

Jet Fuel Production from Olefins for Chevron

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CHEN 4530: Design Project

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Executive Summary

The purpose of this project was to retrofit an existing gasoline production unit involving two alkylation trains and to convert one into a jet fuel production train for Chevron, a petroleum refinery company. This involved the addition of several new pieces of equipment, including a new section called the Dimersol process. The Dimersol process converts propane into isohexene, the main component of the final product, jet fuel, through a black box reactor. From this point in the Dimersol process, the reactor products are taken through two distillation columns, essentially dividing the streams into a butane or lighter stream, which will go through the ISOAKLY Light train, and butane or heavier, which will go through the ISOALKY Heavy train. The ISOALKY Light train will lead to the production of gasoline whereas the ISOALKY Heavy train will lead to the production of jet fuel. Both ISOALKY Light and Heavy trains have their respective black box reactors to further obtain their final products. The final specification requested by Chevron was to get a flash point of 104°F for the jet fuel stream, which exits from the bottoms of the final distillation column at a flow rate of 279 GPM.

The major pieces of equipment needed to obtain this specification were: seven distillation columns, 22 pumps, six heat exchangers, one compressor, two flash drums, three black box reactors, 4 chlorine as well as several control valves, check valves, and vessels. Each piece of equipment played a role in the production of jet fuel efficiently and economically. Equipment was designed with the goal of obtaining enough specs to be able to price the equipment for the economic analysis.

Our economic analysis concludes that the plant would be a profitable investment with an IRR of 226%, which far surpasses the hurdle rate target of 15%, and an ROI of 273%. This economic analysis was performed solely assessing new equipment and related capital and variable costs. However, due to the amount of assumptions and estimates made within this report it is suggested that a more accurate simulation, particularly with regard to the reactors, be made and that a more thorough analysis of the equipment pricing and resulting economic feasibility be done, perhaps with a more rigorous toolset. That being said, even with the skew of other products being minimized, the retrofit addition to the plant still promises to be economically viable and is recommended to move forward with the project.

1 - Project Description, Approach and Management Plan

1.1 - Overall Project Description and Scope

Chevron has charged the team with analyzing the economic viability of retrofitting an existing gasoline refinery to a combined jet fuel and gasoline refinery using a newer, safer process proprietary to Chevron. Along with this retrofit, Chevron has asked that the new isoalkylation process, ISOALKY, is coupled with a Dimersol process to produce the heavier components needed for the jet fuel blend. This combination has never been implemented and is a first for Chevron with plans to start construction at a West Coast plant by 2027. Chevron's proprietary ISOALKY process uses the same equipment as previous processes, thus minimal reactor redesign is required. The overall process has two trains; a light train to produce gasoline, butane and propane, and a heavy train to produce jet fuel and gasoline. Both of these trains utilize products from the new Dimersol process and fluid catalytic cracked (FCC) hydrocarbon feeds from elsewhere at the refinery. Existing equipment will be able to be reconditioned for the light train but all of the equipment spec'd in this analysis for the Dimersol process and heavy ISOALKY train will be built from scratch.

1.2 - Background

This project is being undertaken mostly due to a result of the shifting demand in the hydrocarbon fuels industry. With the rise in electric vehicle demand, particularly along the west coast where the plant is located, demand for light fuels is expected to decrease in upcoming years. Conversely, demand for heavy fuels such as jet fuel is expected to remain constant, and possibly even increase over time as no viable alternative is poised to take its place. The west coast plant currently has two trains producing light fuels and this project seeks to answer whether it would be economically practical to convert one of the trains producing light fuels to a train that produces heavy fuels. A hurdle rate of 15% was set as the minimum requirement for the conversion to be economically feasible. Because this project is primarily a question of economics, designing equipment was a far less rigorous process than it otherwise would be, and many of the conclusions made from this report are made from the economic analysis.

1.3 - Approach and PFD

The general approach the group made was largely outlined by Chevron's team providing documents (Leichty, S. et al., 2024). With how extensive the scope of the process was, the team needed to start simple. First, a block flow diagram was created, essentially outlining the entire system to understand the overall structure, this is outlined in **Figure 1.3.1**. This was the first step to defining the process, as it allowed effective organization of the process, laying out all of the required units and starting to map out the components. In the block flow, the blue pieces of equipment preexisting and the orange pieces of equipment will be added to the process. With guidance from Chevron, the pressures for reactors and columns were added along with the desired number of trays for the columns. Heat exchangers and pumps were generally avoided on this diagram except selected heat exchangers used for heat integration. The block flow diagram also came in handy when sorting out the material balances as there are a large amount of components to track. From this point forward, a process flow diagram (PFD) was beginning to be constructed.

The PFD, similar to the block flow diagram, included more details of the system and every piece of equipment to be used. These pieces of equipment include but are not limited to: the condensers, reboilers,

drums, coolers, heat exchangers, and valves. The distillation columns were used to separate fluids based on volatility and include both the condensers and reboilers. The reboiler drums were used to collect the feed vapor from the tops of the columns. The coolers and heaters were used to cool or heat with various utilities. The heat exchangers take two streams of various temperatures and cross them to heat one and cool the other. Pumps were used to increase the pressures to either overcome the large distance between pieces of equipment or to bring the stream to a certain pressure for an incoming piece of equipment. In between each of these pieces of equipment, were defined temperatures and pressures of each of the streams. The pressure profile was necessary in order to eventually begin the project's Aspen HYSYS simulation, which is detailed more in **Section 6**. Defining the pressures between every piece of equipment would help contextualize where additional pumps or streams were needed, as well as to map out where the pressures, levels, or temperatures would need to fluctuate within the system to ensure a safe and efficient process. Several assumptions were made in order to get an accurate pressure drop throughout the system, such as the pressure drop across a level controller; these are outlined more in detail in **Section 4**. Additionally, in order to get an accurate reading on some of the pressures after the condensers on the tops of the columns, a Cox chart was used, which can be found in **Appendix A**. The PFD is shown below in **Figure 1.3.2**, where it was created in an Excel spreadsheet upon Chevron's request. **Table 1.3.1** goes through the symbols defined in **Figure 1.3.2**. Since **Figure 1.3.2** is very extensive, there are three subfigures that zoom into the various parts. **Figure 1.3.3** shows the Dimersol section of the process, **Figure 1.3.4** shows the ISOALKY Light section of the process, and **Figure 1.3.5** shows the ISOALKY Heavy section of the process.

Table 1.3.1: Key for **Figure 1.3.2**.

Shown in PFD	Definition
P-XX	Pump
C-XX	Cooler
H-XX	Heater
Sph.	sphere
Cl	Chlorine adsorber
Dryer	Mole sieve dryer
Com-XX	Compressor
PR	Partial reboiler
TT	Temperature transmitter
LC	Level control
	Check valve
	Valve
	Can vary with Aspen simulation

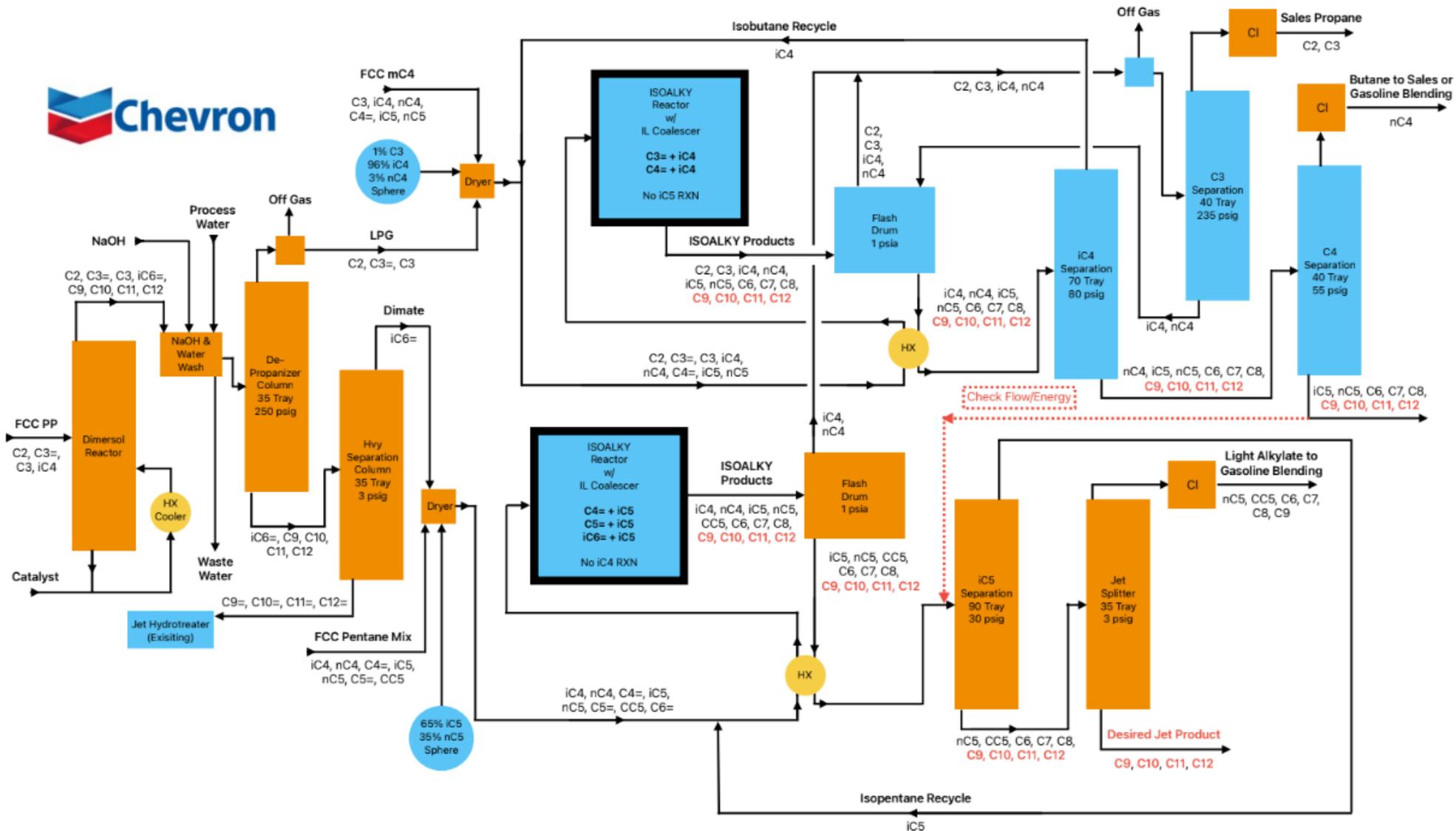


Figure 1.3.1: Box flow diagram for the entire process.

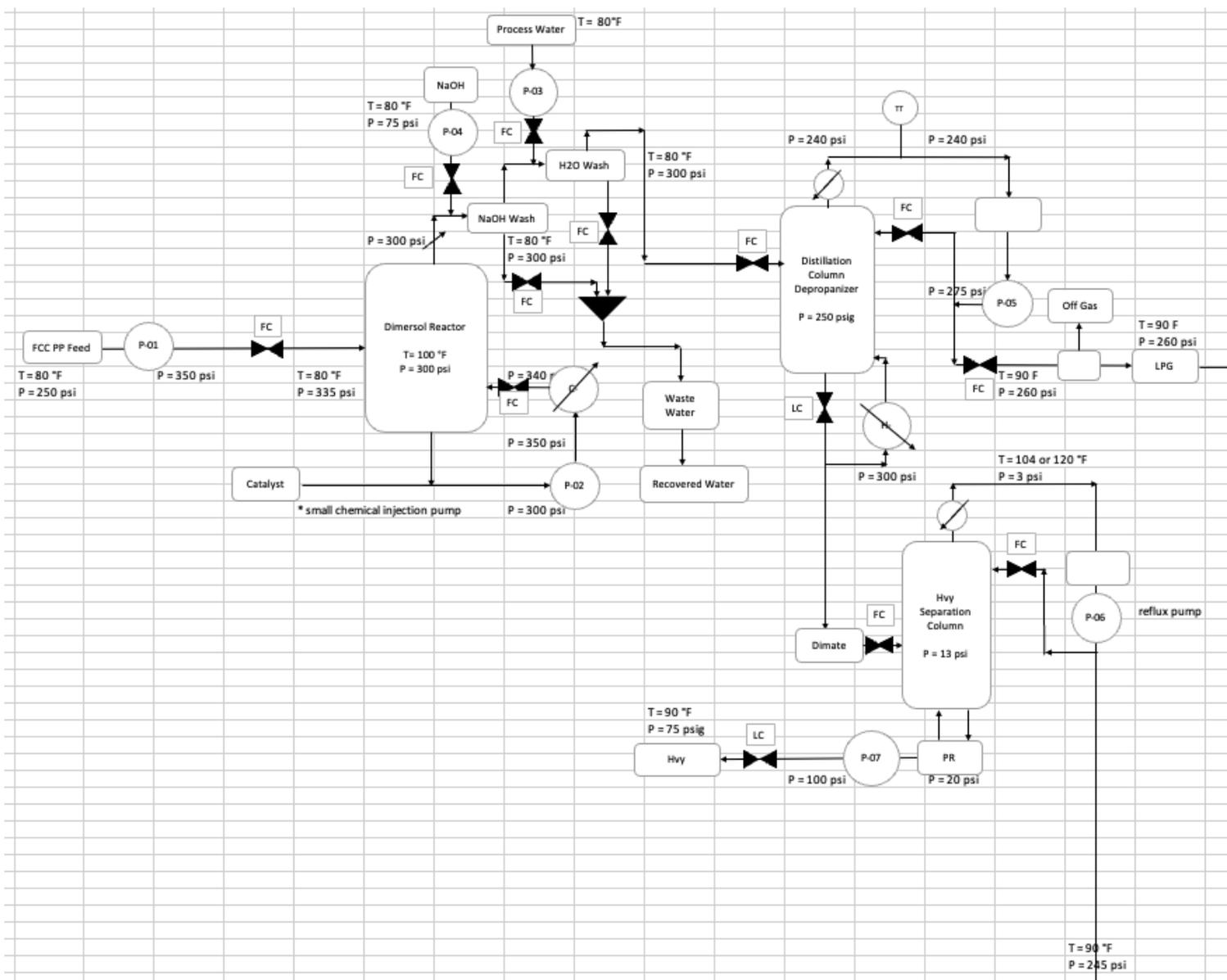


Figure 1.3.3: Dimersol section of PFD.

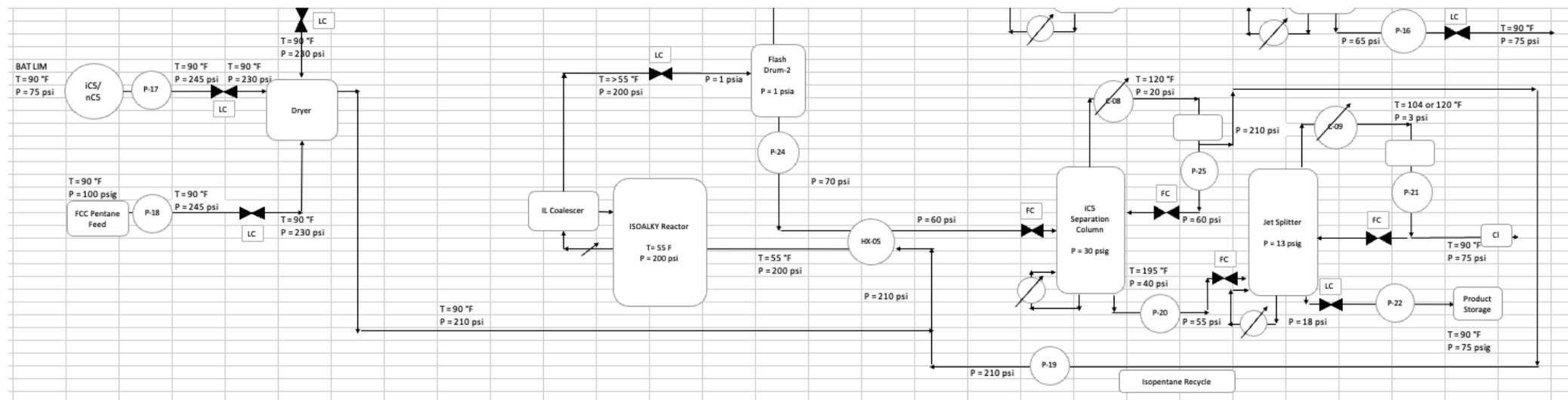


Figure 1.3.5: ISOALKY Heavy Train section of PFD.

1.4 - Project Management

The design team was composed of five members: Blaine Biedger, Bree Edwards, Bergen Evans, Lydia Flackett, and Joe Sullivan. Joe Sullivan was chosen to be the project manager. This allowed us to better facilitate collaboration among team members. To begin the project, a Gantt chart was created detailing the project requirements and when each item was to be completed and can be found below in **Figure 1.4.1**. During this process, tasks were evenly distributed among all members of the team. At the start of the project Bree, Blaine and Lydia worked on the material and energy balances while Bergen worked on the PFD and Joe built the block flow diagram. Once these tasks were completed work started on the simulation. Simulation took a bulk of the time and was done by Joe, Bergen and Bree. Design started while the simulation was being wrapped up, generating the necessary documentation for quick analysis upon the finalization of the simulation. Specifically, pumps and compressors were designed by Lydia, heat exchangers by Bergen and Blaine, distillation columns, filters and dryers by Bree, chlorine absorbers by Bree and Blaine, and reactors by Joe and Blaine. Heat integration began once the simulation was finalized and was completed by Bergen. In the final stages of the project the economic analysis was compiled by Blaine and Bree. This report was assembled by the entire team. Along the way the team had weekly meetings with the liaisons at Chevron as well as bi-weekly meetings with the course professor, Dr. Young. These meetings were instrumental to keeping the project on track as this allowed for input on any barriers hindering progress. Additionally, the team met at least once a week to set weekly action items and discuss the project progress.

