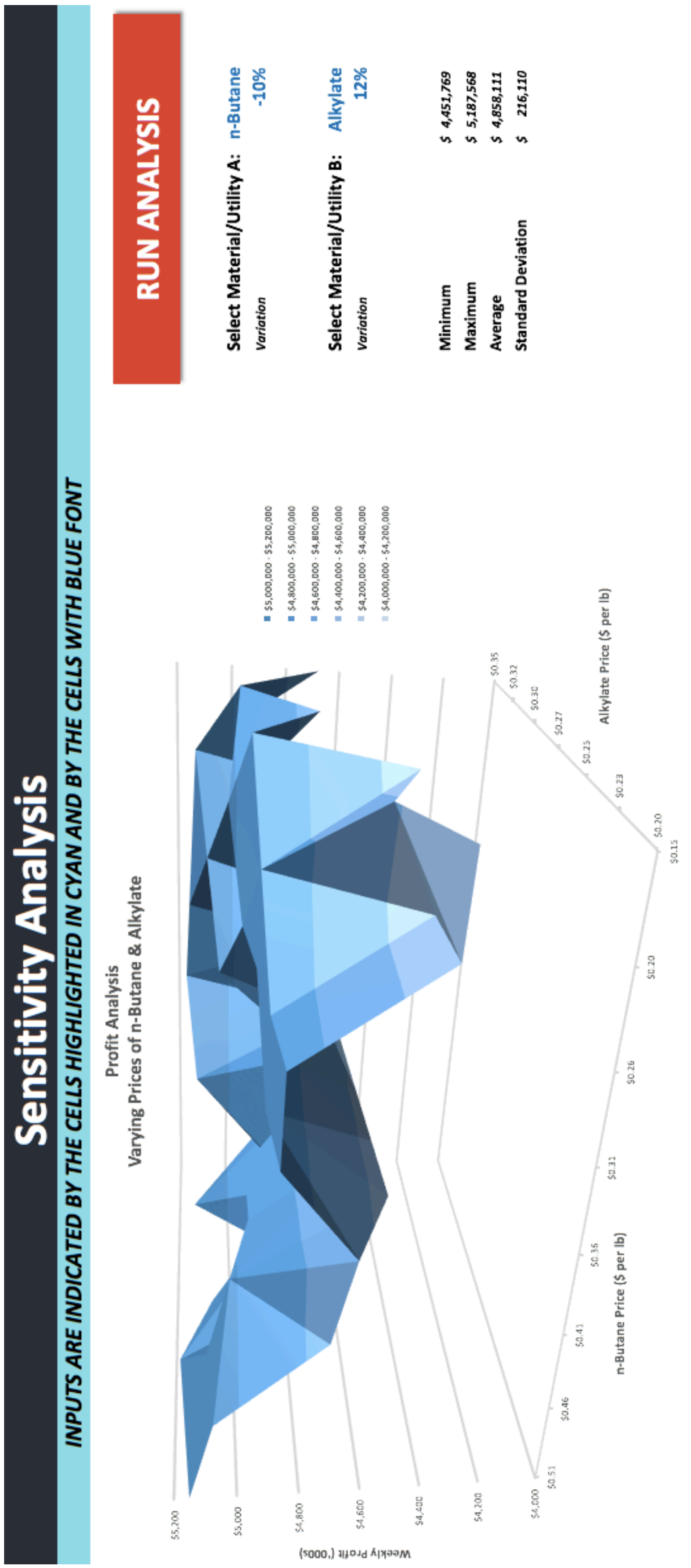


Figure 2: Sensitivity Analysis

Investment Analysis

INPUTS ARE INDICATED BY THE CELLS HIGHLIGHTED IN CYAN AND BY THE CELLS WITH BLUE FONT

	EXTRACTIVE DISTILLATION	MTBE PRODUCTION	EXTRACTION OF 1-BUTENE	METATHESIS	ALKYLATION	HYDROGENATION	OLEFIN ISOMERIZATION	SKELETAL ISOMERIZATION
Current Capacities	18,225,385 lb/week	8,476,923 lb/week	2,119,231 lb/week	14,834,615 lb/week	3,712,892 lb/week	8,576,220 lb/week	215,314 lb/week	################
Capacity Use Pre-Expansion	95%	100%	100%	18%	17%	16%	0%	0%
Capacity Use Post-Expansion	100%	87%	100%	20%	19%	16%	0%	0%

Investment Analysis

Bottleneck		*MTBE PRODUCTION*
Current Capacity		*8,476,923 lb/week*
Percent Expansion		*20%*
Cost per lb	*$*	*25.00*
New Capacity		*10,172,308 lb/week*
Investment Cost	*$*	*42,384,615*
Previous Profit	*$*	*5,151,353*
New Profit	*$*	*5,336,422*
Incremental Profit	*$*	*185,069*
Annual Incremental Profit	*$*	*9,623,597*
Annual Interest Rate		*12.0%*
Lifetime		*10 years*

Discounted Cash Flow Analysis

Break Even Between Years	6-7
NPV	$ 11,990,855.55

Year	Discounted Cash Flow	NPV
0	$ -	$ (42,384,615)
1	$ 8,592,498	$ (33,792,118)
2	$ 7,671,873	$ (26,120,245)
3	$ 6,849,886	$ (19,270,359)
4	$ 6,115,970	$ (13,154,388)
5	$ 5,460,688	$ (7,693,701)
6	$ 4,875,614	$ (2,818,087)
7	$ 4,353,227	$ 1,535,140
8	$ 3,886,810	$ 5,421,949
9	$ 3,470,366	$ 8,892,315
10	$ 3,098,541	$ 11,990,856

Figure 3: Investment Analysis

Clicking on the “Investment Analysis” button will execute that runs the macro. It first optimizes the process using the original capacities. The macro will then optimize the process using the new capacity for the selected process. It will then take the profit before the expansion and after the expansion, calculate an incremental weekly profit, and annualize it in order to do a discounted cash flow analysis using the interest rate and years previously selected by the user. The output of this analysis includes the investment cost, the discounted future cash flows, the year by which the investment is expected to break even, and the net present value of the investment.

A number of assumptions have been made when constructing the investment analysis feature. The interest rate is assumed to remain constant throughout the life of the investment. Future versions could allow for a variable interest rate that could be provided by the company’s econometric forecasting for each year in the period, increasing the accuracy of the discounted cash flow analysis. Another assumption is that prices for utilities and chemicals are constant over this time frame. This assumption reduces the calculation accuracy, as prices are almost certain to change. Future versions could include the option of changing the set of chemical prices yearly as the forecasting wing of the company sees fit. Adding this functionality would only improve the calculations for the first few years at best, however. Since price volatility, especially in the current economic climate, makes long term forecasting lose a lot of predictive power, adding this functionality would only improve the calculations for the first few years at best. Capacity expansion also assumes that construction will not impact current operations. The user is expected to consider all costs in the expansion process, including any start up costs when the expansion is integrated into the existing process. Ideally these are condensed in the per pound cost that the user inputs.

Profit Breakdown

The Profit Breakdown sheet gives a graphical depiction of the profit breakdown by product. The waterfall chart automatically updates when the optimization model is run and/or when the user changes the price inputs in the landing page. As was noted in the Landing Page section, the profit breakdown is calculated based on the difference between the product revenue and the operating cost of the unit that produces it. In the case of the MTBE production, the costs of skeletal isomerization have been included when calculating the profit. Similarly, the cost of olefin isomerization has been taken into account when determining the profit of 1-butene distillation. These combinations were made because the isomerization units do not directly produce a sellable product, as their functions are to increase production of the process units their costs have been combined with. This method of calculating profit results in an accurate total plant profit, but it does not include the cost of requisite upstream processes in the production of downstream products like alkylate and propylene. Future versions of the optimization program would spread these costs out and provide a more accurate account of the profit breakdown.

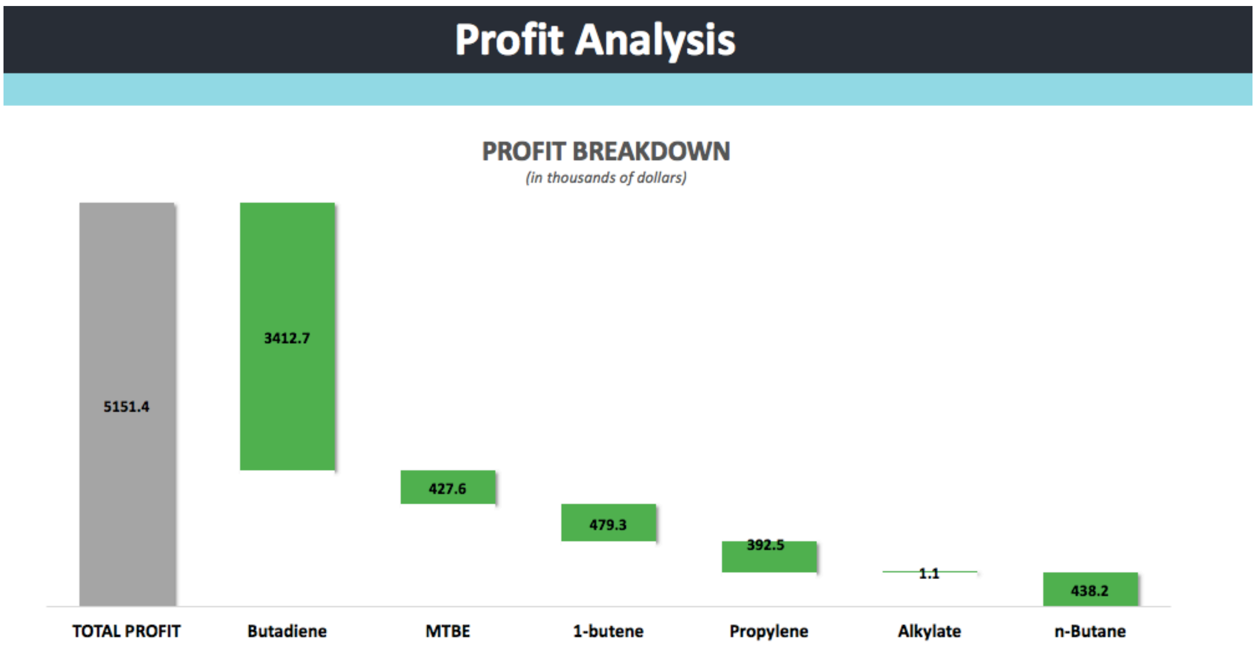


Figure 4: Profit Analysis

Detailed Flow Diagram

The user can get a clearer visual of the plant operations on this sheet. The possible connections between the plant processes are shown along with the percentage of a unit's output intermediate stream that is sent along a particular path. The percentages update automatically with every run of the optimization macro from the Landing Page. Product streams are shown as dashed lines, but the flow rates must be recorded from the Landing Page. The group