Team Members :
 Lydia Flackett, Bree Edwards,
 Bergen Evans, Blaine Biediger, & Joe Sullivan



Chevron JET Fuel



CT MANAGER: Joe Sullivan START DATE: 01/26/24 END DATE: 05/04/24 LAST UPDATE: 03/01/24

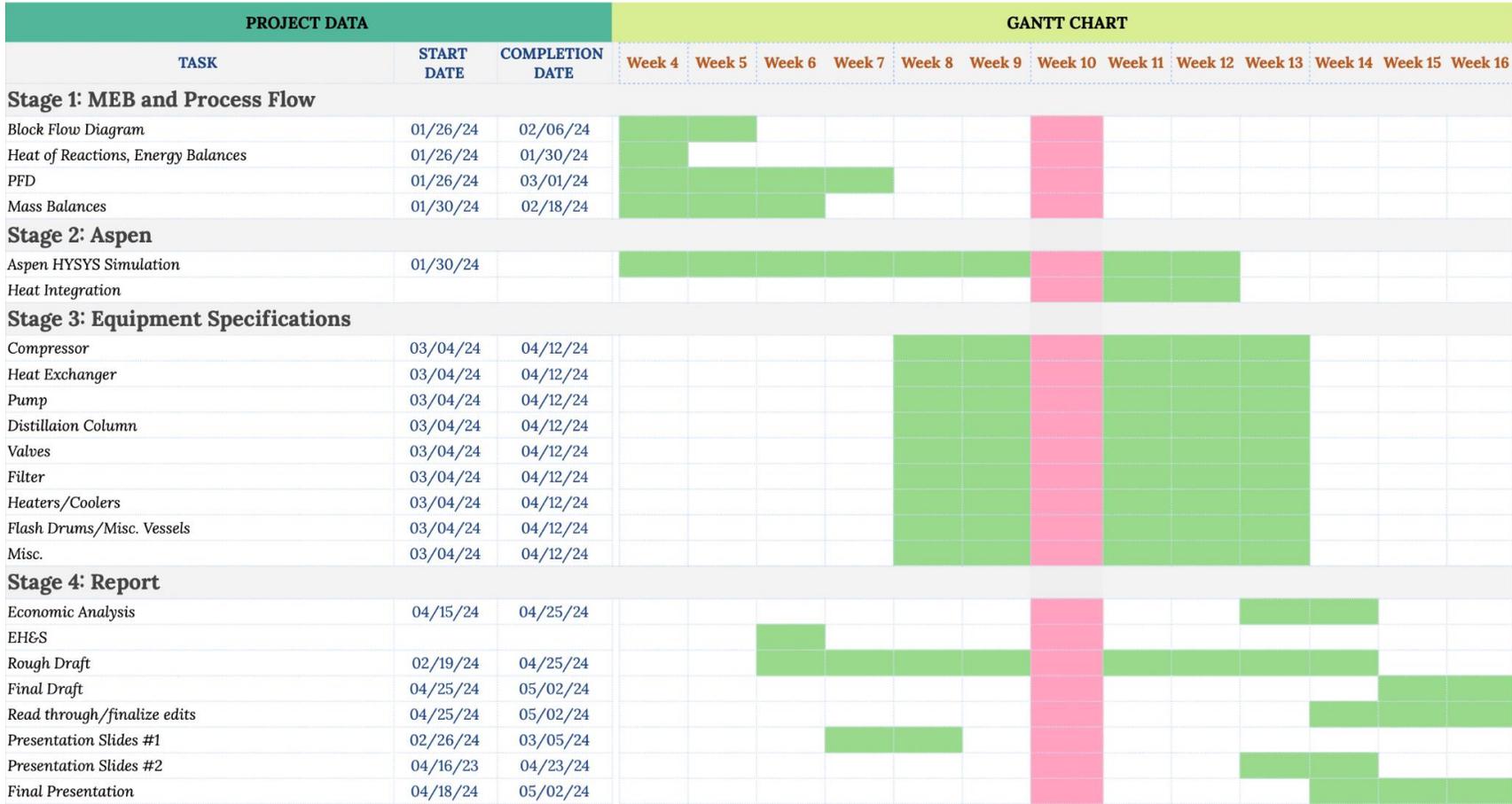


Figure 1.4.1: Gantt chart for the project.

2 - Environmental, Health & Safety Considerations

2.1 - State and Federal Regulations/Permits

This plant conversion will take place at one of Chevron's West Coast refineries. Refineries must consider regulations in air quality, hazardous waste treatment and disposal, and environmental health and safety.

The Clean Air Act is a federal law that indicates the procedures that must be followed to control emissions. In California, the local air districts can grant permits to corporations that are within the allowed limits. California has three levels of control that apply to air quality: Federal BACT, Federal lowest achievable emissions rate (LAER), and the CA BACT. The Federal BACT are required standards for areas that already meet the national ambient air quality standards. LAER are stricter standards due to being located in an area that does not already meet the national ambient air quality standards. California also allows for air districts to require stricter standards than the federal government (*Stationary Source Permitting*). The plant must have received one of these permits to be operational.

Hazardous waste treatment and disposal is an important consideration for all industries. The department of toxic substance control (DTSC) states that waste is hazardous if, "it is a listed waste, characteristics waste, used oil and mixed wastes" (*Managing Hazardous Waste*). The type of hazardous waste will dictate what permit type will be required. More on waste stream considerations is discussed in more detail in **Section 2.2**.

The plant must be up to code with the required personnel safety equipment. This includes personal protective equipment (PPE), fire extinguishers, first aid, emergency exit plans, electrical safety, ventilations, safety ladders, and more. As well as personal safety equipment, the plant must also have records for cleanliness, equipment verification, and personnel qualifications (California, *Cal/OSHA - Laws and Regulations*).

2.2 - Waste Stream Considerations

All the components within this process (excluding water) are considered hazardous waste and need to be disposed of properly. The DTSC provides general requirements for generators of used oil in California. These requirements are slightly stricter than federal regulations. Used oil is allowed to be recycled back into the process if the generator can prove that it meets the specification for recycled oil. Most large generators of oil hazardous waste have containers (portable tanks) that can be transported to disposal centers (*Used Oil Generator Requirements 2021*). The DTSC requires that producers of used oil give in depth stream compositions that are entering and leaving the process to ensure that nothing is left out (*DTSC Hazardous Waste Generator Requirements 2022*). This steam classification is also needed to ensure that the plant is in accordance with the California Water Code. The water code states that each generator of waste must indicate any waste that could affect the quality of water within the state. Lastly, as all of the hazardous waste is flammable, the waste contents need to be stored in designated drums to prevent ignition.

This process has a water wash, thus wastewater must be considered. There are many programs within California to handle wastewater treatment. The National Pollutant Discharge Elimination System Wastewater is a federal program that issues permits to regulate the discharge of municipal wastewater. The Waste Discharge Requirements regulates all discharges of waste to land (California State Water Resources Control Board, 2019).

2.3 - Primary Safety, Environmental, and Health Concerns

The largest safety concern would be personnel safety. This is discussed in more depth in **Section 2.7**. Environmental concerns are also vital to consider as working with oil and gas can have a large environmental impact should anything go wrong. This is discussed more in **Section 2.1** and **Section 2.2**. If the permits are attained and safety standards are followed then the environmental impact will be limited.

2.4 - MSDS Summary Table for All Components

Shown below in **Table 2.4.1** is the summarized MSDS data for each of the chemicals within this process as well as their flash point, flammability, health, reactivity, and other special considerations.

Table 2.4.1: MSDS Summary Table.

Chemical	Flash Point (°C)	Flammability	Health	Reactivity	Special Considerations
Ethane (C2)	-104	4	1	0	Always transport in closed containers due to flammability concerns
Propane (C3)	-104	4	2	0	Always transport in closed containers due to flammability concerns
Propylene (C3=)	-107.78	4	1	0	Always transport in closed containers due to flammability concerns
Butane (C4)	-60	4	1	0	Always transport in closed containers due to flammability concerns
Butene (C4=)	-80	4	1	0	Always transport in closed containers due to flammability concerns
Isobutane (iC4)	-83.15	4	1	0	Always transport in closed containers due to flammability concerns
Pentane (C5)	-40	4	0	0	Always transport in closed containers due to flammability concerns
Pentene (C5=)	-18	4	1	1	Always transport in closed containers due to flammability concerns
Isopentane (iC5)	-51	4	1	0	Always transport in closed containers due to flammability concerns
Cyclopentane (CC5)	-25	1	3	0	Always transport in closed containers due to flammability concerns
Hexane (C6)	-26	3	2	0	Always transport in closed containers due to flammability concerns
Isohexane (iC6)	-33	3	3	0	Always transport in closed containers due to flammability concerns
Heptane (C7)	-4	3	3	0	Always transport in closed containers due to flammability concerns
Octane (C8)	13	3	3	0	Always transport in closed containers due to flammability concerns
Nonene (C9)	24	3	2	0	Always transport in closed containers due to flammability concerns
Decane (C10)	46	2	3	0	Take precautionary measures against static discharges
Undecane (C11)	60	2	3	0	Take precautionary measures against static discharges
Dodecane (C12)	71	2	1	0	Take precautionary measures against static discharges
Water (H2O)	N/A	0	0	0	N/A
Caustic (NaOH)	N/A	0	3	1	Wash after handling due to health concerns

Information found from online SDS's which can be found in the reference section and links to PDF copies are in **Appendix B.

2.5 - Plant Safety Equipment

There are many types of hazards that could occur within the plant. If process machinery were to fail it is essential to have equipment that could lessen the impact. This could include insulation, pressure release valves, temperature controllers, fire extinguishers, and spill kits. Insulation is used to ensure that the equipment is the proper temperature for operation. Pressure release valves need to be implemented into

control systems that could become overpressurized. Temperature controllers can be used to keep the system at the proper working temperature (other controllers can and should be implemented). Fire extinguishers should be nearby in case of fire. Much like fire extinguishers, spill kits need to be available to clean up any spills that could occur. Lastly, it is vital that employees wear PPE to protect themselves. PPE is discussed in more detail in **Section 2.7**.

2.6 - Safe Plant Operating Procedures

There are five main types of safe operating procedures (SOP) that must be considered for this process: safety equipment, emergency evacuation drills, safety training, standard operating procedures of machinery, and risk assessment.

Safety equipment is imperative when working in a potentially harmful environment. The specific safety precautions can be found in **Section 2.7**. The SOP for equipment safety would also include how to keep plant equipment in proper working order.

Evacuation procedures are vital for personnel safety. Should something happen, all workers need to be trained on the proper evacuation procedures. Drills should be conducted so that everyone is prepared to respond calmly in the event of an emergency. These drills should also include where to find safety equipment and how to shut down machinery.

Safety training is needed so that all employees are aware of all the safety procedures even if it is not specific to their particular job. This safety training needs to be conducted using EHS standards.

Personnel should be trained on the proper operating procedures of the machinery. This should include how to keep the machinery in good working order. Employees should be able to determine if parts are defective and immediately report those defects to a supervisor. Along with operating procedures, the shut down procedure needs to be learned as machinery will need to be turned off for maintenance or in case of an emergency.

All personnel need to be aware of the possible problems that could arise with machinery. Along with being aware of the issues they need to be trained in how to avoid dangerous situations. Employees must not take any unnecessary risks and follow all safety procedures already in place.

2.7 - Employee Safety Precautions and Personal Protection Equipment

PPE is the very first line of defense against a hazard. Employees can wear helmets, gloves, safety glasses, respiratory protection, and closed toed shoes can all be worn to eliminate dangers to oneself. Employees should be trained on the OSHA PPE standards. This would ensure that all employees know how to properly use their PPE and be able to recognize if something is defective. Hard hats should always be worn when there is a chance of danger of a head injury from an impact. Gloves are required when hands can be exposed to punctures, chemical burns, thermal burns, and absorption of harmful substances. Safety glasses should be used when exposure to flying particles, liquid chemicals, chemical gasses, or acids or caustic liquids. Respiratory protection is recommended when there is a potential for breathing contaminated or oxygen deficient air. Proper shoes should be worn to prevent foot injury (*Personal Protection Equipment*). Along with PPE, proper eyewash and showers should be available in case of an accident. Lastly, there needs to be proper disposal areas.

2.8 - Worst Case Scenario

The worst case scenario would be if an explosion or fire were to occur. Most of the components within this process are highly flammable thus a fire is more likely to spread. Due to this, an explosion could not only impact the plant itself, but also surrounding areas. Plant personnel could be severely harmed during a scenario like this as well. If proper safety procedures are followed then an accident is unlikely.

2.9 - Failure Mode and Effects Analysis

In **Table 2.9.1** below, the fail mode and effects analysis (FMEA) can be found. FMEA is a potential hazard analysis, specifically the one below is done on a distillation column. The FMEA provides insight into precautions that can be taken to prevent plant hazards. **Figure 2.9.1** depicts the occurrence probability scale used to construct the FMEA analysis.

Rating	Occurrence	
	Probability of Failure	Criteria
10	Very High: New technology/new design with no history	≥ 100 per thousand pieces ≥ 1 in 10
9	High: Failure is inevitable with new design, new application, or change in duty cycle/operating conditions	50 per thousand pieces 1 in 20
8	High: Failure is likely with new design, new application, or change in duty cycle/operating conditions	20 per thousand pieces 1 in 50
7	High: Failure is uncertain with new design, new application, or change in duty cycle/operating conditions	10 per thousand pieces 1 in 100
6	Moderate: Frequent failures associated with similar designs or in design simulation and testing.	2 per thousand pieces 1 in 500
5	Moderate: Occasional failures associated with similar designs or in design simulation and testing.	.5 per thousand pieces 1 in 2,000
4	Moderate: Isolated failures associated with similar design or in design simulation and testing.	.1 per thousand pieces 1 in 10,000
3	Low: Only isolated failures associated with almost identical design or in design simulation and testing.	.01 per thousand pieces 1 in 100,000
2	Low: No observed failures associated with almost identical design or in design simulation and testing.	$\leq .001$ per thousand pieces 1 in 1,000,000
1	Very Low: Failure is eliminated through preventative control	Failure is eliminated through preventative control

Figure 2.9.1: FMEA occurrence rating (Christiansen, 2023)

Table 2.9.1: FMEA Study of a Distillation Column

													Action Results				
Function	Potential Failure Mode	Potential Effects of Failure	S	Potential Effects of Failure	O	Current Process Controls	D	R P N	C R I T	Recommended Action	Responsibility and Target Completion Date	Action Taken	S	O	D	R P N	C R I T
Distillation Column	Overflow	Equipment Damage	6	Spillage, stream mixing, lack of separation	2	Establish needed flow	1	12	N	Have spill kits Equipment maintenance Flowmeters added	Facilities ; routinely	Flowmeters added	6	2	1	12	N
Distillation Column	Flow excessively slows	Less separation	3	Decrease in column efficiency	1	Establish needed flow	2	6	N	Equipment maintenance Flowmeters added	Facilities ; routinely	Flowmeters added	3	1	2	6	N
Distillation Column	Over pressurized	Equipment Damage	6	Spillage, stream mixing	1	Calculations on proper pressure	1	6	N	Equipment maintenance Pressure indicators	Facilities ; routinely	Pressure indicators added	6	1	1	6	N
Distillation Column	Uncontrolled Temperature Increase	Equipment Damage	7	Spillage, explosion	1	Calculations on proper temperature	1	7	N	Equipment maintenance Temperature indicators	Facilities ; routinely	Temperature indicators added	7	1	1	7	N
Distillation Column	Incorrect material introduced	Equipment Damage	6	Explosion, lack of separation	1	Proper stream controls established	1	6	N	Equipment maintenance	Facilities ; routinely	Flow monitoring added	6	1	1	6	N

** S = severity of event, O = probability of occurrence, D = probability of detection, RPN = S, O, D multiplied together for assessment of risk

** Rankings were made based on the occurrence of rating found in **Figure 2.9**

3 - Impacts and Ethics of the Project

As with any chemical plant design project it is paramount to consider the ethics of the process and potential consequences that could arise. Concerning internal welfare within the Chevron workforce, the health and safety of the operators should be the foremost ethical concern of the plant. **Section 2** of this report outlines the suggested precautions that should be taken while operating the plant and handling materials, safety equipment to keep on site, and actions to take in the event of a live hazard or worst case scenario.

Concerning the macroscopic impacts of this project; which encompasses market and environmental impacts. Jet fuel demand is expected to remain constant into the future, thus the drive for this plant's resources to be redirected from gasoline to jet fuel. If this demand continues to rise in future as it is projected to, producing a large amount of it may have an impact on the market value of jet fuel. Whether this impact is substantial to the stock portfolio of Chevron or the larger fuel market could vary based on how economically feasible the process is deemed to be. Another major consideration is the contribution of using jet fuel to power aircraft. This coupled with the concern of potential release of off gas from the Dimersol and ISOALKY Light processes fully encircle the span of the environmental impacts of this project. Regarding this matter, there are several considerations regarding the ultimate destination of the off gas, such as whether it will be released to the atmosphere or not. If the gas is released to the atmosphere it may cause additional environmental impacts.