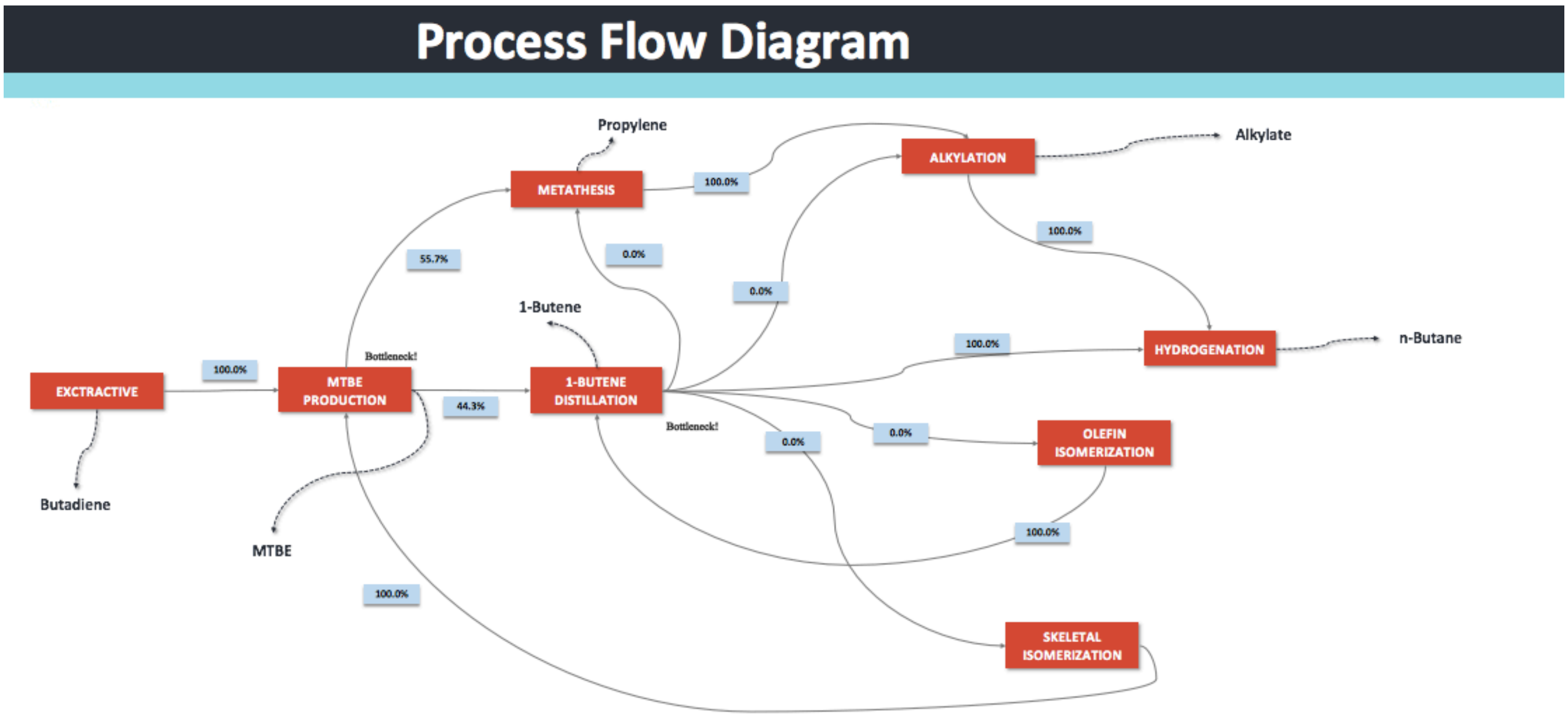


Figure 5: Process Flow Diagram

excluded the product flow rates because the large numbers would overcrowd the diagram while only providing information that the user could easily find on another page.

Feed Information

This sheet is preloaded with different compositions of crude C4 based on the production specifications of the Dow Chemical Company. The medium, high, and low butadiene content compositions displayed in the table are the ones referenced in the drop down menu on the Landing Page. Additionally, there are two columns for custom compositions of crude C4. These columns have been included because it is unlikely that the company's own crude C4 composition and the composition of the crude C4 available for purchase will match those of the selected Dow Chemical options. After lab sampling of both the internal and external crude C4, the user can input the results in the custom columns of the table. These can also be referred to in the dropdown menus on the Landing Page. If the compositions inputted by the user lie outside the Dow Chemical specs shown below the table, the green circle will turn red next to the outlier species. To help prevent user error, if the sum of the custom percentages does not equal 100%, the cell in the last row will turn red.

FEED INFORMATION

INPUTS ARE INDICATED BY THE CELLS HIGHLIGHTED IN CYAN AND BY THE CELLS WITH BLUE FONT

DOW CHEMICAL CRUDE C4

Composition of Incoming C4

Ideally would be derived from lab results

Feed Sample	DOW Chemical (Medium Butadiene)	DOW Chemical (High Butadiene)	DOW Chemical (Low Butadiene)	Custom A	Custom B
1,3-Butadiene	45.0%	60%	30%	51%	58%
isobutylene	25.0%	15%	30%	23%	21%
1-butene	12.0%	15%	15%	9%	7%
2-butene	10.0%	10%	14%	9%	6%
n-butane	6.0%	0%	8%	8%	6%
isobutane	1.0%	0%	2%	0%	2%
1,2 butadiene	1.0%	0%	1%	0%	0%
TOTAL	100.0%	100.0%	100.0%	100.0%	100.0%

Typical Crude C4 Compositions from Dow Chemical

	Minimum	Maximum
1,3-Butadiene	30%	60%
isobutylene	10%	30%
1-butene	5%	16%
2-butene	0%	14%
n-butane	0%	8%
isobutane	0%	2%
1,2 butadiene	0%	1%

Figure 6: Feed Information

Pricing Information

The most recent prices the group could locate for the chemicals and utilities relevant to the plant are located in the table on the left of this sheet. Source and date information are located in each row, with the majority of prices coming from Platt and Argus within the several months of the report's publishing. It should be noted that these prices are not from the same point in time, and with the recent volatility in the industry, the varied timeframes may cause the results of the optimization program to return unrealistic profit margins, as well as inaccurate split fractions. It is therefore recommended that the company frequently update the prices of the chemicals with their most up to date information. The custom column was created for this purpose, although all other columns can also be updated. For some chemicals like MTBE, crude C4, and alkylate, the prices quoted are often on a volume basis. Since the optimization program operates on a mass flow basis, the Pricing Information sheet converts the price per volume to price per pound in the table on the right. The user simply needs to input the price per gallon and the remaining cells in the table will autofill with the price per pound in cents.

Pricing Information

INPUTS ARE INDICATED BY THE CELLS HIGHLIGHTED IN CYAN AND BY THE CELLS WITH BLUE FONT

Prices

($ per lb)

Material	MED	LOW	HIGH	CUSTOM	Source	Month	Year
Ethylene	0.18	0.153	0.20	0.18	Platt	January	2016
Propylene	0.3	0.255	0.34	0.30	Platt	January	2016
1-Butene	0.665	0.64	0.69	0.665	Argus	August	2015
Methanol	0.405	0.34425	0.2926125	0.405	Platt	January	2016
MTBE	0.2346	0.19941	0.26	0.23	Platt	January	2016
Butadiene	0.415	0.36	0.47	0.415	Argus	August	2015
n-Butane	0.5106	0.5075	0.5138	0.5106	Argus	August	2015
i-Butane	0.5112	0.5088	0.5138	0.5112	Argus	August	2015
Crude C4	0.01	1.2593	1.5088	0.01	Argus	August	2015
isobutylene	0.575	0.55	0.6	0.575	Argus	August	2015
Alkylate	0.2017	0.2009	0.27	0.2017	OPIS	February	2016
Hydrogen	8	8	8	8			
Electricity	0.06			0.06			
Steam (150 psig)	10.5			10.5			
Cooling water	0.02			0.02			
Process water	0.2			0.2			
boiler feed water	0.5			0.5			
Natural Gas	3.2			3.2			
Chilled Water	4			4			
Steam (50 psig)	6.6			6.6			

Density Calculations			
Alkylate	5.93 lb/gal		
	119.64	119.14	120.14
Crude C4	5.09 lb/gal		
	704.5	768	641
MTBE	6.18 lb/gal		
	1.45	1.2325	1.63
	145	123.25	163.4875

Figure 7: Pricing Information

Process Sheets (Extractive Distillation)

The sheets for each of the plant processes have the same basic structure and function, so for brevity the report will base the discussion of the process sheets on the Extractive Distillation sheet. Any differences in other process sheets will be noted.

Since extractive distillation is the first process in the plant, its sheet is unique in that it is set up with additional information about the crude C4 feed. The selected compositions for the internal and external crude C4 feeds are displayed in the top left of the sheet. Below the percentage compositions are the mass flows for each of the relevant chemicals in each of the feeds. The block diagram for the process is seen to the right of these tables. For the streams shown, the mass flow rates are shown in the large table underneath the diagram. All processes have a main table similar to this one in which the mass flows of input, intermediate, and output streams are calculated. The output stream for butadiene extraction is Raffinate-1, whose mass flow rates are referenced as one of the input flow streams of the MTBE production sheet. The rest of the intermediate streams are linked between processes as depicted in the Detailed Flow Diagram.

The process parameters of: distillation effectiveness, cell J33; fraction of unrecovered butadiene hydrogenated, cell O49; and fractional conversion of hydrogenated butadiene, cells R49-51, are used in calculating the mass flows of the intermediate streams and hydrogen input. The required hydrogen is then converted to lbs per lb butadiene product for the butadiene material cost cell on the Landing Page. For other processes with additional inputs like MTBE production, metathesis, and alkylation, the additional input is also calculated on the right of the main process stream table and is changed to a lb per lbs product basis. Other processes also have parameters that affect performance that can be tuned to the user's preference. This freedom allows the user to account for changes in the plant's efficiency as the plant ages or between routine maintenance.

The butadiene extraction utility data is collected on the right of the sheet. The data for each process has been selected from the sources listed in each process description. The utility requirements are then combined with the utility prices on the Landing Page to provide a total utility bill per lb of product for a given process. This number is then brought back to the Landing Page in the utility cost row for the processes. Capacity conversions are shown next to the utility information.

Using the Model

When using the model, the user must first provide the amount of available crude C4 feed coming from upstream processes in the company, as well as its composition and the composition of the crude C4 available for purchase. The model will update the profit and mass flow rates for the given split fractions immediately after each input value is changed. The results will not be optimized, however, until the user clicks on the "Run Simulation" button. Once the user has selected the desired chemical and utility prices on the Pricing Information sheet, the user can select capacity restraints for each of the processes. It should be noted that over constraining the processes can cause the available crude C4 flow to be insufficient or overload the processes, depending on the constraints selected. For example, if a high flow requirement is desired for every process that receives an input from 1-butene distillation, there might not be enough flow through the distillation process to satisfy the constraints for the other processes. Conversely, if a high flow minimum is imposed on the 1-butene distillation and low maximums are imposed on the downstream units, there might be too much flow to meet the constraints downstream. If the selected constraints, which can be changed by the user, are not met, the circle in the "percent capacity used" column will change from green to red for the process. Once the prices and capacity constraints have been selected, the user can run the simulation to optimize the plant by clicking on the "Run Simulation" button. The Process Information table will then display the optimal split fractions for the plant along with capacity usage and product information. The external C4 will then be set to the optimal value, resulting in the total profit being maximized. If the change in external C4 and the split fractions cannot satisfy capacity constraints, an error window will pop up after running the optimization stating that the constraints could not be met. Adjustments to the capacity constraints or external C4 composition can be made to attempt to satisfy the constraints, rerunning the simulation after each change. In the design team's experience, overloaded processes in the downstream part of the plant can be rectified by increasing butadiene content in the external crude C4 composition if adjusting the capacity constraints is not possible. If the user exhausts all possible adjustment options and the constraints are not satisfied, they should consider taking action like selling available crude C4 or inputting additional feed at different points in the plant, depending on if the plant is overfull or running dry. The user can perform trial-and-error to determine how much available crude needs to be sold, but the model does not easily allow for the addition of external feed at multiple points in the plant.

Assuming the constraints are met, the user now has the optimal amount of external crude C4 to be purchased and the resulting profits. Now the user may turn their attention to the Sensitivity Analysis page. The user can then select the two prices that they want to vary from the drop down menus. The increments of change can be inputted as percentages for each variable. Clicking on the "Run Analysis" button will present the relationship between the variables' prices and the total profit.

The Investment Analysis page is straightforward to use. After running the optimization on the Landing Page, running the Investment Analysis by clicking the button will automatically locate the bottleneck of the plant under the current conditions. If there is no bottleneck, which is unlikely given the proportional utility assumption, the analysis will report back that there is none. The user needs to simply input the percent expansion of the unit's capacity, the interest rate, and the lifetime of the expansion. The cost per lb added capacity must also be provided by the user through an outside costing analysis for the unit. Once the inputs are entered, the additional profit per year are displayed, and the present value for the additional profit and the expansion project are given in the table. The requisite lifetime for the project to turn a profit is displayed above the table.

Case Study

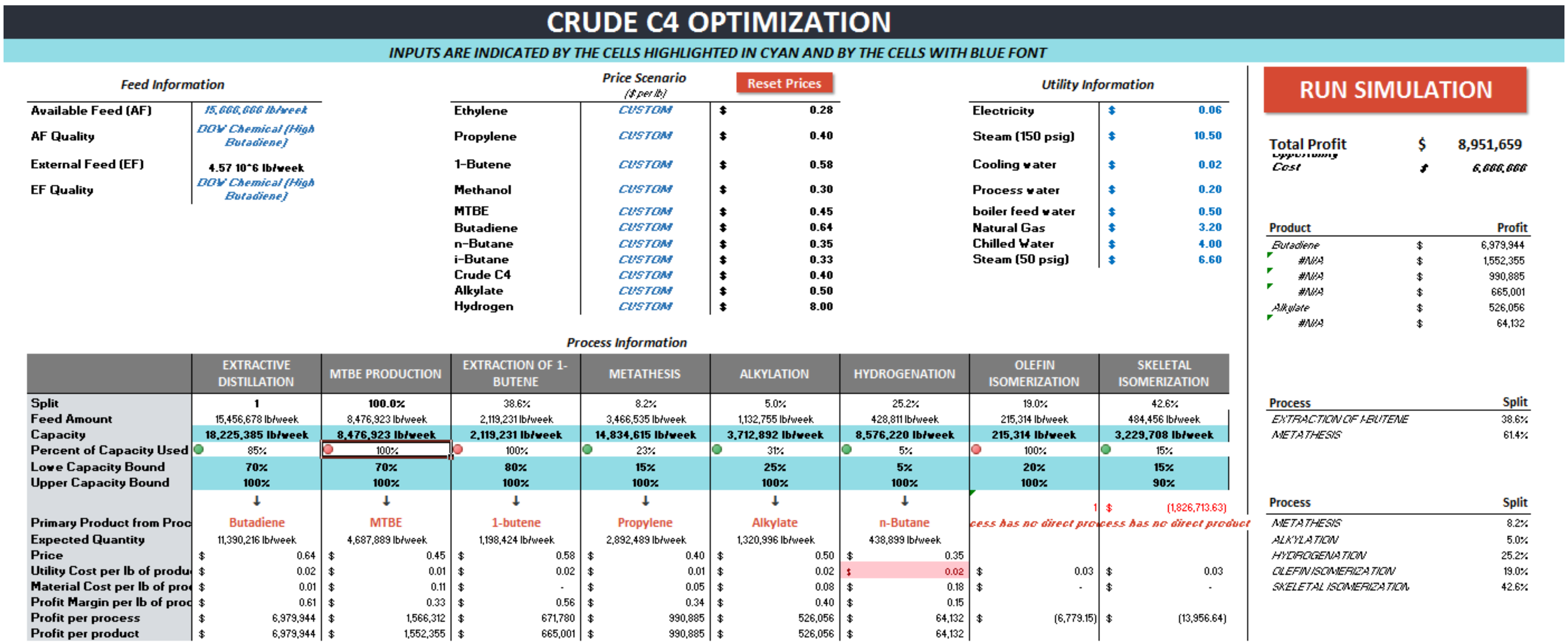
To give a more concrete example of how the model is used, consider the pricing scenario as shown in Figure 8.