4 - Design and Economic Premises

Assumptions:

Material Balances:

- Dimersol reactor : Heavier carbons are C10 + C11 + C12 and the molecular weight is averaged
- Water wash : 95% of wash goes straight through to waste water
- Depropanizer column : 99% of water leaves in the tops
- Heavy separation column : 99% of water leaves in the tops
- iC4 reactions only in the iC4 train and iC5 reactions only in the iC5 train

Energy Balances:

*These assumptions were provided by Chevron

- The heat of formation and heat of reaction values are for standard conditions (25C and 1 bar)
- Values were not extrapolated for other temperatures and pressures

Process Flow Diagram:

- 15 psi pressure drop across level and flow control valves
- 7 psi pressure drop across temperature control valves
- 10 psi pressure drop across coolers, heaters, and heat exchangers
- Temperature transmitter pressure drop negligible
- 20 psi pressure drop across the dryers
- Dimersol reactor conditions specified in Dimersol paper

Simulation:

- iC9= Simulated As 1-Nonene
- iC10= Simulated As 1-Dodecene
- iC11= Simulated As 1-Undecene
- Simulated As 4-Methyl-1-Pentene
- 2M,5E-Pentane Simulated As 2M,3E-Pentane
- DMHeptane Simulated As 2,3M-Heptane
- TMHeptane Simulated As 3,3,5M-Heptane
- DMOctane Simulated As 2,7M-Octane
- iC11 Simulated As nC11
- iC12 Simulated As nC12
- All reactors are black box reactors
- Dimersol:
 - Catalyst will not be modeled
 - Dimersol reactor is simplified from normal bypass cooling loop configuration
 - NaOH wash is simplified from regenerative recycle loop
 - Water wash is simplified from regenerative recycle loop
 - 100% of the water is removed in the wash step as opposed to a practical percentage
- ISOALKY Light Train:
 - Reactor is simplified to exclude complex refrigeration and catalyst recycle
 - 100% of the iC4 in the products stream is recovered in the recycle
- ISOALKY Heavy Train:
 - Reactor is simplified to exclude complex refrigeration and catalyst recycle
 - 100% of the iC5 in the products stream is recovered in the recycle

Pumps:

- All elevation gains are 50 ft
- All lengths of pipes are 500 ft
- The density of the fluid is an average of in/out from ASPEN
- The use of heuristic 38 to determine total pressure change

Heat Exchangers:

- Properties of chilled brine were estimated as that of cooling water

Economics:

- 6 year operational cycle starting in 2027
- 4% annual inflation rate
- 10% capital cost
- 30 day accounts receivable
- 15% hurdle rate
- Materials and products were priced at the following rates:
 - Sales Propane: \$89.54/bbl
 - Sales Butane: \$88.81/bbl

- Sales Motor Alkylate: \$126.50/bbl
- Sales Jet: \$149.29/bbl
- FCC PP Stream: \$91.84/bbl
- FCC C4= Stream: \$102.16/bbl
- FCC C5= Stream: \$111.06/bbl
- iC4 Stream: \$89.11/bbl
- iC5 Stream: \$112.25/bbl
- HP Steam: \$30.03/klb
- LP Steam: \$27.38/klb
- Electricity: \$0.42/kWh
- Cooling Water: \$10/year per GPM
- ISOALKY Ionic Liquid: \$1,000,000 initial cost, \$10,000 yearly cost.
- Dimersol Catalyst: \$1.62/bbl
 - This was adjusted for inflation from \$0.4/bbl listed in 1977.
- 24% income tax rate
- 5 operators with a yearly wage of \$112k, including benefits
- Maintenance costs are 5% of investment
- Plant operates at 100% capacity from beginning of operational cycle

5 - Material and Energy Balances

5.1 - Material Balances

The amount of material fed into the process was provided by Chevron and can be found in **Table 5.1.1** below. The iC4 and iC5 spheres are able to be drawn from in order to satisfy mass balance requirements after the recycle in the light ISOALKY reaction train. The Excel spreadsheet of all the mass balances can be found in **Appendix C**. The Dimersol values were found in *The IFP Dimersol Process for Dimerization of Propylene into Isohexenes*. This provided ratios and flow rates entering into the Dimersol process, these values can be found in **Table 5.1.2** and **Table 5.1.3**. Due to the fact that the reactor information is largely proprietary, the reactor mass balances were based on reaction yields provided by Chevron in the Excel spreadsheet Alkylate to Jet_Conceptual Yield for CU, this Excel can be found in **Appendix C**. Using these yields, the mass balances were calculated to emulate ideal reactor conditions, assuming 100% selectivity, which is not necessarily realistic.

Table 5.1.1: Feed Component Values

Component	FCC PP	FCC mC5	FCC mC4	iC4 Makeup from Sphere	iC5 Makeup from Sphere
C2	0.5				
C3=	75				
C3	23.5		2.5	1	
iC4	1	4.9	34.3	96	
nC4		3.5	7	3	
C4=		16.3	46.9		
iC5		37.5	7.8		65
nC5		4.3	1.5		35
C5=		33			
Cyclopentane		0.5			
iC6		0			
Total	100	100	100		100
Flow rate (bpd)	7000	6000	13000	Unlimited	Up to 3000

Table 5.1.2: Dimersol component Values

Feed			
	Vol %	BPSD	Lbs/HR
Propylene	71	2,700	20,550
Propane	29	1,103	8,170
Products			
	Vol %	BPSD	Lbs/Hr
Propylene	4.2	135	1,030
Propane	34.6	1,103	8,170
Dimate	61.2	1,952	19,520

Table 5.1.3: Properties of Dimate

	Wt. %
Isohexenes	92
Nonenes	6.5
Heavier	1.5

** Heavier was split into an average of C10, C11, and C12

5.2 - Energy Balances

There were no energy balances performed for this process. The Dimersol and ISOALKY reactors are black box reactors, thus Chevron provided us with the necessary heat of reactions to complete the Aspen HYSYS simulation. However, had the values been calculated the methodology would have been to use the following equation to determine the change in enthalpy per component:

$$\Delta H = \Delta H_f + \int_{T_{ref}}^T C_p dT$$

This equation uses a reference temperature and the final temperature of the reactor, specific heat of the component, and the heat of formation for the component. Once the enthalpies are calculated, then the heat of reaction can be computed using the following equation:

$$H_{rxn} = (H_{out}) - (H_{in})$$

Table 5.2.1 and **Table 5.2.2** indicate the heat of formations for each component, the needed chemical equations that occur, and the heat of reaction.

Table 5.2.1 : Heat of formations for all components

Component	Heat of formations (kJ/mol)
iC4	-134.5
iC5	-153.3
C3=	20.4
C4=	-11.3
C5=	-58.2
C6=	-73
iC7	-229
iC8	-250
iC9	-275
iC10	-301
iC11	-327

Table 5.2.2 : Chemical equations with heats of formations

Reaction	Heat of Formation (kJ/mol)
iC4 + C2= → iC6	-122
iC4 + C3= → iC7	-115
iC4 + C4= → iC8	-104
iC4 + C5= → iC9	-82
iC4 + C6= → iC10	-94
iC5 + C2= → iC7	-128
iC5 + C3= → iC8	-117
iC5 + C4= → iC9	-110
iC5 + C5= → iC10	-89.5
iC5 + C6= → iC11	-101

6 - Process Simulation

Aspen HYSYS was selected as the simulation software for this analysis. Aspen Plus and HYSYS are both good process simulation platforms but in industry Plus is more common for chemicals and pharmaceuticals whereas HYSYS is more prevalent in the petroleum industry (Abdullah, 2023). The first step in any simulation is defining the components and property packages. There were some issues with finding the components that Chevron had desired and some assumptions had to be made, this can be found in **Section 4**. **Table 6.1** shows the component list used in the HYSYS simulation. When looking for the appropriate property package for this simulation, SRK and Grayson-Streid were the top two choices. For completeness, time was spent researching possible property packages using the Aspen Help Guide.

SRK, Soave-Redlich-Kwong model, was ultimately chosen because Grayson-Streid was not compatible with NaOH in the simulation. SRK offers similar results to a Peng-Robinson model which was the next choice, all of which are good for modeling hydrocarbon or petroleum processes. Two distinct advantages that SRK has are analysis of heavy components and analysis of components at vacuum conditions. Nonane and heavier are present in the simulation so this was a necessary package. Although there are no vacuum conditions the flash drum does operate at a low pressure of 1 psig which is near enough to utilize this functionality. Additionally, SRK is enhanced for the computation of hydrocarbon-hydrocarbon pairs (Aspen HYSYS V14 Help). After the proper components and property packages were confirmed, the process could be built using the PFD as a reference point. This was especially useful as it had all the desired equipment and pressures of each stream.

On the first iteration of the simulation, the plan was to put the entire process into one simulation flowsheet. This turned out to be too big for HYSYS to handle, therefore the process was split into three simulations; the Dimersol process, the light ISOALKY process and the heavy ISOALKY process. **Figures 6.1.1, 6.2.1 and 6.3.1** respectively detail these process flowsheets in HYSYS. Each of these processes features a black box reactor as Chevron provided the parameters of the reactors in the form of mass balances

and conversions. Details of the Dimersol process were supplied by the paper discussed in the material balances section. The main purpose of the simulation was to design the separation trains and verify the mass balances.

The final HYSYS simulation achieves a 0% tolerance for both overall and reactor mass balances for the Dimersol process. For the light ISOALKY process, a tolerance of 0.014 % for the overall mass balances and 0.004% for the reactor was achieved. Finally, the heavy ISOALKY train achieves an overall tolerance of 0.162% and a reactor tolerance of 0.033%. A summary of the full results of the simulation can be found in **Tables 6.2 and 6.3** along with typical refinery information such as API, specific gravity, molecular weight, RVP and flash point.

Table 6.1: HYSYS Component List

Common Name	IUPAC	HYSYS	Carbon Number
Ethane	Ethane	Ethane	C2
Propane	Propane	Propane	C3
Propene	1-Propene	Propene	C3
Isobutane	Isobutane	i-Butane	C4
n-Butane	Butane	n-Butane	C4
Butene	1-Butene	1-Butene	C4
Isopentane	Isopentane	i-Pentane	C5
n-Pentane	Pentane	n-Pentane	C5
Cyclopentane	Cyclopentane	Cyclopentane	C5
Pentene	(2E)-2-Pentene	cis2-Pentene	C5
Dimethyl-Butane	2,3-Dimethylbutane	23-Mbutane	C6
Methyl-Pentane	2-Methylpentane	2-Mpentane	C6
Methyl-Pentane	3-Methylpentane	3-Mpentane	C6
Isohexene	4-Methyl-1-pentene	4M-1-pentene	C6
Dimethyl-Pentane	2,3-Dimethylpentane	23-Mpentane	C7
Dimethyl-Pentane	2,4-Dimethylpentane	24-Mpentane	C7
Trimethyl-Pentane	2,2,4-Trimethylpentane	224-Mpentane	C8
Dimethyl-Hexane	2,4-Dimethylhexane	24-Mhexane	C8
Dimethyl-Hexane	2,5-Dimethylhexane	25-Mhexane	C8
Ethyl-Methyl-Pentane	3-Ethyl-2-methylpentane	2M-3Epentane	C8
Trimethyl-Hexane	2,2,5-Trimethylhexane	225-Mhexane	C9
Trimethyl-Hexane	2,3,5-Trimethylhexane	235-Mhexane	C9
Dimethyl-Heptane	2,3-Dimethylheptane	23-Mheptane	C9
Nonene	1-Nonene	1-Nonene	C9
Trimethyl-Heptane	3,3,5-Trimethylheptane	335-Mheptane	C10
Dimethyl-Octane	2,7-Dimethyloctane	27-Moctane	C10
Decene	1-Decene	1-Decene	C10
n-Undecane	Undecane	n-C11	C11
Undecene	1-Undecene	1-Undecene	C11
n-Dodecane	Dodecane	n-C12	C12
Dodecene	1-Dodecene	1-Dodecene	C12
NaOH	Sodium Hydroxide	NaOH	N/A

Water	Water	H ₂ O	N/A
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Table 6.2: Refinery Table Detailing Various Properties for Major Streams in Aspen HYSYS.

Stream	In/Out	Temperature (F)	Pressure (psig)	Molar Flow (lbmol/hr)	Mass Flow (lb/hr)	Volumetric Flow (GPM)	Volumetric Flow (BPD)	Enthalpic Flow (Btu/hr)	API	Specific Gravity (60/60)	Molecular Weight	RVP (psig)	Flash Point (F)
FCC Prop Feed	Feed	80.00	250	1246.32	53088.3	205.00	7028.50	-1.31E+07	141.8	0.518	42.6	153.60	--
LPG Off Gas	Product	121.85	240	48.21	2120.7	8.31	284.82	-1.76E+06	145.8	0.510	44.0	243.80	--
Dimersol LPG Overhead	Product	122.16	250	284.86	12600.1	49.29	1689.98	-1.23E+07	145.4	0.511	44.2	240.90	--
Dimate	Product	140.26	228	417.64	35132.2	104.95	3598.36	-1.32E+07	80.0	0.669	84.2	3.38	--
Dimersol Heavy Sep Bottoms	Product	369.18	85	23.37	3051.7	8.28	283.95	-1.04E+06	60.6	0.737	130.6	20.24	93.02
iC4 Sphere	Feed	80	150	323.39	18743.4	66.60	2283.43	-2.14E+07	120.0	0.563	58.0	39.43	--
FCC Mixed C4= Feed	Feed	80	150	1912.87	110663.7	379.21	13001.48	-7.34E+07	111.0	0.583	57.9	32.99	--
iC5 Sphere	Feed	90	75	759.83	54823.1	175.00	6000.00	-5.78E+07	94.4	0.626	72.2	0.28	--
FCC Mixed C5= Feed	Feed	90	100	816.98	54949.3	175.02	6000.68	-3.69E+07	94.0	0.628	67.3	10.12	--
Sales Propane	Product	115.71	265	339.26	14884.3	58.96	2021.47	-1.70E+07	148.9	0.505	43.9	227.40	--
Sales Butane	Product	109.04	100	146.73	8528.4	29.23	1002.17	-9.18E+06	111.1	0.583	58.1	45.50	--
Mogas from C4 Train	Product	293.32	95	1149.36	120956.8	350.69	12023.78	-1.04E+08	73.7	0.690	105.2	65.31	--
Mogas from Jet Splitter	Product	120.22	60	478.10	40995.9	124.49	4268.22	-4.11E+07	83.44	0.658	85.8	3.11	--
Jet A	Product	402.50	75	690.11	103673.9	279.33	9576.89	-7.43E+07	59.2	0.742	150.2	18.19	103.90

Table 6.3: Properties for Each Stream Coming In and Out of the Dimersol Reactor

Stream	In/Out	Temperature (F)	Pressure (psig)	Molar Flow (lbmol/hr)	Mass Flow (lb/hr)	Volumetric Flow (GPM)	Volumetric Flow (BPD)	Enthalpic Flow (Btu/hr)	API	Specific Gravity (60/60)	Molecular Weight	RVP (psig)	Flash Point (F)
Dimersol Reactants	In	80.91	300	1246.32	53088.3	205.00	7028.50	-1.31E+07	141.8	0.518	42.6	158.70	--
Dimersol Products	Out	100.00	300	774.08	52904.8	170.83	5857.11	-3.01E+07	97.1	0.619	68.3	66.25	--
ISOALKY iC4 Reactants	In	71.79	230	9024.16	516146.1	1829.53	62726.74	-5.37E+08	119.1	0.564	57.2	35.93	--
ISOALKY iC4 Products	Out	55.00	200	8083.40	516165.8	1763.84	60474.45	-5.78E+08	110.4	0.585	63.9	19.66	--
ISOALKY iC5 Reactants	In	75.75	185	8324.09	599989.4	1914.38	65636.02	-5.99E+08	94.3	0.627	72.1	-1.87	--
ISOALKY iC5 Products	Out	55.00	200	7498.51	599792.8	1863.36	63886.74	-6.33E+08	88.4	0.644	80.0	-7.43	--

6.1 - Dimersol

The Dimersol process, **Figure 6.1.1**, is a proprietary process that has never been coupled with an alkylation process to produce jet fuel. This process takes a FCC mix of propylene with a small amount of catalyst to produce isohexene and heavy dimate. This isohexene olefin is the main desired product as it provides a high carbon number base for the alkylation process downstream. Downstream separation columns with reflux ratios of between 1.5 and 2.5, split the products into a C4- stream, a pure isohexene stream and a heavy olefin stream.

Some simplifying assumptions were made, **Section 4**, in the process of building the Dimersol simulation. These assumptions were needed to get the columns to converge. Under normal operating conditions, the Dimersol reactor operates with a side draw, which is pumped through a cooler to maintain the desired ambient temperature of the reaction. This side draw/recycle proved problematic and could not be properly implemented in HYSYS. The available units for reactors are far too complex to implement in this simulation in addition to the basic applications that the units were meant for. None of the reactor units available in HYSYS can accommodate a side draw loop. Due to this, the thermodynamics of the reaction were modeled simply as a heater and cooler. As for the black box reactor the reactant stream was subject to the heating and cooling of the reaction as the Dimersol cooling loop is assumed to be 99% reactants. After these heating operations, the stream was terminated and a new stream started as the products. The composition of the product stream was then derived from the mass balance table created beforehand and stream properties from the PFD.