	Price Scenario ($ per lb)	Reset Prices	
Ethylene	CUSTOM	$	0.28
Propylene	CUSTOM	$	0.40
1-Butene	CUSTOM	$	0.58
Methanol	CUSTOM	$	0.30
MTBE	CUSTOM	$	0.45
Butadiene	CUSTOM	$	0.64
n-Butane	CUSTOM	$	0.35
i-Butane	CUSTOM	$	0.33
Crude C4	CUSTOM	$	0.40
Alkylate	CUSTOM	$	0.50
Hydrogen	CUSTOM	$	8.00

Utility Information		
Electricity	$	0.06
Steam (150 psig)	$	10.50
Cooling water	$	0.02
Process water	$	0.20
boiler feed water	$	0.50
Natural Gas	$	3.20
Chilled Water	$	4.00
Steam (50 psig)	$	6.60

Figure 8: Pricing Scenario for Case Study

Assume an available feed of 15,000,000 lb/week of crude C4 at the composition given by high butadiene Dow Chemical crude C4, and the crude C4 available for purchase has the same composition. Figure 9 has the results of the optimization model for this situation, with the process flow constraints given in the Process Information table. The optimization has the optimal purchase of the external crude C4 at 4.57 * 10^6 lbs/week. The valuation of a week's worth the internal C4, the opportunity cost, is calculated at $6,000,000. The weekly profit from operating the plant is calculated at $8,951,659. Therefore, the benefit from running the plant is $2,951,659/week or roughly $153.5million per year. Notable results are that the MTBE unit and 1-butene distillation are at 100% capacity. This arises from the fact that the MTBE unit has a higher capacity than the 1-butene distillation column, and the MTBE unit can send the difference in capacity to the metathesis unit. The olefin isomerization unit is also operating at maximum capacity, while the skeletal isomerization unit is operating against the lower bound of its flow constraints. This suggests that the plant would need to operate below the lower constraint of the skeletal isomerization unit for the plant to reach an unconstrained profit maximum.



CRUDE C4 OPTIMIZATION

INPUTS ARE INDICATED BY THE CELLS HIGHLIGHTED IN CYAN AND BY THE CELLS WITH BLUE FONT

RUN SIMULATION

Feed Information

Available Feed (AF)	15,666,666 lb/week
AF Quality	DOW Chemical (High Butadiene)
External Feed (EF)	4.57 10^6 lb/week
EF Quality	DOW Chemical (High Butadiene)

Price Scenario ($ per lb) — Reset Prices

Ethylene	CUSTOM	$	0.28
Propylene	CUSTOM	$	0.40
1-Butene	CUSTOM	$	0.58
Methanol	CUSTOM	$	0.30
MTBE	CUSTOM	$	0.45
Butadiene	CUSTOM	$	0.64
n-Butane	CUSTOM	$	0.35
i-Butane	CUSTOM	$	0.33
Crude C4	CUSTOM	$	0.40
Alkylate	CUSTOM	$	0.50
Hydrogen	CUSTOM	$	8.00

Utility Information

Electricity	$	0.06
Steam (150 psig)	$	10.50
Cooling water	$	0.02
Process water	$	0.20
boiler feed water	$	0.50
Natural Gas	$	3.20
Chilled Water	$	4.00
Steam (50 psig)	$	6.60

Total Profit	$	8,951,659
Opportunity Cost	$	6,666,666

Product		Profit
Butadiene	$	6,979,944
#N/A	$	1,552,355
#N/A	$	990,885
#N/A	$	665,001
Alkylate	$	526,056
#N/A	$	64,132

Process Information

	EXTRACTIVE DISTILLATION	MTBE PRODUCTION	EXTRACTION OF 1-BUTENE	METATHESIS	ALKYLATION	HYDROGENATION	OLEFIN ISOMERIZATION	SKELETAL ISOMERIZATION
Split	1	100.0%	38.6%	8.2%	5.0%	25.2%	19.0%	42.6%
Feed Amount	15,456,678 lb/week	8,476,923 lb/week	2,119,231 lb/week	3,466,535 lb/week	1,132,755 lb/week	428,811 lb/week	215,314 lb/week	484,456 lb/week
Capacity	18,225,385 lb/week	8,476,923 lb/week	2,119,231 lb/week	14,834,615 lb/week	3,712,892 lb/week	8,576,220 lb/week	215,314 lb/week	3,229,708 lb/week
Percent of Capacity Used	85%	100%	100%	23%	31%	5%	100%	15%
Lowe Capacity Bound	70%	70%	80%	15%	25%	5%	20%	15%
Upper Capacity Bound	100%	100%	100%	100%	100%	100%	100%	90%
	↓	↓	↓	↓	↓	↓	1	$ (1,826,713.63)
Primary Product from Proc	Butadiene	MTBE	1-butene	Propylene	Alkylate	n-Butane	cess has no direct pro	cess has no direct product
Expected Quantity	11,390,216 lb/week	4,687,889 lb/week	1,198,424 lb/week	2,892,489 lb/week	1,320,996 lb/week	438,899 lb/week		
Price	$ 0.64	$ 0.45	$ 0.58	$ 0.40	$ 0.50	$ 0.35		
Utility Cost per lb of produ	$ 0.02	$ 0.01	$ 0.02	$ 0.01	$ 0.02	$ 0.02	$ 0.03	$ 0.03
Material Cost per lb of pro	$ 0.01	$ 0.11	$ -	$ 0.05	$ 0.08	$ 0.18	$ -	$ -
Profit Margin per lb of proc	$ 0.61	$ 0.33	$ 0.56	$ 0.34	$ 0.40	$ 0.15		
Profit per process	$ 6,979,944	$ 1,566,312	$ 671,780	$ 990,885	$ 526,056	$ 64,132	$ (6,779.15)	$ (13,956.64)
Profit per product	$ 6,979,944	$ 1,552,355	$ 665,001	$ 990,885	$ 526,056	$ 64,132		

Process	Split
EXTRACTION OF 1-BUTENE	38.6%
METATHESIS	61.4%

Process	Split
METATHESIS	8.2%
ALKYLATION	5.0%
HYDROGENATION	25.2%
OLEFIN ISOMERIZATION	19.0%
SKELETAL ISOMERIZATION	42.6%

Figure 9: Landing Page after simulation was done using the price scenario for the case study.

Examining the 3D Sensitivity Analysis page, an interesting relationship to examine is the effect of varying isobutane and alkylate prices on the total profit of the plant. The general trend of the 3D graph (Figure 10) is rising profits as the price spread between the chemicals is the largest, with the alkylate at a high price and isobutane at a low price. This is shown on the graph with lower profit at the near right corner and higher profit towards the back left of the graph. The steeper slope from right to left indicates that a change in alkylate price has much more of an impact of the profit than a change in isobutane price. This relationship makes sense because the isobutane requirement roughly one pound of isobutane per four pounds of alkylate. The standard deviation of the profit ranges is $73,336, which is a relatively small figure compared to the profits in the $8million range. This small standard deviation indicates that the plant profit is relatively robust to five percent variations in the prices of isobutane and alkylate. Looking at the Profit Breakdown sheet (Figure 11), the alkylate represents a small portion of the overall profit. Therefore, the small deviations in overall profit in response to chemical price changes in the alkylate process makes sense. Butadiene and MTBE price changes would show a greater standard deviation in the overall profit.

The Investment Analysis page shows an interesting but not unexpected result (Figure 12). The bottleneck selected by the user is the MTBE production. Although the 1-butene column is also operating at 100% capacity, additional flow through the MTBE column would allow the metathesis and alkylation processes to fill out more while still keeping the 1-butene column operating at max capacity. Expanding the 1-butene column would only take away flow from the metathesis pathway, since the MTBE process bottleneck restricts the downstream flow. In this scenario the user is evaluating a 15% expansion of the MTBE unit. For a sample expansion cost, $45.00 per lb/week is used. Note that this value has not been calculated using costing models and is solely intended for the purpose of highlighting the Investment Analysis function. The user would have to perform these calculations when using the Investment Analysis sheet. An interest rate of 12% annually and a project lifetime of 15 years is selected. The cost of expansion is calculated at roughly $57million, and the break even point of the expansion is between years two and three after the capacity is expanded. The net present value of the process over its 15 year lifespan is $123 million.

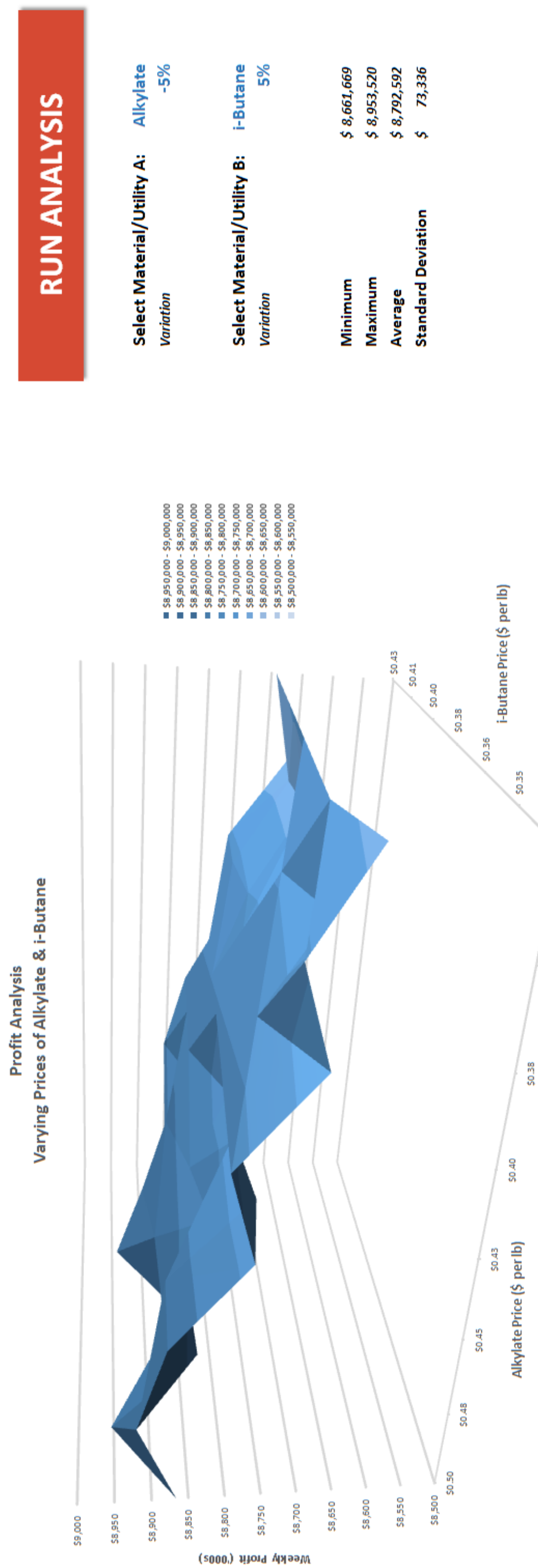


Figure 11: Sensitivity Analysis results for the pricing scenarion in the case study

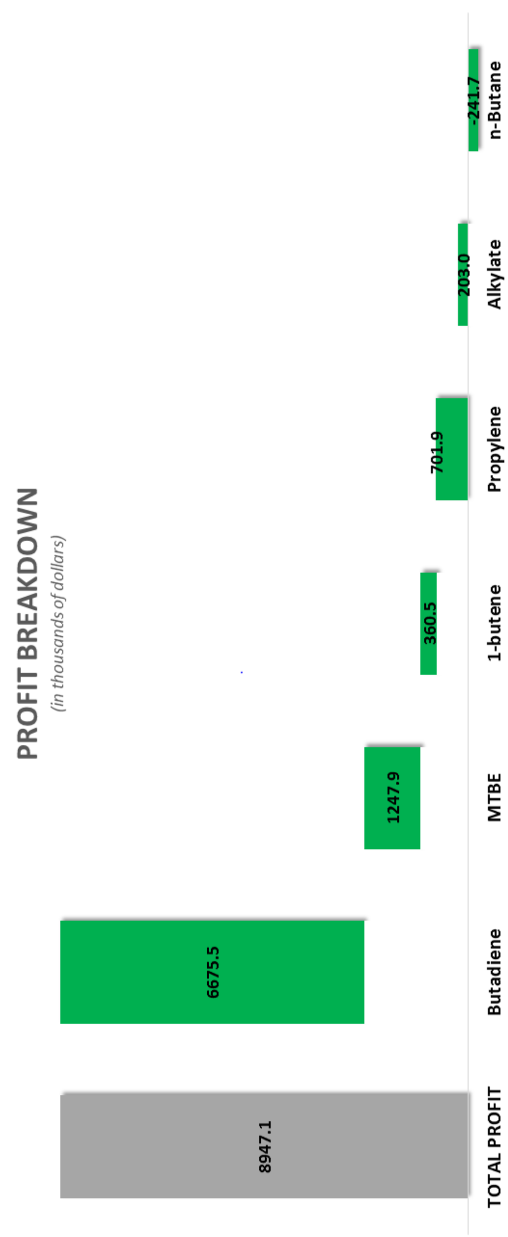


Figure 10: Profit Breakdown for the price scenario in the case study.