Downstream from the reactor, the product goes through two separate wash steps; a caustic (NaOH) wash and a water wash. Both wash steps are meant to be run with recycles that purify and regenerate the wash component. Adding these two wash cycles accurately to the simulation made convergence more difficult. Due to this, these wash systems were simplified to unit mixers adding the washing agent and then removing 100% of the agent from the process stream using component separators. Originally water was being removed at 95% but this led to issues downstream in one of the columns. In addition, this column still struggled with converging when the water was removed. To simplify more, ethane was removed from the process stream, allowing the column to converge. The ethane was then handled outboard for the rest of the analysis. The three products of this process were the liquid propane gas to be fed to the light ISOALKY train, the pure isohexene (dimate) to be fed to the heavy ISOALKY train and the heavy olefin byproduct to be sent to a jet hydrotreater elsewhere in the plant.

The main obstacles that needed to be overcome were the convergence of the column, building in the recycles and the reactor side draw recycle. Most of these were overcome by simplifying the system but the column required some extra attention after the previously mentioned simplifications were made. Although the column producing the LPG converged, the convergence was suboptimal. Up until now, Aspen simulations involving columns were run as total condensers and total reboilers leaving no off-gas stream from the overhead. In this simulation, the partial condenser was required to purge the system of any vapor produced at the desirable operating conditions. For columns with more than two product streams, HYSYS requires three specs to set convergence, in other words, three degrees of freedom. With three parameters to modify, optimizing this column proved a little tricky and took more time than expected. Results from this simulation can be seen in **Tables 6.1.1 and 6.1.2** including flow rates and compositions.

Table 6.1.1: Composition of Dimersol Reactor Inlet and Exit Streams

Dimersol							
		In			Out		
		Mass	Volume	Mole	Mass	Volume	Mole
		(lb/hr)	(GPM)	(mol/hr)	(lb/hr)	(GPM)	(mol/hr)
	Total Flow	53088.3	205.00	1246.32	52904.8	170.83	774.08
CN	Component	Mass Percent	Volume Percent	Mole Percent	Mass Percent	Volume Percent	Mole Percent
C2	Ethane	0.35%	0.50%	0.49%	0	0	0
C3	Propane	22.94%	23.41%	22.16%	23.02%	28.10%	35.67%
C3	Propene	75.63%	75.09%	76.56%	3.79%	4.51%	6.16%
C4	i-Butane	1.08%	1.00%	0.79%	1.09%	1.19%	1.28%
C4	n-Butane	0	0	0	0	0	0
C4	1-Butene	0	0	0	0	0	0
C6	23-Mbutane	0	0	0	0	0	0
C6	2-Mpentane	0	0	0	0	0	0
C6	3-Mpentane	0	0	0	0	0	0
C6	4M-1-pentene	0	0	0	66.33%	61.36%	53.87%
C9	225-Mhexane	0	0	0	0	0	0
C9	235-Mhexane	0	0	0	0	0	0
C9	23-Mheptane	0	0	0	0	0	0
C9	1-Nonene	0	0	0	4.69%	3.96%	2.54%
C10	335-Mheptane	0	0	0	0	0	0
C10	27-Moctane	0	0	0	0	0	0
C10	1-Decene	0	0	0	0.36%	0.30%	0.18%
C11	n-C11	0	0	0	0	0	0
C11	1-Undecene	0	0	0	0.36%	0.30%	0.16%
C12	n-C12	0	0	0	0	0	0
C12	1-Dodecene	0	0	0	0.36%	0.29%	0.15%
-	NaOH	0	0	0	0	0	0
-	H2O	0	0	0	0	0	0

Table 6.1.2: Heavies From Dimersol

Heavies from Dimersol				
		Mass	Volume	Mole
		(lb/hr)	(GPM)	(mol/hr)
	Total Flow	3051.7	8.28	23.37
CN	Component	Mass Percent	Volume Percent	Mole Percent
C9	225-Mhexane	0	0	0
C9	235-Mhexane	0	0	0
C9	23-Mheptane	0	0	0
C9	1-Nonene	81.25%	81.67%	84.04%
C10	335-Mheptane	0	0	0
C10	27-Moctane	0	0	0
C10	1-Decene	6.25%	6.18%	5.82%
C11	n-C11	0	0	0
C11	1-Undecene	6.25%	6.10%	5.29%
C12	n-C12	0	0	0
C12	1-Dodecene	6.25%	6.03%	4.85%
-	NaOH	0	0	0
-	H2O	0	0	0

6.2 - Light ISOALKY Train

In the light ISOALKY train, **Figure 6.2.1**, feeds of FCC mixed C4's, the Dimersol LPG, and a makeup iC4 sphere are reacted and run through a separation train, again with reflux ratios between 1.5 and 2.5, to produce sales propane, sales butane, and motor alkylate or gasoline. This mimics the existing process for producing gasoline, but uses the new ISOALKY reaction process that in turn changes the reactor product composition and the resulting product distribution. It is desired to separate as much of the propane and butane for sale as possible. One important part of the ISOALKY process is that the reaction conditions require a volumetric ratio of at least 8:1 of isobutane to total olefins and is the reason for isobutane recycling.

The main simplifying assumption that was made while creating the light ISOALKY simulation was to use a black box reactor driven by the mass balances similar to that in the Dimersol process. The ISOALKY process is proprietary to Chevron and utilizes a complex refrigeration unit in addition to recycling the ionic catalyst. Along with the black box, the heat of reaction was modeled as a simple heater. At the request of Chevron, a heat integration unit was implemented to precool the reactor inlet stream and preheat a cool process inlet stream to the first column in the separation train. The cooled process stream is an effluent of the flash drum.

An important unit that was required by Chevron to achieve a cheaper pre-separation step of the lighter products from this reactor was a flash drum. This flash drum operates at 1 psig and 18°F achieving partial separation of C5- components including a majority of the propane in the vapor stream. The stream is compressed back into a liquid and run through a column to separate the propane for sale as a side product. The heavy product from this stream is recycled back to the process stream and fed into the iC4 recycle column. Many different configurations and operating conditions for the flash drum were tested to optimize the amount of propane sequestered. During this case study it was found that the amount of C4- and C5+ always varied by the same proportion when the operating conditions were changed. The goal of implementing this unit was to separate C3's and C4's into the vapor allowing for more efficient separation of the sales propane and iC4 downstream, however analysis of the process found this was not the case. Furthermore, HYSYS had trouble running the bottoms stream from the propane separator back into the flash drum as originally planned. This was overcome by bypassing the flash drum and directly mixing the bottoms stream with the liquid outlet stream of the flash drum.

Another aspect of the simulation that proved difficult to converge was using a black box. Like the Dimersol process, this process has a stream that ends at the reactants side of the reactor and has a new stream that starts on the products side, all driven by the mass balances. With the iC4 recycle stream produced on the products side of the black box feeding to the reactants side, HYSYS could no longer iterate the process independently. It was not a huge issue but did take some time to sort out and further iteration may yield a tighter HYSYS mass balance tolerance.

One final assumption that was made for this simulation was that there were only iC4 reactions occurring. Examination of the composition of the streams, as seen in **Tables 6.2.1-6.2.4**, reveals that there would be more alkylation reactions occurring that produce more of the higher carbon number products. Assuming that only the iC4 reactions were occurring, there are 2 reaction pathways present with a total of 22 components to track. Additional reaction tracking would increase the complexity and scope of the project and was deemed unnecessary.

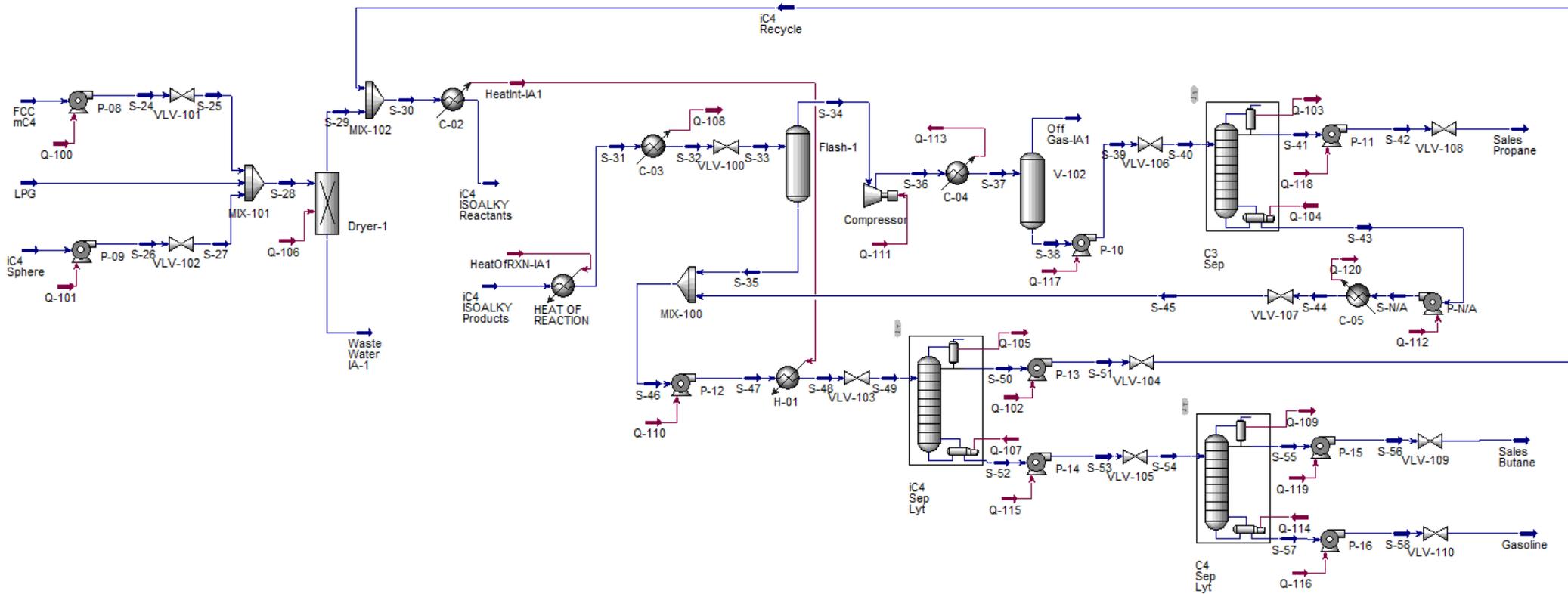


Figure 6.2.1: ISOALKY Light Process PFD from Aspen HYSYS

Table 6.2.1: Composition of ISOALKY Light Reactor Inlet and Outlet Streams

ISOALKY Light							
		In			Out		
		Mass	Volume	Mole	Mass	Volume	Mole
		(lb/hr)	(GPM)	(mol/hr)	(lb/hr)	(GPM)	(mol/hr)
	Total Flow	516146.1	1829.53	9024.16	516165.8	1763.84	8083.40
CN	Component	Mass Percent	Volume Percent	Mole Percent	Mass Percent	Volume Percent	Mole Percent
C2	Ethane	0.04%	0.06%	0.08%	0.04%	0.07%	0.09%
C3	Propane	4.67%	5.19%	6.05%	4.65%	5.36%	6.73%
C3	Propene	0.39%	0.42%	0.53%	0	0	0
C4	i-Butane	80.91%	81.12%	79.61%	70.26%	73.07%	77.19%
C4	n-Butane	1.61%	1.56%	1.59%	1.61%	1.62%	1.77%
C4	1-Butene	10.25%	9.72%	10.44%	0	0	0
C5	i-Pentane	1.79%	1.62%	1.42%	2.78%	2.60%	2.46%
C5	n-Pentane	0.35%	0.31%	0.28%	0.35%	0.32%	0.31%
C5	Cyclopentane	0	0	0	0	0	0
C5	cis2-Pentene	0	0	0	0	0	0
C6	23-Mbutane	0	0	0	0.90%	0.79%	0.67%
C6	2-Mpentane	0	0	0	0.26%	0.23%	0.19%
C6	3-Mpentane	0	0	0	0.13%	0.11%	0.10%
C6	4M-1-pentene	0	0	0	0	0	0
C7	23-Mpentane	0	0	0	1.31%	1.10%	0.83%
C7	24-Mpentane	0	0	0	0.87%	0.75%	0.56%
C8	224-Mpentane	0	0	0	9.41%	7.92%	5.26%
C8	24-Mhexane	0	0	0	1.34%	1.12%	0.75%
C8	25-Mhexane	0	0	0	1.34%	1.13%	0.75%
C8	2M-3Epentane	0	0	0	1.34%	1.09%	0.75%
C9	225-Mhexane	0	0	0	1.52%	1.24%	0.75%
C9	235-Mhexane	0	0	0	0.30%	0.24%	0.15%
C9	23-Mheptane	0	0	0	0.20%	0.16%	0.10%
C9	1-Nonene	0	0	0	0	0	0
C10	335-Mheptane	0	0	0	0.48%	0.38%	0.21%
C10	27-Moctane	0	0	0	0.16%	0.13%	0.07%
C10	1-Decene	0	0	0	0	0	0
C11	n-C11	0	0	0	0.71%	0.56%	0.29%
C11	1-Undecene	0	0	0	0	0	0
C12	n-C12	0	0	0	0.02%	0.02%	0.01%
C12	1-Dodecene	0	0	0	0	0	0
-	NaOH	0	0	0	0	0	0
-	H2O	0	0	0	0	0	0

Table 6.2.2: Composition and Properties of Sales Propane

Sales Propane				
		Mass	Volume	Mole
		(lb/hr)	(GPM)	(mol/hr)
	Total Flow	14884.3	58.96	339.26
CN	Component	Mass Percent	Volume Percent	Mole Percent
C2	Ethane	1.23%	1.75%	1.80%
C3	Propane	98.50%	98.01%	98.00%
C3	Propene	0	0	0
C4	i-Butane	0.27%	0.24%	0.20%
C4	n-Butane	0	0	0
C4	1-Butene	0	0	0

Table 6.2.3: Composition and Properties of Sales Butane

Sales Butane				
		Mass	Volume	Mole
		(lb/hr)	(GPM)	(mol/hr)
	Total Flow	8528.4	29.23	146.73
CN	Component	Mass Percent	Volume Percent	Mole Percent
C2	Ethane	0	0	0
C3	Propane	0	0	0
C3	Propene	0	0	0
C4	i-Butane	2.41%	2.50%	2.41%
C4	n-Butane	97.59%	97.50%	97.59%
C4	1-Butene	0	0	0

Table 6.2.4: Composition and Properties of Motor Alkylate from Light Train

Motor Alkylate from Light Train				
		Mass	Volume	Mole
		(lb/hr)	(GPM)	(mol/hr)
	Total Flow	120956.8	350.69	1149.36
CN	Component	Mass Percent	Volume Percent	Mole Percent
C2	Ethane	0	0	0
C3	Propane	0	0	0
C3	Propene	0	0	0
C4	i-Butane	0	0	0
C4	n-Butane	0.01%	0.01%	0.01%
C4	1-Butene	0	0	0
C5	i-Pentane	11.85%	13.10%	17.29%
C5	n-Pentane	1.48%	1.62%	2.16%
C5	Cyclopentane	0	0	0
C5	cis2-Pentene	0	0	0
C6	23-Mbutane	3.84%	3.97%	4.69%
C6	2-Mpentane	1.10%	1.15%	1.34%
C6	3-Mpentane	0.55%	0.57%	0.67%
C6	4M-1-pentene	0	0	0
C7	23-Mpentane	5.59%	5.52%	5.87%
C7	24-Mpentane	3.73%	3.80%	3.91%
C8	224-Mpentane	40.17%	39.81%	37.00%
C8	24-Mhexane	5.74%	5.62%	5.29%
C8	25-Mhexane	5.74%	5.67%	5.29%
C8	2M-3Epentane	5.74%	5.47%	5.29%
C9	225-Mhexane	6.47%	6.21%	5.31%
C9	235-Mhexane	1.29%	1.23%	1.06%
C9	23-Mheptane	0.86%	0.82%	0.71%
C9	1-Nonene	0	0	0
C10	335-Mheptane	2.04%	1.89%	1.51%
C10	27-Moctane	0.68%	0.65%	0.50%
C10	1-Decene	0	0	0
C11	n-C11	3.04%	2.82%	2.05%
C11	1-Undecene	0	0	0

C12	n-C12	0.09%	0.08%	0.05%
C12	1-Dodecene	0	0	0
-	NaOH	0	0	0
-	H2O	0	0	0

6.3 - Heavy ISOALKY Train

Similarly, the heavy train, as shown in **Figure 6.3.1**, uses feeds of FCC mixed C5's, the isohexene product from the Dimersol process and a makeup iC5 sphere to produce gasoline and jet fuel. This train encompassed a majority of the retrofit of the project. All of the equipment, except for the reactor, will need to be built from scratch. Like the light train, the heavy train features an isoalkane recycle but this time it uses isopentane in place of the isobutane used in the light train. As with the other simulations, the reflux ratios for this train were kept between 1.5 and 2.5. As the desired product of this train is the jet fuel, higher carbon number reactants are key to obtaining a higher flash point. Flash point is the minimum temperature for an ignitable vapor to form. A flash point of 104°F is required for the jet fuel to meet the spec for Jet A classification and to account for degradation during transport to airports. With the drive to shift the product catalog to reflect market demand, coupling this process with the Dimersol process is what drives the greater production of heavier hydrocarbon products.

Keeping in tune with the light ISOALKY train, here too a black box reactor is implemented, ignoring the refrigeration and ionic liquid catalyst aspects of the ISOALKY process. Originally the heavy train had a flash drum to separate C4 and send it to the light train to better be utilized there. A case study on the use of a flash drum was also conducted on the heavy train with the same results and an added complication. At any operating condition, iC5 was vaporized and lost through the vapor stream. Due to these findings, the decision was made to forgo the use of this unit in the heavy train. Additionally, the hope was to heat integrate the cooled liquid process stream from the flash drum to the ISOALKY reactant stream to preheat the cooled flash drum effluent stream for separation and cool the reactants to the desired temperature, but this wasn't possible without the flash drum. Aside from the issues with implementing a flash drum step in the separation train there were some issues with the iC5 recycle.

The heavy ISOALKY train is less complicated than the light train but still required some effort to converge the overall and reactor balances. When the flash drum was removed there was no way for the C4 and lighter components to leave the system. Upon each iteration, C3's and C4's built up in the recycle loop with no decrease indicating an equilibrium. An attempt to separate these components downstream from the iC5 column using a flash drum was made but had the same results as putting it upstream of the column. This is most likely the cause of the greater discrepancy in the mass balance tolerance in this train than in the light train. It would be recommended to have an additional column in the iC5 recycle loop to remove the lighter components, mimicking the separation train in the light simulation. Adding an additional column would allow for the C4 and lighter components to be separated and used elsewhere or sold. This points out one of the biggest issues with separating the process into three separate simulations. If the entire process were in the same simulation it might be possible to use the light separation train to effect a more efficient separation for the heavy train.

Further analysis of the process by simulating it in its entirety may prove beneficial but is outside the scope of this project. Other advantages that may be seen by combining the simulations, would be the ability to run the gasoline product from the light train through the heavy train separation section. This stream

contains heavy hydrocarbons that can potentially be added to the jet product to increase the yield of the process. A refinery table of the heavy ISOALKY simulation results can be seen in **Tables 6.3.1-6.3.3**

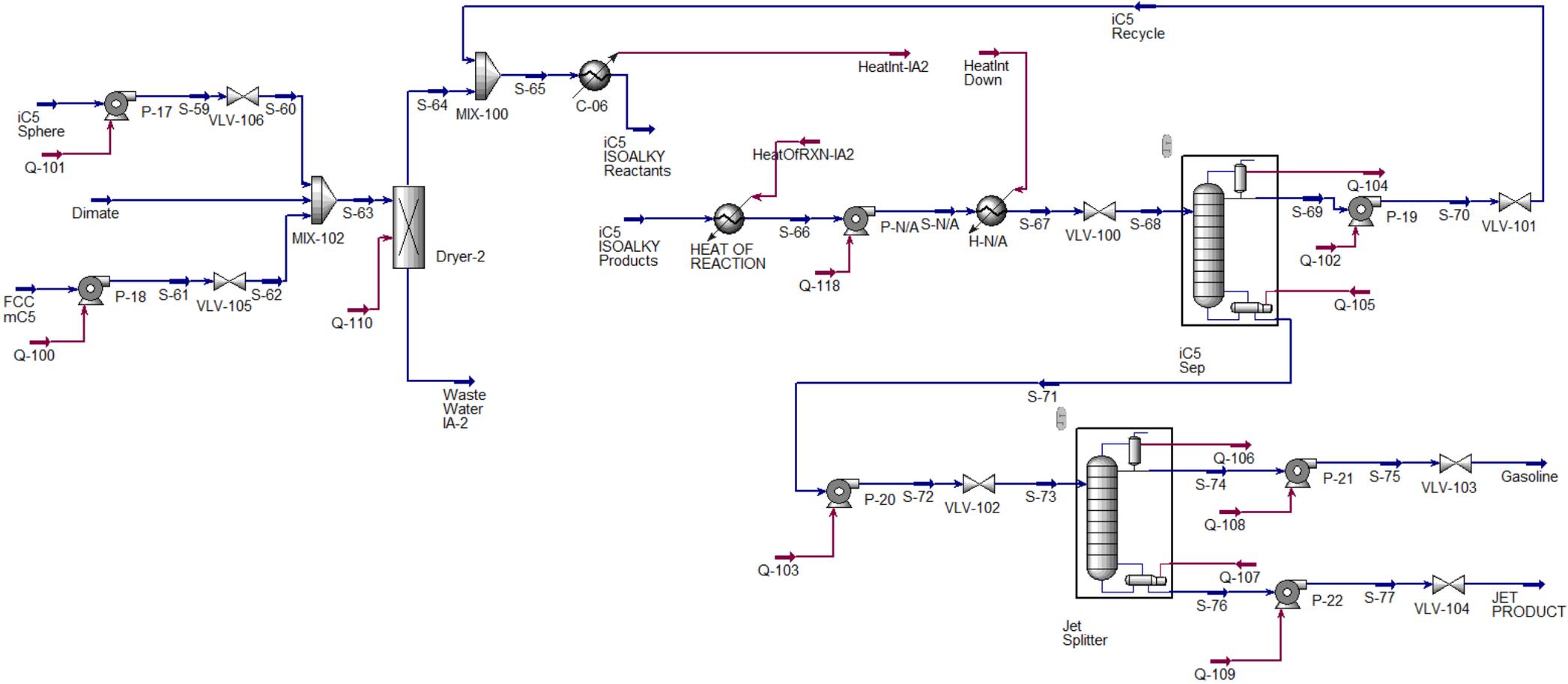


Figure 6.3.1: ISOALKY Heavy Process PFD from Aspen HYSYS.

Table 6.3.1: Composition of ISOALKY Heavy Reactor Inlet and Outlet Streams

ISOALKY Heavy							
		In			Out		
		Mass	Volume	Mole	Mass	Volume	Mole
		(lb/hr)	(GPM)	(mol/hr)	(lb/hr)	(GPM)	(mol/hr)
	Total Flow	599989.4	1914.38	8324.09	599792.8	1863.36	7498.51
CN	Component	Mass Percent	Volume Percent	Mole Percent	Mass Percent	Volume Percent	Mole Percent
C4	i-Butane	0.80%	0.90%	1.00%	0.40%	0.46%	0.55%
C4	n-Butane	1.01%	1.09%	1.26%	0.72%	0.79%	0.99%
C4	1-Butene	1.41%	1.49%	1.82%	0	0	0
C5	i-Pentane	83.21%	83.54%	83.13%	76.35%	78.72%	84.64%
C5	n-Pentane	4.47%	4.44%	4.47%	2.01%	2.05%	2.23%
C5	Cyclopentane	0.06%	0.05%	0.06%	0.05%	0.05%	0.06%
C5	cis2-Pentene	3.18%	3.02%	3.27%	0	0	0
C6	23-Mbutane	0	0	0	0.44%	0.43%	0.41%
C6	2-Mpentane	0	0	0	0.13%	0.12%	0.12%
C6	3-Mpentane	0	0	0	0.06%	0.06%	0.06%
C6	4M-1-pentene	5.85%	5.47%	5.01%	0	0	0
C7	23-Mpentane	0	0	0	0.29%	0.27%	0.23%
C7	24-Mpentane	0	0	0	0.19%	0.18%	0.15%
C8	224-Mpentane	0	0	0	0.59%	0.55%	0.42%
C8	24-Mhexane	0	0	0	0.08%	0.08%	0.06%
C8	25-Mhexane	0	0	0	0.08%	0.08%	0.06%
C8	2M-3Epentane	0	0	0	0.08%	0.08%	0.06%
C9	225-Mhexane	0	0	0	2.11%	1.89%	1.32%
C9	235-Mhexane	0	0	0	0.42%	0.37%	0.26%
C9	23-Mheptane	0	0	0	0.28%	0.25%	0.18%
C9	1-Nonene	0	0	0	0	0	0
C10	335-Mheptane	0	0	0	4.13%	3.56%	2.32%
C10	27-Moctane	0	0	0	1.38%	1.22%	0.77%
C10	1-Decene	0	0	0	0	0	0
C11	n-C11	0	0	0	7.88%	6.82%	4.03%
C11	1-Undecene	0	0	0	0	0	0
C12	n-C12	0	0	0	2.31%	1.98%	1.08%
C12	1-Dodecene	0	0	0	0	0	0
-	NaOH	0	0	0	0	0	0

-	H2O	0	0	0	0	0	0
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Table 6.3.2: Composition and Properties of Motor Alkylate from Heavy Train

Motor Alkylate from Heavy Train				
		Mass	Volume	Mole
		(lb/hr)	(GPM)	(mol/hr)
	Total Flow	40995.9	124.49	478.10
CN	Component	Mass Percent	Volume Percent	Mole Percent
C2	Ethane	0	0	0
C3	Propane	0	0	0
C3	Propene	0	0	0
C4	i-Butane	0	0	0
C4	n-Butane	0	0	0
C4	1-Butene	0	0	0
C5	i-Pentane	35.74%	37.71%	42.48%
C5	n-Pentane	16.85%	17.60%	20.02%
C5	Cyclopentane	0.80%	0.70%	0.98%
C5	cis2-Pentene	0	0	0
C6	23-Mbutane	6.49%	6.42%	6.46%
C6	2-Mpentane	1.85%	1.86%	1.84%
C6	3-Mpentane	0.93%	0.91%	0.92%
C6	4M-1-pentene	0	0	0
C7	23-Mpentane	4.23%	3.98%	3.62%
C7	24-Mpentane	2.82%	2.74%	2.41%
C8	224-Mpentane	8.70%	8.23%	6.53%
C8	24-Mhexane	1.24%	1.16%	0.93%
C8	25-Mhexane	1.24%	1.17%	0.93%
C8	2M-3Epentane	1.21%	1.10%	0.91%
C9	225-Mhexane	17.40%	15.96%	11.63%
C9	235-Mhexane	0.50%	0.45%	0.33%
C9	23-Mheptane	0.01%	0.01%	0.01%
C9	1-Nonene	0	0	0

Table 6.3.3: Composition and Properties of Jet Product

Jet A Product				
		Mass	Volume	Mole
		(lb/hr)	(GPM)	(mol/hr)
	Total Flow	103673.9	279.33	690.11
CN	Component	Mass Percent	Volume Percent	Mole Percent
C8	224-Mpentane	0	0	0
C8	24-Mhexane	0	0	0
C8	25-Mhexane	0	0	0
C8	2M-3Epentane	0.01%	0.01%	0.02%
C9	225-Mhexane	5.32%	5.50%	6.23%
C9	235-Mhexane	2.24%	2.29%	2.63%
C9	23-Mheptane	1.62%	1.65%	1.90%
C9	1-Nonene	0	0	0
C10	335-Mheptane	23.87%	23.73%	25.20%
C10	27-Moctane	7.96%	8.11%	8.40%
C10	1-Decene	0	0	0
C11	n-C11	45.61%	45.51%	43.83%
C11	1-Undecene	0	0	0
C12	n-C12	13.37%	13.19%	11.79%
C12	1-Dodecene	0	0	0
-	NaOH	0	0	0
-	H2O	0	0	0

7 - Equipment Design and Specifications

7.1 - Pumps

Pumps are used throughout the process in order to transport fluid from one piece of equipment to another. This process utilizes 22 theoretical pumps, however, 71 pumps are needed in order to accommodate the flow rates and required head. The dimersol process contains seven pumps, the light ISOALKY train contains nine pumps, and the heavy ISOALKY train contains six pumps. The pump curves used for sizing are all Fristam FPR pumps. All sizing pump curves can be found in **Appendix E**. Each pump is designed to be larger than needed in order to avoid cavitation and prevent overflow issues if problems arise. The FPR pumps were chosen because they can handle high flow rates and discharge pressures. These pumps contain a front loading seal and fewer parts than other options thus making maintenance easier. All the pumps are centrifugal pumps to lower maintenance costs and due to the size versatility.

Pumps must work against the rise in elevation, length of pipe, and control valves. These factors alter the change in pressure for each pump. The rise in elevation and length of pipes for each pump were assumed to be 50 ft and 500 ft, respectively. This ensures that the pipes connect properly to all pieces of equipment. **Tables 7.1.1 , 7.1.2, and 7.1.3** show the calculation values used to determine the head and overall capacity of the pumps for the dimersol, light ISOALKY train, and heavy ISOALKY train. **Tables 7.1.4, 7.1.5, and 7.1.6** show the pump sizing values and chosen pump models (FPR- Centrifugal Pump 2023).

For economic purposes, the 71 pumps were not priced because Chevron requested a different method. This is discussed in more detail in **Section 9.1**. The pumps were designed using the pump curves provided in design rather than finding new ones thus the flow rates and head requirements were much higher than the pumps could accommodate. More powerful pumps should be used when actually designing pumps for this process.

Sample hand calculations and equations used to determine pump sizing (P-01):

Known:

Pressure In = 250 psi	Pressure Out = 315 psi
Length of Pipe = 500 ft	Pipe Elevation Gain = 50 ft
Density of Fluid = 31.415 lb/ft ³	(in/out average from ASPEN)
Density of Water at 70 F = 62.3 lb/ft ³	
Overall Capacity = 207.86 GPM	(from ASPEN)
NPSHA (pump 1 in series) = 436.2	(from ASPEN)
NPSHA (pump 2 in series) = 996.29	(from ASPEN)

Calculated Values:

Heuristic 38 : For liquid flow, assume a pipeline pressure drop of 2 psi / 100 ft of pipe and a control valve pressure drop of at least 10 psi. For each 10-ft rise in elevation, assume a pressure drop of 4 psi.

$$\text{Pipeline pressure drop} = \frac{2 \text{ psi}}{100 \text{ ft}} * 500 \text{ ft} = \mathbf{10 \text{ psi}}$$

$$\text{Control valve pressure drop} = \mathbf{10 \text{ psi}}$$

$$\text{Elevation pressure drop} = \frac{4 \text{ psi}}{10 \text{ ft}} * 50 \text{ ft} = \mathbf{20 \text{ psi}}$$

$$\text{Total change in pressure} = (315 - 250) + 10 + 10 + 20 = \mathbf{105 \text{ psi}}$$

$$\text{Total Head} = (\text{Total change in pressure} * 144 \text{ in}^2/\text{ft}^2) / \text{Density of fluid} = (105 * 144) / 31.415 \\ = \mathbf{481.3 \text{ ft}}$$

$$\frac{\text{Total Change in Pressure}}{\text{Density of Fluid}} * \frac{144 \text{ in}^2}{\text{ft}^2}$$

$$\text{Head per unit} = \text{total head} / \# \text{ pumps in series} = \frac{481.3 \text{ ft}}{2} = \mathbf{240.65 \text{ ft}}$$

$$\text{Capacity per unit} = \text{overall capacity} / \# \text{ pumps in parallel} = \frac{207.86 \text{ GPM}}{1} = \mathbf{207.86 \text{ GPM}}$$

$$\text{Change in pressure per unit} = \text{total change in pressure} / \# \text{ pumps in series} = \frac{105 \text{ psi}}{2} \\ = \mathbf{52.5 \text{ psi}}$$

Pump Curve Values and Calculations:

Model = 3542 RPM = 3500 Inlet = 3 in Outlet = 2.5 in
Impeller Diameter = 195 mm = 7.68 in Motor HP = 30 HP NPSHR = 7 ft

Must account for the fact that the pump curve HP is based on water at 70F and the fluid density is different, thus the HP needed must be adjusted.

$$\text{Adjust BHp} = \text{motor HP} * (\text{density of fluid} / \text{density of water at 70F}) = 30 * (31.415 / 62.3) = \mathbf{15.13 \text{ HP}}$$

Heuristic 39: Estimate the theoretical horsepower THp for pumping a liquid:

$$\text{THp} = (\text{GPM}) * (\text{pressure increase, psi}) / 1714 = (207.86 * 52.5) / 1714 = \mathbf{6.37 \text{ HP}}$$

$$\text{Unit efficiency} = \text{THp} / \text{adjust BHp} = \frac{6.37}{15.13} * 100 = \mathbf{42.09}$$

Table 7.1.1: Dimersol Pump Calculations

	P- 01	P - 02	P - 03	P - 04	P - 05	P - 06	P - 07
Pressure In (psi)	250	280	60	75	240	3	20
Pressure Out (psi)	315	300	315	315	265	243	100
Length of Pipe (ft)	500	500	500	500	500	500	500
Elevation of Pipe (ft)	50	50	50	50	50	50	50
P_Length (psi)	10	10	10	10	10	10	10
P_Elevation (psi)	20	20	20	20	20	20	20
P_ Control Valve (psi)	10	10	10	10	10	10	10
Δ Pressure (psi)	105	60	295	280	65	280	120
Density of Fluid (lb/ft ³)	31.415	31.4	62.835	92.24	28.325	39.09	36.51
Head (ft)	481.3	275.16	676.06	437.12	330.45	1031.7	473..29
Overall Capacity (GPM)	207.86	207.96	35.33	88.12	54.71	110.54	10.28