Investment Analysis

INPUTS ARE INDICATED BY THE CELLS HIGHLIGHTED IN CYAN AND BY THE CELLS WITH BLUE FONT

	EXTRACTIVE DISTILLATION	MTBE PRODUCTION	EXTRACTION OF 1-BUTENE	METATHESIS	ALKYLATION	HYDROGENATION	OLEFIN ISOMERIZATION	SKELETAL ISOMERIZATION
Current Capacities	18,225,385 lb/week	8,476,923 lb/week	2,119,231 lb/week	14,834,615 lb/week	3,712,892 lb/week	8,576,220 lb/week	215,314 lb/week	3,229,708 lb/week
Capacity Use Pre-Expansion	85%	100%	100%	23%	32%	5%	100%	15%
Capacity Use Post-Expansion	87%	100%	100%	28%	40%	5%	20%	15%

Investment Analysis

Bottleneck		*MTBE PRODUCTION*
Current Capacity		*8,476,923 lb/week*
Percent Expansion		*15%*
Cost per lb	*$*	*45.00*
New Capacity		*9,748,462 lb/week*
Investment Cost	*$*	*57,219,231*
Previous Profit	*$*	*8,936,447*
New Profit	*$*	*9,447,165*
Incremental Profit	*$*	*510,718*
Annual Incremental Profit	*$*	*26,557,325*
Annual Interest Rate		*12.0%*
Lifetime		*15 years*

Discounted Cash Flow Analysis

Break Even Between Years	2-3
NPV	$ 123,659,111.50

Year	Discounted Cash Flow	NPV
0	$ -	$ (57,219,231)
1	$ 23,711,897	$ (33,507,333)
2	$ 21,171,337	$ (12,335,996)
3	$ 18,902,979	$ 6,566,983
4	$ 16,877,660	$ 23,444,643
5	$ 15,069,339	$ 38,513,983
6	$ 13,454,767	$ 51,968,750
7	$ 12,013,185	$ 63,981,935
8	$ 10,726,058	$ 74,707,993
9	$ 9,576,838	$ 84,284,831
10	$ 8,550,748	$ 92,835,579
11	$ 7,634,596	$ 100,470,175
12	$ 6,816,604	$ 107,286,779
13	$ 6,086,253	$ 113,373,033
14	$ 5,434,155	$ 118,807,188
15	$ 4,851,924	$ 123,659,112

Figure 12: Investment Analysis results from pricing scenario in case study.

Unit Operations Descriptions

Butadiene Extraction

Extractive Butadiene Distillation is the first process in the block diagram, and thus the first decision point for the process optimizations model. This process removes butadiene from the mixed crude C4 stream. The resulting butadiene stream is high in purity. Butadiene is used to produce several types of rubbers. Extractive distillation is necessary because the similarities in volatilities between the products in the C4 stream prevent the use of conventional distillation. The specific process described in this report is the BASF butadiene process, which requires the use of N-methylpyrrolidinone (NMP) as a solvent.[11] NMP is not corrosive, which allows for carbon steel to be used in the plant without the risk of corrosion.[2]

BASF butadiene extractive distillation requires three processes. These processes are extractive distillation, degassing, and distillation. The extractive distillation has an overhead product containing butenes and a bottoms product containing crude butadiene. The solvent is recovered during the degassing process, while the butadiene is purified using the distillation process, which allows for a purity of 99.7% or higher. The unrecovered butadiene is then selectively hydrogenated to 90% butenes and 10% butanes before proceeding on to the subsequent processes of the plant.[18]

MTBE Production

Methyl tertiary butyl ether (MTBE) is an oxygenate commonly used in gasoline, although its use has been declining as environmental concerns have surfaced. MTBE and other oxygenates became popular in the 1990s as concerns arose about the air pollution resulting from lead octane enhancers, a problem partially alleviated by the use of oxygenates. However, by the late 1990s and early 2000s, the popularity of MTBE declined due to problems with groundwater contamination and leaks in underground storage tanks.

The specific process used in this report is the Ethermax Process, licensed by UOP.[15] This process converts 99% of isobutylene. The process requires an adiabatic reactor, where the primary reaction occurs. The effluent runs to a distillation column, where the bottoms is the MTBE product. Unreacted components are fed through a fractionator to promote conversion. The methanol in the overhead from the distillation column is then recovered through a system of separations. Although this was the process with the best characteristics the group could find, its capacity created a crippling bottleneck on the rest of the plant. In order to show off the model's capabilities, the group assumed that the plant had access to multiple trains of the Ethermax process.

Metathesis

The metathesis reaction produces propylene from 2-butene, 1-butene and ethylene. The specific process detailed in this project report is the UOP Oleflex Process.[12] In the propylene production process, a feed of liquefied petroleum gas is depropanized to separate and remove the butanes and other hydrocarbons. It is then sent to an Oleflex unit and reacted. The two resulting product streams are a vapor that is rich in hydrogen, as well as a liquid that is rich in both propane and propylene.

1-Butene Distillation

1-Butene distillation allows for the recovery of high purity 1-butene. The 1-butene monomer can be very profitable if it is pure. In a series of two distillation columns, the heavy hydrocarbons are removed in the bottoms stream first, while 1-butene is removed as the bottoms from the second distillation column. This process requires no butadiene or isobutene.[17]

Skeletal Isomerization

Skeletal Isomerization involves isobutylene, 1-butene, and 2-butene. At high temperature, these constituents reach chemical equilibrium. Skeletal isomerization allows for the product to be fed to an MTBE unit and convert the isobutylene into profit. The process described in this report is the skeletal isomerization process (SKIP) process, introduced by the Texas Olefins Company.[9] A feed of 1 and 2-butenes are first vaporized, and steam is added. The stream is heated to reaction temperature, which falls between 480-550° C. Next, the stream is reacted in a fixed-bed reactor, where some of the 1- and 2-butenes are converted to isobutylene. Following reaction and equilibrium, the stream is cooled in a heat exchanger and a water-quench column. The hydrocarbons are then separated from the stream and depropanized to recover the isobutylene for use in other processes.

The SKIP process, like other similar processes introduced by other companies, is often included following an MTBE process. The isobutylene is then recycled back to the MTBE unit for further production of the profitable MTBE. An alternative option for setup is to include two MTBE units with a SKIP unit between them.