Table 7.1.2: Light ISOALKY Train Pump Calculations

	P- 08	P - 09	P - 10	P - 11	P - 12	P - 13	P - 14	P-15	P-16
Pressure In (psi)	150	150	100	225	1	70	90	45	65
Pressure Out (psi)	275	275	250	280	141	225	100	115	110
Length of Pipe (ft)	500	500	500	500	500	500	500	500	500
Elevation of Pipe (ft)	50	50	50	50	50	50	50	50	50
P_Length (psi)	10	10	10	10	10	10	10	10	10
P_Elevation (psi)	20	20	20	20	20	20	20	20	20
P_ Control Valve (psi)	20	20	20	20	20	20	20	20	20
Δ Pressure (psi)	165	165	190	95	180	195	50	110	85
Density of Fluid (lb/ft ³)	35.86	34.39	33.22	28.87	38.59	33.66	35.52	35.21	35.11
Head (ft)	662.67	690.90	823.72	473.93	671.68	834.35	202.7	449.87	348.67
Overall Capacity (GPM)	379.75	57.37	463.63	97.88	2348.76	2257.89	66.14	68.75	348.21

Table 7.1.3: Heavy ISOALKY Train Pump Calculations

	P- 17	P - 18	P - 19	P - 20	P-21	P-22
Pressure In (psi)	75	100	20	40	3	18
Pressure Out (psi)	245	245	210	55	75	90
Length of Pipe (ft)	500	500	500	500	500	500
Elevation of Pipe (ft)	50	50	50	50	50	50
P_Length (psi)	10	10	10	10	10	10
P_Elevation (psi)	20	20	20	20	20	20
P_ Control Valve (psi)	20	20	20	20	20	20
Δ Pressure (psi)	210	185	230	55	112	112
Density of Fluid (lb/ft ³)	38.19	38.415	36.39	38.34	39.3	36.25
Head (ft)	791.83	693.48	910.14	206.57	410.38	444.91
Overall Capacity (GPM)	176.56	175.94	1538.26	464.22	128.35	351.86

Table 7.1.4: Dimersol pump sizing values

	P- 01	P - 02	P - 03	P - 04	P - 05	P - 06	P - 07
Head per Unit (ft)	240.65	275.16	338.03	218.56	330.45	343.82	236.65
Δ Pressure per Unit (psi)	52.50	60	147.50	140.00	65	93.33	60.00
# Units in Series	2	1	2	2	0	3	2
# Units in Parallel	0	0	0	0	0	0	0
Capacity per Unit (GPM)	207.86	207.96	35.33	88.12	54.71	110.54	10.28
Total # pumps	2	1	2	2	1	3	2
NPSHA : pump 1 (ft)	436.2	566.5	170.3	141.7	6.5333	7.183	1.0181
NPSHA : pump 2 (ft)	996.29	N/A	401.2	187.2	N/A	25.6	4.198
NPSHA : pump 3 (ft)	N/A	N/A	N/A	N/A	N/A	59.8	
Pump line	Fristam Centrifugal						
Model	3542	3452	3452	742	3452	3452	742
RPM	3500	3500	3500	3500	3500	3500	3500
Inlet Diameter (in)	3	3	3	2.5	3	3	2.5
Outlet Diameter (in)	2.5	2	2	2	2	2	2
Impeller Diameter (mm)	195	230	240	190	240	245	195
Impeller Diameter (in)	7.68	9.06	9.45	7.48	9.45	9.65	7.68
Motor (HP)	30	40	30	20	30	40	10
Adjust BHp (HP)	15.13	20.16	30.26	29.61	13.64	25.10	5.86
THp (HP)	6.37	7.28	3.04	7.20	2.07	6.02	0.36
NPSHR (ft)	7	10	6	3.3	6	7	0.8
Pump Efficiency (%)	42.09	36.11	10.05	24.31	15.21	23.98	6.14

** All pumps are from the Fristam Centrifugal pump line, the pump types are FPR, and the pump material is carbon steel.

Table 7.1.5: Light ISOALKY train pump sizing values

	P- 08	P - 09	P - 10	P - 11	P - 12	P - 13	P - 14	P-15	P-16
Head per Unit (ft)	331.33	345.45	411.86	236.9	335.8	278.1	202.7	224.94	348.67
Δ Pressure per Unit (psi)	82.5	82.5	95	47.5	90	65	50	55	85
# Units in Series	2	2	2	2	2	3	0	2	0
# Units in Parallel	0	0	0	0	5	5	0	0	0
Capacity per Unit (GPM)	379.75	57.37	463.63	97.88	469.7	451.6	66.14	68.75	348.21
Total # pumps	2	2	2	2	10	15	1	2	1
NPSHA : pump 1 (ft)	496	464.1	109.2	5.702	980.7	908.2	30.17	3.0841	21.55
NPSHA : pump 2 (ft)	612.7	787.7	281.95	25.985	1101.5	1019.3	N/A	10.873	N/A
NPSHA : pump 3 (ft)						1674			
Pump line	Fristam Centrifugal								
Model	3552	3452	3552	742	3552	3552	742	742	3552
RPM	3500	3500	3500	3500	3500	3500	3500	3500	3500
Inlet Diameter (in)	3	3	3	2.5	3	3	2.5	2.5	3
Outlet Diameter (in)	2.5	2	2.5	2	2.5	2.5	2	2	2.5
Impeller Diameter (mm)	235	245	250	200	230	215	180	190	230
Impeller Diameter (in)	9.25	9.65	9.84	7.87	9.06	8.46	7.09	7.48	9.06
Motor (HP)	75	30	85	20	85	60	15	15	60
Adjust BHp (HP)	43.16	16.56	45.32	9.27	52.65	32.41	8.55	8.48	33.81
THp (HP)	18.28	2.76	25.70	2.71	24.67	17.13	1.93	2.21	17.27
NPSHR (ft)	15	6	20	4	20	17	2	2	15
Pump Efficiency (%)	43.35	16.67	56.71	29.27	46.85	52.84	22.56	26.02	51.07

** All pumps are from the Fristam Centrifugal pump line, the pump types are FPR, and the pump material is carbon steel.

Table 7.1.6: Heavy ISOALKY Train Pump Sizing Values

	P- 17	P - 18	P - 19	P - 20	P - 21	P - 22
Head per Unit (ft)	395.9	346.7	303.4	206.57	205.2	222.5
Δ Pressure per Unit (psi)	105	92	76.7	55	56	56
# Units in Series	2	2	3	0	2	2
# Units in Parallel	0	0	4	0	0	0
Capacity per Unit (GPM)	176.56	175.94	384.6	464.22	128.35	351.86
Total # pumps	2	2	12	1	2	2
NPSHA : pump 1 (ft)	287.6	342.7	421.3	38.23	5.928	22
NPSHA : pump 2 (ft)	699.587	1070.3	1017.2	N/A	20.49	83.57
NPSHA : pump 3 (ft)			1252.7			
Pump line	Fristam Centrifugal					
Model	3552	3552	3552	3452	742	3452
RPM	3500	3500	3500	3500	3500	3500
Inlet Diameter (in)	3	3	3	3	2.5	3
Outlet Diameter (in)	2.5	2.5	2.5	2	2	2
Impeller Diameter (mm)	240	225	215	245	190	230
Impeller Diameter (in)	9.45	8.86	8.46	9.65	7.48	9.06
Motor (HP)	60	50	60	60	20	50
Adjust BHp (HP)	36.78	30.83	35.05	36.92	12.62	29.09
THp (HP)	10.82	9.50	17.20	14.90	4.19	11.50
NPSHR (ft)	10	10	15	25	5.5	15
Pump Efficiency (%)	29.41	30.8	49.08	40.34	33.24	39.52

** All pumps are from the Fristam Centrifugal pump line, the pump types are FPR, and the pump material is carbon steel.

7.2 - Compressor

There is one compressor used in the entire process, it is found in the light ISOALKY train. The compressor was used to increase the pressure after the flash drum (FLASH-1) due to it being at 1 psi. This ensures that the heat exchanger and following column can work properly. **Table 7.2.1** below shows the compressor calculation values and **Table 7.2.2** shows the compressor sizing values. The compressor curve used to size the compressor can be found in **Appendix F**.

While it was found that 28 compressors would need to be used in order to handle pressure and flowrate, for pricing purposes Chevron requested another formula be used which can be found in **Section 9.2**.

Table 7.2.1 : Compressor Calculation Values

Variable	Value
Flow In (lbs/hr)	125,200
Pressure In (psi)	15.7
Pressure Out (psi)	124.7
Temperature In (K)	263
Calculated Temperature Out (K)	333.23
ASPEN Temperature Out (K)	328.27
Efficiency (%)	100
Density (lb/ft ³)	0.727
Reference Pressure (psi)	14.7
Reference Temperature (K)	288.2
Pressure Ratio	7.95
Corrected Flow (lbs/hr)	111,980
Corrected Flow (lbs/min)	1,866.3
Corrected Volumetric Flow (ft ³ /min)	2567.2
Cp/Cv	1.13

Table 7.2.2 : Compressor Sizing Values

Total # of Compressors	28
Change in flow per unit (lbs/min)	183.37
Change in pressure per unit (psi)	54.4
Pressure ratio per unit	3.97
# units in parallel	14
# units in series	2
Company name	ATP Turbo
Model	GTX5544R
Compressor Type	Turbocharger Compressor
Efficiency (%)	74
RPM	69,000
Watts	5,300

HP	7.12
----	------

Sample hand calculations and equations used to determine compressor sizing :

Know Values :

Flow Rate In = 125,000 lb/hr	(From Aspen)
Pressure In = 1 psi	(From Aspen)
Pressure Out = 110 psi	(From Aspen)
Temperature In = 263 K	(From Aspen)
Temperature Out = 328.27 K	(From Aspen)
Efficiency = 100 %	(From Aspen)
Density = 0.727 lb/ft ³	(From Aspen)
Reference Pressure = 14.7 psi	
Reference Temperature = 288.2 K	
Cp/Cv = 1.13	(From Aspen)

Calculated Values:

$$\text{Absolute Pressure In} = \text{Pressure In} + \text{Reference Pressure} = 1 \text{ psi} + 14.7 \text{ psi} = \mathbf{15.7 \text{ psi}}$$

$$\text{Absolute Pressure Out} = \text{Pressure Out} + \text{Reference Pressure} = 110 \text{ psi} + 14.7 \text{ psi} = \mathbf{124.7 \text{ psi}}$$

$$\begin{aligned} \text{Calculated Temperature Out} &= \text{Temperature In} * \left(\frac{\text{Absolute Pressure Out}}{\text{Absolute Pressure In}} \right)^{((Cp/Cv - 1)/ Cp/Cv)} \\ &= 263K * \left(\frac{124.7 \text{ psi}}{15.7 \text{ psi}} \right)^{(1.13-1)/1.13} = \mathbf{333.23 \text{ K}} \end{aligned}$$

$$\text{Pressure Ratio} = \left(\frac{\text{Absolute Pressure Out}}{\text{Absolute Pressure In}} \right) = \frac{124.7 \text{ psi}}{15.7 \text{ psi}} = \mathbf{7.95}$$

$$\begin{aligned} \text{Corrected Flow} &= \text{Flow Rate In} * \sqrt{\frac{\text{Temperature In}}{\text{Reference Temperature}}} * \frac{P_{ref}}{P_{in,abs}} \\ &= 125000 \text{ lb/hr} * \sqrt{\frac{263K}{288.2 K}} * \frac{14.7 \text{ psi}}{1 \text{ psi}} \\ &= \mathbf{111980 \text{ lb/hr}} \end{aligned}$$

$$\text{Change in pressure per unit} = \frac{\text{Absolute Pressure Out} - \text{Absolute Pressure In}}{2} = \frac{124.7 \text{ psi} - 15.7 \text{ psi}}{2} = \mathbf{54.5 \text{ psi}}$$

$$\text{Pressure Ratio per unit} = \frac{\text{Pressure Ratio}}{2} = \frac{7.95}{2} = \mathbf{3.97}$$

$$\text{Change in flow per unit} = \frac{\text{Corrected Flow}}{14} * 1/60 \text{ min} = \frac{111980 \text{ lb/hr}}{14} * 1/60 \text{ min} = \mathbf{183.37 \text{ lb/min}}$$

7.3 - Heat Exchangers

Heat exchangers are instruments that transfer heat between two streams of fluid. In a shell and tube heat exchanger, one stream is passed through many small tubes while the other is run through the shell, a casing that encompasses the tubes and allows the shell-side fluid to wash over the tubes. The process stream passes through one of these sides whereas the other side is a utility stream brought exclusively to heat or cool the process. There are six total heat exchangers in the process, one in the dimersol process, four in the light ISOALKY train, and one in the heavy ISOALKY train.

The first step in designing the heat exchangers is to collect relevant data from the Aspen simulation. This includes the process stream inlet and outlet temperatures, heat duty of the exchanger, and process stream density and heat capacity. Based on the temperature change in the process stream a utility was chosen to sufficiently cool or heat the process stream. For most of the exchangers this utility was chosen to be chilled brine, or cooling water. After choosing the utility, the process stream was assigned to the tube-side according to Heuristic 55 due to its higher volatility and heat compared to the utility fluids. Pressure drops across the tubes were determined when designing the PFD, and the shell-side pressure drop was estimated as 5-7 psi according to Heuristic 31.

The next goal was to determine the number of shell and tube passes required for each heat exchanger via the correction factor, F_T . To determine the correction factor, R and S values specific to each heat exchanger were calculated based on the temperature changes across the streams via the following equations:

$$R = \frac{\text{Hot Temperature In} - \text{Hot Temperature Out}}{\text{Cold Temperature Out} - \text{Cold Temperature In}}$$

$$S = \frac{\text{Cold Temperature Out} - \text{Cold Temperature In}}{\text{Hot Temperature In} - \text{Cold Temperature In}}$$

The inlet and outlet temperatures of the utility streams were chosen with the goal of having a ΔT greater than a ΔT_{\min} determined via Heuristic 26. The log-mean temperature difference, ΔT_{\ln} , was also found at this point for future use. With R and S calculated, graphs of correction factors correlation to R and S for heat exchangers of varying tube and shell passes were used to find an acceptable F_T . To be acceptable the point where R and S intersect must yield an F_T greater than 0.85. All correction factor graphs can be found in **Appendix G**.

With F_T available, the final component necessary to calculate the area is the heat transfer coefficient, U. This coefficient was estimated using a table of heat transfer coefficients for various tube and shell fluid combinations. With U, F_T , ΔT_{\ln} , and Q, the heat duty, the area of the exchanger could be calculated via the following equation:

$$\text{Area} = \frac{\text{Heat Duty}}{\text{Heat Transfer Coeff.} * F_T * LMTD}$$

Volumetric flow rate through the tube and shell was calculated using heat duty, temperature difference, and stream properties density and heat capacity. As mentioned above, Aspen provided these properties for the process stream, however the utility stream required these to be found via literature. An assumption that the density and heat capacity of the utilities were approximately that of water at the same

temperature was made, and the densities and heat capacities at the inlet and outlet temperatures were averaged along the shell. The flowrate was found using the following equation:

$$\text{Volumetric Flow} = \frac{\text{Heat Duty}}{\text{Density} * \text{Heat Capacity} * \Delta T}$$

After obtaining these specifications the exchanger can now be sized. First, a table was used to choose the tubes' outer diameter, gauge, and cross-sectional area. Length was chosen as 16ft to start and adjusted as needed. The outer area per tube, number of tubes, and tube fluid velocity were calculated using the chosen dimensions and stream properties and placed into the following equations:

$$\text{Surface Area per Tube} = \pi * \text{tube outer diameter} * \text{tube length}$$

$$\text{Number of Tubes} = \text{Area} / \text{Surface Area per Tube} / \text{Number of Tube Passes}$$

$$\text{Velocity} = \text{Volumetric Flow} / \text{Cross Sectional Area per Tube} / \text{Number of Tubes}$$

Heat exchanger design mandates that the velocity of the fluid in the tube be between 1 to 10 ft/s, which was the main basis on which dimensions and other exchanger properties were chosen. With the velocity in the accepted range, miscellaneous properties that do not affect the streams such as the baffle cut and spacing were chosen according to Heuristic 54. As for material, Carbon Steel was chosen as suggested by the Chevron liaisons. Below are sample hand calculations for the heat exchanger in the Dimersol process. **Table 7.3.1** details all the specifications of each of the six heat exchangers.

Sample hand calculations and equations used to determine heat exchanger sizing (HX-01):

Known Values via Aspen:

Hot Temperature In: 1211 °F Hot Temperature Out: 80.7 °F

Heat Duty: 4.59E+07 Btu/hr Heat Transfer Coefficient: 20 Btu/°F-ft²-hr

Process Heat Capacity: 0.75 Btu/lb-°F

Process Density: 31.4 lb/ft³

Chosen Values:

Cold Temperature In: 0 °F Cold Temperature Out: 60 °F

Utility Heat Capacity: 0.99 Btu/lb-°F

Utility Density: 62.4 lb/ft³

Tube Length: 10 ft

Tube Outer Diameter: 0.75 in

Tube Cross Sectional Area: 0.182 ft²

Calculated Values:

Temperature Differences:

Hot Temp. Out - Cold Temp. In = 80.7 - 0 = **80.7°F**

Hot Temp. In - Cold Temp. Out = 1211 - 60 = **1151°F**

Log-Mean Temperature Difference:

$$\text{LMTD} = \frac{80.7 - 1151}{\ln(80.7/1151)} = \mathbf{403^\circ\text{F}}$$

$$\frac{T_{H,o} - T_{H,i}}{\ln(T_{h,o}) - \ln(T_{H,i})}$$

R, S, & F_T:

$$R = \frac{1211 - 80.7}{60 - 0} = \mathbf{18.8}$$

$$S = \frac{60 - 0}{1211 - 0} = \mathbf{0.05}$$

Estimating F_T using Correction Factor curves found in **Appendix G**:

$$F_T = \mathbf{0.85}$$

1 Shell Pass, 2 Tube Passes

Heat Transfer Area:

$$\text{Area} = \frac{4.59E7}{20 * 0.85 * 403} = \mathbf{6700 \text{ ft}^2}$$

For pricing purposes calculations could stop here, however tube velocity must be confirmed to be between 1 and 10 ft/s

Tube-Side Volumetric Flow Rate:

$$\text{Volumetric Flow} = \frac{4.59E7}{0.75 * 31.4 * (1121 - 80.7)} = \mathbf{32365 \text{ ft}^3/\text{hr}}$$

Surface Area per Tube:

$$\text{Surface Area per Tube} = 0.75 * 12 * \pi * 10 = \mathbf{565 \text{ ft}^2}$$

Number of Tubes:

$$\text{Number of Tubes} = \frac{6700}{565 * 2} = \mathbf{6 \text{ tubes}}$$

Tube Velocity:

$$\text{Velocity} = \frac{32365}{6 * 0.18} = \mathbf{30015 \text{ ft/hr}; 8.34 \text{ ft/s}}$$

Table 7.3.1: Specifications of Process Heat Exchangers

Property	HX-01	HX-02	HX-03	HX-04	HX-05	HX-06
Tube Fluid	Process	Process	Process	Process	Process	Process
Tube Flow Rate (ft ³ /hr)	32365	21259	56844	68988	9129	40694
Tube Inlet Temp. (°F)	1211	126	138	131	193	176
Tube Outlet Temp. (°F)	81	81	63	101	3	76
Shell Fluid	Chilled Brine	Chilled Brine	Chilled Brine	Cooling Water	Chilled Brine	Chilled Brine
Shell Flow Rate (ft ³ /hr)	652	10801	8055	10098	1022	6690
Shell Inlet Temp. (°F)	0	0	0	51	0	0
Shell Outlet Temp. (°F)	60	60	30	80	60	45
Total Heat Duty (Btu/hr)	4.59E+07	3.01E+07	3.76E+07	1.89E+07	1.21E+07	4.17E+07
Heat Transfer Area (ft ²)	6700	24338	9525	19760	20081	8349
Passes (Shell : Tube)	1 : 2	1 : 2	1 : 2	1 : 2	3 : 6	2 : 4
Shell Diameter (in)	4	4	4	4	4	4
Tube X-Sectional Area (ft ²)	0.18	0.18	0.34	0.18	0.18	0.18
Tube Number	6	27	7	22	8	8
Tube Length (ft)	10	16	20	16	16	10
Tuber Inner Diameter (in)	0.48	0.48	0.67	0.48	0.48	0.48
Tube Gauge	10	10	8	10	10	10
Tube Spacing (in)	1	1	1	1	1	1
Tube Velocity (ft/s)	8.3	1.2	7.5	4.8	1.9	8.4
Baffle Cut (in)	0.8	0.8	0.8	0.8	0.8	0.8
Baffle Spacing (in)	3	3	3	3	3	3
Heat Transfer Coeff. (Btu/hr-°F-ft ²)	20	20	50	20	20	50
Material	Carbon Steel					
Tube Pressure Drop (psi)	10	10	10	10	10	10
Shell Pressure Drop (psi)	5	5	7	5	5	5

7.4 - Flash Drum

Only one flash drum was implemented and designed in this process. Because the scope of this project is more about the economics of the project, the flash drum was not designed extensively. To this end the only requirement for designing the flash drum was to obtain a volume to use for pricing. Chevron specified a five minute residence time for flash drums. The flow rate into the flash drum was found to be 2613 GPM. By multiplying the flow rate by the residence time the volume required for the vessel, 13065 gal, is obtained. Flash drums are a simple vessel that allows for a stream to separate based on vapor liquid equilibrium. The flash drum operates at a pressure of 1 psig and a temperature of 18 °F so exotic and expensive materials are not needed.

7.5 - Filters, Dryers and Chlorine Absorbers

7.5.1 - Filters/Dryers

The filters and dryers were designed using the same filter cartridge targeted for high flow systems made by Brother Filtration. These filters can be implemented in a dryer setting to obtain the same functionality as a traditional dryer with the added bonus of removing other contaminants to purify the wastewater stream simultaneously. Sizing of the filters was determined based on the inlet flow rate and **Figure 7.5.1.1**. From the size of the filter, the filter area could be determined by dividing the volume in m^3 by the height of the filter in m . Final equipment specifications are presented in **Table 7.5.1.1**. From the provided document from Chevron, the dryers have a residence time of 10 mins because they feed products streams. Likewise, the washers have a residence time of 5 mins because they do not feed product streams.

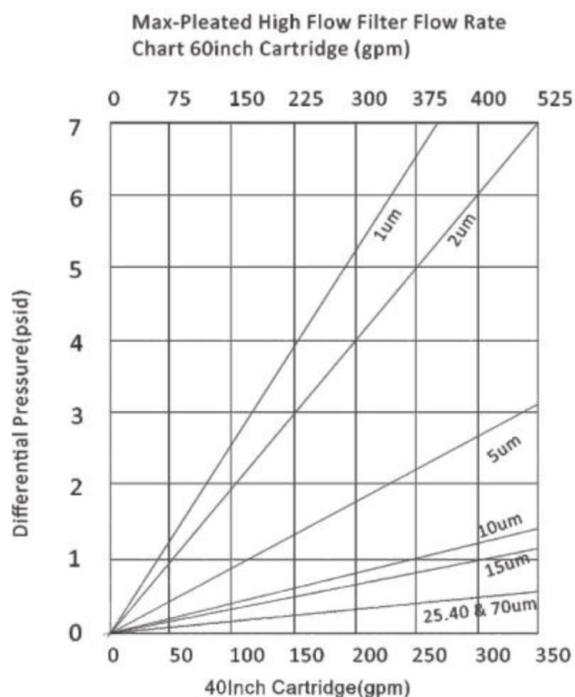


Figure 7.5.1.1: Flow Rate vs Pressure for 40 and 60 in Cartridge Filters

Table 7.5.1.1: Filter Specifications

Equipment Name	Volume (Gal)	Flow Rate (GPM)	Residence Time (min)	Area (ft^2)
Dryer-1	4960	496	10	40.4
Dryer-2	4550	455	10	37.1
Wash-NaOH	1220	245	5	15.0
Wash-H2O	1030	207	5	12.6

7.5.2 - Chlorine Adsorbers

The chlorine absorbers were designed based on compatibility for both gas and liquid streams, as well as a material that could be priced with a cost reference website or spreadsheet. The decision to use four of the same type of absorbers was determined for ease of cost analysis later in the design process. For the absorbents, molecular sieves were used in this application. The precise nature of the separation made molecular sieves a good candidate for this use because of their tunability based on molecule size (ScienceDirect, n.d.). By making the molecular size of the sieve on the order of magnitude of the chlorine molecule that is being absorbed out of the propane, butane, and gasoline product streams, this will ensure that the sieves are not absorbing extraneous material that would alter the composition of these streams. The provided Cost Formulas Excel spreadsheet was used to price the molecular sieves and the volume of absorbers was equal to the volume of the vessel to emulate a packed bed absorption setup.

For the absorption vessel, a simple horizontal tank with round ends was chosen to contain the absorbents. The material used here was carbon steel & API, which is defined by the Matche Cost Reference website as a vessel that meets the American Petroleum Institute's standards and regulations (Matches, n.d.). The specification of all chlorine absorbers can be found in **Table 7.5.2.1**. The names of the equipment are correlated to the boxes labeled "Cl" box diagram, **Figure 1.3.1**, with CL-1 being the top most chlorine absorber and CL-4 being the one on the very bottom. There should be a fourth chlorine absorber on the bottoms stream of the C4 Separation Column but this is not included in **Figure 1.3.1**. Residence time is based on the provided document from Chevron citing that vessels that do not feed a process should have a time of 5 mins (Leichty, S. et al., 2024). From this, the flow rate could be multiplied by the residence time to determine a volume for the absorber units.

Table 7.5.2.1: Chlorine Absorber Specifications

Equipment Name	Volumn (Gal)	Flow Rate (GPM)	Residence Time (min)
CL-1	439	87.9	5.00
CL-2	328	65.6	5.00
CL-3	1430	287	5.00
CL-4	623	124	5.00

7.6 - Distillation Columns

The distillation columns were specified in Aspen HYSYS. The purpose of these columns varied from Dimersol to ISOALKY light and heavy trains. The Depropanizer Column, or LPG Sep, was used to separate light propane gas components: ethane, propane, and propylene from heavy components: isohexene, nonane, decane, dodecane, and undecane. The Heavy Separation Column, or Heavy Sep, was used to separate the dimate from the heavy olefin components, specifically nonene and heavier. The dimate was

composed of primarily isohexene, with trace amounts of nonene and heavier components. The columns in the ISOALKY Light and Heavy trains are primarily intended to separate out the component they are named after out of the tops and every other component out the bottoms. The one exception to this is the Jet Splitter in the ISOALKY Heavy train. This column separated nonane and lighter from the top to comprise the Light Alkylate to Gasoline Blending product stream. Out of the bottoms is the desired jet fuel, which is composed of nonane and heavier components. It should be noted that the separation was less than ideal for all columns. As a result, there are trace amounts of contaminants throughout the process. These values are compiled as part of the stream compositions in **Tables 6.1.1, 6.2.1 and 6.3.1**.

Using the capability to add column internals; the tray type, tray spacing, and diameter were modified until there were no weeping or flooding issues in any tray. No modifications were made to tray number, because the Aspen was fully converged at this point and any major changes would have caused discontinence in the convergence. This process was repeated for all 3 Aspen files. The results of this troubleshooting for the Dimersol Aspen file is in **Table 7.6.1**. All names of the columns are matched to their respective labels in the Aspen file for ease of cross reference.

Table 7.6.1: Dimersol Column Specifications

Dimersol						
Column Name	Tray/Packing Type	Number of Passes	Tray Spacing (ft)	Diameter (ft)	Number of Trays	Total Height (ft)
LPG Sep	Bubble Cap	1	2.3	10.0	55	126.5
Heavy Sep	Bubble Cap	1	1.5	8.30	35	52.5

Likewise, for the ISOALKY Light and Heavy processes, these results are presented in **Table 7.6.2** and **Table 7.6.3** respectively.

Table 7.6.2: ISOALKY Light Column Specifications

ISOALKY Light						
Column Name	Tray/Packing Type	Number of Passes	Tray Spacing (ft)	Diameter (ft)	Number of Trays	Total Height (ft)
C3 Sep	Sieve	2	3.5	6.37	40	140
iC4 Sep Lyt	Sieve	4	2.8	22.0	70	196
C4 Sep Lyt	Bubble Cap	1	1.9	9.10	40	75.6

Table 7.6.3: ISOALKY Heavy Column Specifications

ISOALKY Heavy						
Column Name	Tray/Packing Type	Number of Passes	Tray Spacing (ft)	Diameter (ft)	Number of Trays	Total Height (ft)
iC5 Sep	Sieve	4	2.6	23.0	90	234
Jet Splitter	Sieve	1	2.9	7.72	35	101.5

7.7 - Reactor

$$(\$600,000 + 17.72(\text{height})^{2.392})^{1.41}$$

Because reactors in this project were treated as black box reactors, no internals needed to be designed and the reactor design itself was kept to only determining its volume for pricing purposes. Similar to the flash drum the reactor requires a certain residence time. Chevron has specified the residence time for the Dimersol reactor to be five minutes. The flow rate into the reactor was found to be 205 GPM via Aspen. Multiplying the flow rate and residence time yields a reactor size of 1025 gallons. The reactor itself is assumed to be a continuous stir tank reactor as this most closely resembles its actual function. Reactors for the ISOALKY processes were not required to be designed.

	Cost Per Gal of Product
Ingredients	\$2.74
Utilities	\$0.68
Catalysts	\$0.25
Byproduct Credits	-\$1.91

Total	\$10,544,000
Lang Factor Total	\$52,142,000

	Annual Cost
Operating Labor & Benefits	\$560,000
Maintenance	\$4,205,000

8 - Utilities Summary and Heat Integration

A method that reduces the amount of utilities and therefore the total cost of utilities is heat integration, wherein one process stream may be used to heat another process stream and vice versa instead of importing outside utilities. While this generally reduces the cost of utilities, the trade off is that the amount of heat exchangers required tends to be greater than a non-heat integrated system. Subsequently, in estimating the cost of heat exchangers overall, the non-heat integrated process was priced along with the heat integrated process that was simulated in Aspen Energy Analyzer. Aspen Energy Analyzer is used to incorporate heat integration into an already existing Aspen Simulation, in this case Aspen HYSYS. Manual calculations were completed in **Section 7.3** for the utility needs, these are displayed below in **Table 8.1**.

While these simulations are based off of their respective processes (Dimersol, ISOALKY Light, & ISOALKY Heavy), the reality is that all of these processes would be connected. Therefore, for a connected system there heat integration would be more effective at minimizing the utility costs. Additionally, the Aspen HYSYS files that are being used for the energy analysis include heat duties as a means of requiring heat, while this was necessary for the simulation, the values for cost for several of these streams is higher than predicted. Therefore, when doing the cost analysis in **Section 9**, hand-calculated utility costs were used as detailed in **Appendix H**.

Table 8.1: Utility Needs Based on HX Design (Section 7.3)

Component	Tube Fluid	T _{in} -T _{out} (°F)	Shell Fluid	T _{out} -T _{in} (°F)
HX-01	Process	1130	Chilled Brine	60
HX-02	Process	45	Chilled Brine	60
HX-03	Process	75	Chilled Brine	30
HX-04	Process	30	Chilled Brine	29
HX-05	Process	190	Chilled Brine	60
HX-06	Process	100	Chilled Brine	45

The values calculated up above can then be compared to the utilities that were chosen by the Aspen HYSYS simulations. Since there are three different Aspen HYSYS simulations based on the section of the process, three different Aspen Energy Analyzer files were run to correlate to each simulation. The Aspen Energy Analyzer File information is displayed below, in the order of: the Dimersol Process, the ISOALKY Light Train Process, and the ISOALKY Heavy Train Process. For each Aspen Energy Analyzer file, there were 5 base cases in which the simulation recommended the heat integration applied. Once these were retrofitted in the built in retrofit mode, these all converged and the lowest cost, lowest area, and highest HI application was selected and improved from there. Below are the tables chosen from the chosen design for each process.

Starting with the Dimersol process, the utilities chosen were: air, refrigerant 1, HP Steam, Fired Heat (1000), LP Steam, and cooling water. The target values for the load in (kJ/h) and flow rate (kg/h) for these are listed below in **Table 8.2**.

Table 8.2: Utility Targets for Dimersol Aspen HYSYS Simulation.

Utility	Target Load (kJ/h)	Target Flow Rate (kg/h)
Air	1.983e+007	3966810.89
Refrigerant 1	3.469e+004	8673.45
HP Steam	1.546e+007	9079.74
Fired Heat (1000)	1.377e+006	2294.23
LP Steam	8.085e+005	368.12
Cooling Water	7.193e+005	34389.91

The utility needs for both the Dimersol process without heat integration and with heat integration are listed in **Tables 8.3** and **8.4**, respectively. Both go through the Cost Index in (Cost/s), load (kJ/h) and what % of target was obtained. As seen from the tables below, LP Steam was not needed in either the simulation with or without heat integration, this entirely depends on the design chosen so this is not

surprising. Although, with the application of heat integration, the needs for air and refrigerant 1 were eliminated. The use of HP Steam increased by a bit, seeing that the % of target increased by about 4%, however the Fired Heat (1000) decreased by a significant amount. While these are decent modifications, the amount of cooling water increased by a significant amount, however, since cooling water is easily sourced and inexpensive.

Table 8.3: Utility Needs for Dimersol Aspen HYSYS Simulation Without Heat Integration.

Utility	Cost Index (Cost/s)	Load (kJ/h)	% of Target
Air	5.338e-006	1.922e+007	96.89
Refrigerant 1	3.682e-002	4.840e+007	1.395e+005
HP Steam	1.130e-002	1.628e+007	105.3
Fired Heat (1000)	5.712e-002	4.480e+007	3516
LP Steam	0	0	0
Cooling Water	0	0	0

Table 8.4: Utility Needs for Dimersol Aspen HYSYS Simulation with Heat Integration.

Utility	Cost Index (Cost/s)	Load (kJ/h)	% of Target
Air	0	0	0
Refrigerant 1	0	0	0
HP Steam	1.174e-002	1.691e+007	109.4
Fired Heat (1000)	6.358e-004	5.386e+005	39.13
LP Steam	0	0	0
Cooling Water	1.203e-003	2.039e+007	2835

In **Tables 8.5** and **8.6** below, the cost index, area, number of shells, and load are all compared for the heat exchangers without and with heat integration, respectively. The optimal heat integration addition would minimize the amount of area, the number of shells, and the load the heat exchanger requires as it would minimize the costs. While several more heat integration units were added the total load and area do have a general trend of decreasing, however with the total amount of units the system without as many heat integration units may be preferable for many of the streams.