Olefin Isomerization

Olefin Isomerization, also commonly known as butene isomerization or positional isomerization, involves the conversion of 2-butene to 1-butene. The process described here is the Comonomer Production Technology (CPT) by CB&I.[4] However, specific utility requirements were unavailable for any commercial olefin isomerization technology. Using a ratio comparing the utility costs of existing skeletal and olefin isomerization technologies, it was possible to obtain an estimate for olefin isomerization, at approximately 38% of the utility cost of skeletal isomerization.[8] The CPT Process includes two sections. In the first section, 2-butene is isomerized to 1-butene. The stream is vaporized and preheated before being fed to a reactor where the 2-butene is isomerized over a catalyst. The product stream contains both 1- and 2-butene at thermal equilibrium. The second section is the fractionation section where 1- and 2-butene are separated using a butene fractionator. The 1-butene is the overhead product, while the 2-butene is the bottoms which is then recycled to the isomerization reaction. However, since our plant already has its own 1-butene distillation, our olefin process only represents this first section.

Olefin isomerization allows for a large increase in 1-butene recovery, which then allows it to be sold for profit.

Alkylation

Alkylation is a process by which trimethylpentane or "alkylate" is formed from isobutane, isobutylene and 2-butene. Alkylate is a component for motor fuel, which was popular in the 1940s. However, with the decline in popularity of MTBE due to serious environmental concerns, it is possible that alkylate will increase in value in the coming years. The specific process listed here is the STRATCO Alkylation process by Dupont, which uses sulfuric acid.[13] According to the process description, there are five sections of the process, which include the reaction section, the refrigerator section, the effluent treating section, the fractionation section and the blowdown section. The reaction section includes the reaction between the hydrocarbon stream and the sulfuric acid catalyst. The refrigeration section removes both heat of reaction as well as light hydrocarbons. In the effluent treating section, free acid, alkyl sulfates and dialkyl sulfates are removed from the stream. The fractionation section follows the effluent treating section, where isobutane is removed and recycled to the reaction section. Finally, in the blowdown section, the acid is degassed and the pH of the wastewater is adjusted.

Hydrogenation

Butenes can be hydrogenated to n-butane, which allows them to be returned to the steam cracker as a feed. This option is typically less desirable than the other unit operations that can be used to process 2-butene. The hydrogenation process listed here is the Hüls Selective Hydrogenation Process (SHP).[14] The selective hydrogenation process can be used with various feed streams, including C3-C5 streams.

Utility and Capacity Requirements

Overall utility information is included below for each of the unit processes. Pricing information was obtained from the *Product and Process Design Principles* Textbook for the cost of electricity, water, gas and steam.[11] Pricing for various acid solutions, including the sulfuric acid and sodium hydroxide for the Alkylation process, were obtained from Alibaba. It should be noted that this project creates an optimization program for an already existing petrochemicals plant, thus it is not necessary to purchase additional equipment for the unit operations because it is assumed that the company already possesses all necessary equipment.

Metathesis (UOP Oleflex)

Utility	Requirement
Electric Power	6500 kW/h
Boiler Feed Water	10 metric tons per hour
Cooling water	6000 m^3 /h
Fuel Gas	13.1 million kcal/h
Capacity	350,000 MTA

Alkylation (Dupont STRATCO)

Utility	Requirement (unit/barrel)
Electric Power	15 kW
Cooling water	1370 gal
Process water	4 gal
Steam	194 lb
Fresh acid	13 lb
NaOH	.05lb
Capacity	240 MT per stream day

MTBE Production (UOP Ethermax)

Utility	Requirement
Electric Power	177 kWh
Medium-Pressure Steam	7.9 mt per hour
Cooling Water	52 cubic meters per hour
Condensate	7.9 metric tons per hour
Capacity	50,000 MTA

Butadiene Extraction (BASF)

Utility	Requirement
Electric Power	100-200 kWh
Medium-pressure	1.5-2.5t
Cooling Water	100-200 cubic meters
Solvent (Cost)	$0.60 (per metric ton product)
Other Chemicals (Cost)	$2.50 (per metric ton product)
Capacity	29,000 to 430,000 MTA

Hydrogenation (Hüls Selective Hydrogenation Process)

Utility	Requirement
Power	46 kWh
Medium pressure steam	798 kg/hr
Condensate	798 kg/hr
Cooling water	51 m^3/hr
Capacity	6373 BPD

Skeletal Hydrogenation (SKIP Process)

Utility	Requirement
Electric Power	234.16 kWh
Medium-pressure	1.735 mt
Low-Pressure	1.739 mt
Cooling Water	6.576 GJ
Natural Gas	1.679 GJ
Capacity	2400 BPD

1-Butene Distillation

Utility	Requirement (unit per ton 1-butene)
Steam	4t
Water, cooling	110 m^3
Power	43 kWh

Conclusion and Recommendations

This report chronicles a project entitled *C4 Operations Optimization*, which involved the creation of a computer model that can optimize operations and processes for an existing petrochemicals plant. Other features of the project include a sensitivity analysis and investment analysis that provide the user with an idea of how the plant profitability will respond to changes in the economic climate and plant capacity. It is recommended that the plant in question begin using this model promptly, as it can increase profits by a considerable margin. For further developments in the model, we recommend modifications to the method by which it takes utility costs into account. Instead of assuming proportional utilities, functions relating utility requirements to throughput could be incorporated into the model. These functions could be derived from plant observation or from ASPEN simulations.

With the current model, profitability is listed by product, but subsequent versions could spread the utility costs so that one product is not absorbing all the utility costs. Another feature that could be added is a set of purity constraints for each product as specified by the company. These would be most applicable in the 1-butene and n-butane product streams, as trace amounts of isobutylene and isobutane, respectively, can enter these product streams and lower purity.

Acknowledgements

We have been lucky to have had the guidance and support of several faculty members at the University of Pennsylvania as well as from industry consultants. Without these individuals, our project would not have been possible.

We would like to first thank Mr. Gary Sawyer for introducing our project and for his constant advice and help throughout the semester. He responded to all emails and questions in a timely and helpful manner, and his suggestions on how to format the program were especially valuable.

We would also like to thank our faculty advisor, Dr. Wen K. Shieh, for his assistance throughout the semester. Dr. Shieh attended all of our weekly meetings and provided advice and support for our project.

We would like to thank Dr. Warren Seider and Dr. Sean Holleran for their guidance and advice during the CBE 459 and 460 design courses. Without this introduction to the senior design process, we would not have been able to successfully complete our project.

We would like to thank Professor Leonard Fabiano for his support and guidance through the senior design process. We especially appreciate him taking the time to review our project and report.

We owe additional thanks to the many industry consultants who met with us on a weekly basis. Our sincere thanks goes to Dr. Ivan Baldychev, Mr. David Kolesar, Mr. Steven Tieri, and Mr. Bruce Vrana.

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