Table 8.5: Heat Exchangers for Dimersol Aspen HYSYS Simulation Without Heat Integration.

	Cost Index	Area (m ²)	Shells	Load (kJ/h)
Condenser@COL1	2.315e+005	949.8	2	6.425e+006
C_01@Main	7.575e+004	208.1	2	4.840e+007
Condenser@COL2	3.010e+005	1207	3	1.279e+007
Reboiler@COL1	2.290e+004	32.32	1	9.659e+006
HeatofRXN@Main	6.885e+014	625.4	2	4.840e+007
Reboiler@COL2	1.873e+004	19.83	1	6.619e+006

Table 8.6: Heat Exchangers for Dimersol Aspen HYSYS Simulation with Heat Integration.

Label	Type	Cold Stream	Hot Stream	Area (m ²)	Shells	Load (kJ/h)
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E-119	Cooler	Cooling Water	Condenser@COL1 to Off Gas	44.76	1	6.425e+006
E-121	Cooler	Cooling Water	S-3 to S-4	1.467	2	2.151e+005
E-120	Process to Process	S-2 to S-3	S-3 to S-4	6854	45	2.184e+007
E-124	Heater	Reboiler@COL1 to Boil Up	HP Steam	32.40	1	2368
E-122	Process to Process	S-2 to S-3	Condenser@COL2 to Reflux	1.704e-002	1	1.352e+007
E-112	Process to Process	S-2 to S-3	S-3 to S-4	1.081e+004	36	2.385e+006
E-125	Heater	Reboiler@COL2 to Boil Up	HP Steam	3.982	1	1.178e+007
E-115	Process to Process	S-2 to S-3	S-3 to S-4	6578	17	7.188e+005
E-117	Heater	Reboiler@COL2 to Boil Up	HP Steam	15.48	1	4.149e+006
E-123	Heater	S-2 to S-3	HP Steam	0.6499	1	7.188e+005
E-111	Heater	S-2 to S-3	Fired Heat (1000)	6.376	1	2.523e+005
E-113	Heater	S-2 to S-3	Fired Heat (1000)	-	-	2.864e+005
E-126	Cooler	Cooling Water	S-3 to S-4	21.48	1	9.599e+005
E-114	Cooler	Cooling Water	S-3 to S-4	2.139e-003	1	692.4
E-116	Process to Process	Reboiler@COL2 to Boil Up	S-3 to S-4	0.6362	1	8.415e+004
E-118	Cooler	Cooling Water	Condenser@COL2 to Reflux	43.25	1	1.279e+007

Table 8.7 below defines the target values for the cost indices and the network performance for the Dimersol process based on the simulation base case results. These are the values that will be used further down below in **Tables 8.8 - 8.11** when considering the % of Target obtained.

Table 8.7: Dimersol Target Values for the Cost Indices and Network Performance.

Heating (kJ/h)	Cooling (kJ/h)	# of Units	Total Area (m ²)	Operating Cost Index (Cost/s)	Capital Cost Index (Cost/s)	Total Cost Index (Cost/s)
1.765e+005	2.059e+007	11	1.076e+004	1.286e-002	3.569e+013	2.985e+005

Down below, **Tables 8.8 - 8.9** outline the file network cost indexes for the simulation base case, without heat integration, and with the heat integration added into the system, respectively. As seen from **Table 8.8**, the % of Target values were well over the expected. However, when looking at **Table 8.9**, many of the % of Target values have been increased to around 100%, which is more anticipated. The only % of Target that is still quite large is the cooling cost, this is expected since the simulation base case for the Dimersol process required a large amount of cooling. Although, as seen from **Table 8.4**, the majority of

these cooling costs are derived from cooling water. This is the preferred utility as again it is easily obtained and inexpensive.

Table 8.8: Dimersol Aspen Energy Analyzer File Network Cost Indexes for Simulation Base Case.

	Cost Index	% of Target
Heating (Cost/s)	6.843e-002	535.0
Cooling (Cost/s)	3.682e-002	4.953e+004
Operating (Cost/s)	0.1052	818.1
Capital (Cost)	6.885e+014	1929
Total Cost (Cost/s)	5.760e+006	1929

Table 8.9: Dimersol Aspen Energy Analyzer File Network Cost Indexes with Heat Integration.

	Cost Index	% of Target
Heating (Cost/s)	1.238e-002	96.70
Cooling (Cost/s)	1.203e-003	1618
Operating (Cost/s)	1.358e-002	105.6
Capital (Cost)	2.164e+013	60.63
Total Cost (Cost/s)	1.810e+005	60.63

Tables 8.10 - 8.11 detail the values for the heating, cooling, number of units and shells, and the total area of each heat exchanger network (HEN) for both the simulation base case and the added heat integration. As with **Tables 8.8 - 8.9** above, the % of Target values became closer to 100% with the heat integration as opposed to the simulation base case for all except the area. This is anticipated from looking at **Table 8.6**. Similar to **Tables 8.8 - 8.9** above, where the area for each heat exchanger not only seemed to increase but the amount of heat exchangers increased overall.

Table 8.10: Dimersol Aspen Energy Analyzer File Network Performance for Simulation Base Case.

	HEN	% of Target
Heating (kJ/s)	6.467e+007	366.4
Cooling (kJ/s)	6.761e+007	328.4
Number of Units	6.00	42.86
Number of Shells	11.00	18.03
Total Area (m ²)	3042	28.27

Table 8.11: Dimersol Aspen Energy Analyzer File Network Performance with Heat Integration.

	HEN	% of Target
Heating (kJ/s)	1.745e+007	98.88
Cooling (kJ/s)	2.039e+007	99.04
Number of Units	16.00	114.3

Number of Shells	111.0	182.0
Total Area (m ²)	2.441e+004	226.8

Figure 8.1 below displays the HEN of the simulation base case and **Figure 8.2** represents the HEN with the heat integration added. For both figures, the horizontal blue lines in the center of the HENs represent the streams that have the lower source temperatures than target temperatures, and the horizontal red lines in the center of the HENs represent the streams that have the higher source temperatures than target temperatures. These stream temperatures are listed in **Table 8.12**. The horizontal blue lines at the top of the figures represent the cold utilities used and the horizontal red lines at the bottom of the figures represent the hot utilities used. The vertical blue lines represent the heat exchangers that operate between the cold utilities and the hot streams, in other words the heaters. The vertical red lines represent the heat exchangers that operate between the hot utilities and the cold streams, the coolers. In **Figure 8.2**, there are also white vertical lines, these operate between the hot and cold streams and they represent the heat integration units.

Table 8.12: Dimersol Temperatures from Figures 8.1 and 8.2 for Their Respective Streams..

Stream	T ^s (°C) (source temperature)	T ^t (°C) (target temperature)
S-3 to S-4	655.1	27
Col2 to RefluxCOL2	59.7	59.5
Col1 to OffGasCOL1	51	49.9
S-2 to S-3	27.1	655.1
ReboilerCOL1 to BoilupCOL1	197.1	199.6
ReboilerCOL2 to BoilupCOL2	184	187

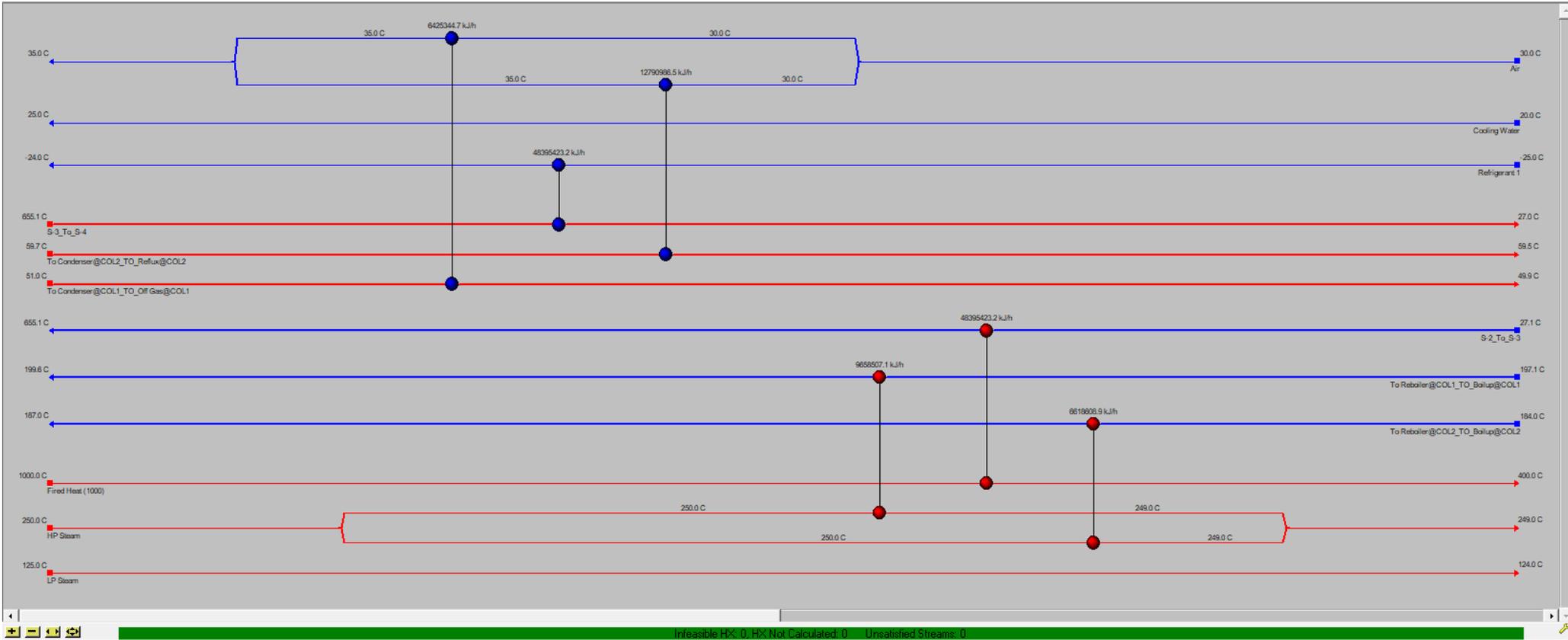


Figure 8.1: HEN diagram for Dimersol Simulation Base Case from Aspen Energy Analyzer.

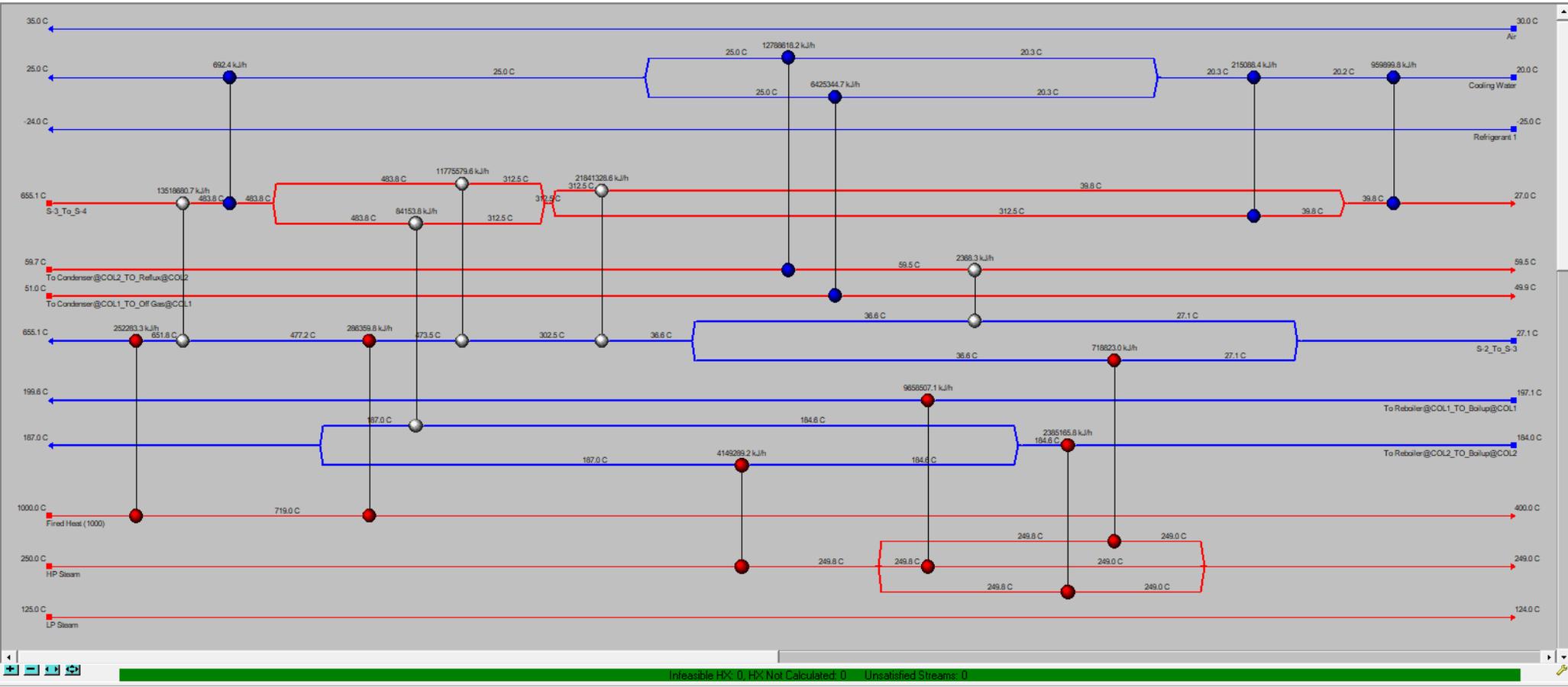


Figure 8.2: HEN diagram for Dimersol Simulation with heat integration from Aspen Energy Analyzer.

As detailed above, the following section will be explained similarly, except with context to the ISOALKY Light Aspen HYSYS Simulation. As detailed in **Table 8.13**, the utilities used in this process are: air, cooling water, refrigerant 1, MP Steam, and LP Steam with the corresponding target load (kJ/h) and target flow rates (kg/h) values that will be used for comparison in the following tables.

Table 8.13: Utility targets for ISOALKY Light Aspen HYSYS Simulation.

Utility	Target Load (kJ/h)	Target Flow Rate (kg/h)
Air	1.225e+008	24493652.04
Cooling Water	1.591e+008	7607581.28
Refrigerant 1	1.632e+006	409090.54
MP Steam	6.328e+007	31934.79
LP Steam	2.193e+008	9986.12

The utility needs are compared for both the ISOALKY Light process with and without heat integration are listed below in **Tables 8.14-8.15**. As seen from these tables below, the % of Target values with the simulation base case were more out of the anticipated range than with the heat integration. Similar to the Dimersol process, the cooling water was the highest % of Target.

Table 8.14: Utility needs for ISOALKY Light Aspen HYSYS Simulation without Heat Integration.

Utility	Cost Index (Cost/s)	Load (kJ/h)	% of Target
Air	5.160e-006	1.858e+007	15.17
Cooling Water	1.489e-002	2.523e+008	158.6
Refrigerant 1	3.704e-002	4.869e+007	2983
MP Steam	0.1597	2.614e+008	413.1
LP Steam	3.041e-002	5.762e+007	26.27

Table 8.15: Utility needs for ISOALKY Light Aspen HYSYS Simulation with Heat Integration.

Utility	Cost Index (Cost/s)	Load (kJ/h)	% of Target
Air	0	0	0
Cooling Water	1.646e-002	2.790e+008	175.3
Refrigerant 1	7.552e-004	9.927e+005	60.81
MP Steam	5.000e-002	8.181e+007	129.3
LP Steam	0.1043	1.975e+008	90.06

Tables 8.16-8.17 outline the heat exchangers and their respective cost index, area, shells, and load for the simulation base case and the system with heat integration, respectively. The general areas and number of shells do seem to decrease with the heat integration included into the system, although the loads of both are similar, although the heat integration included has more units in total.

Table 8.16: Heat Exchangers for ISOALKY Light Aspen HYSYS Simulation without Heat Integration.

	Cost Index	Area (m ²)	Shells	Load (kJ/h)
Condenser@@COL5	2.926e+005	1163	3	7.881e+006
C-02@Main_H-01	1.023e+004	0.2104	1	1.800e+004
Reboiler@COL3	3.236e+005	1325	3	2.522e+008
C-04@Main	6.524e+004	199.0	1	1.988e+007
C-03@Main	8.205e+004	277.4	1	3.599e+007
C-05@Main	5.709e+004	137.1	2	1.276e+007
C-02@Main_H-01	1.008e+004	5.378e-002	1	1.802e+007
Reboiler@COL4	3.572e+004	76.55	1	1.797e+007
Condenser@COL3	6.460e+005	2697	6	2.325e+008
Reboiler@COL5	3.491e+004	73.56	1	9.215e+006
Condenser@COL4	2.897e+005	1149	3	1.069e+007
HeatofRxn@Main	4.859e+004	127.1	1	3.964e+007
C-02@Main_H-01	2.119e+005	845.7	2	3.177e+007

Table 8.17: Heat Exchangers for ISOALKY Light Aspen HYSYS Simulation with Heat Integration.

Label	Type	Cold Stream	Hot Stream	Area (m ²)	Shells	Load (kJ/h)
E-134	Process to Process	S-48 to S-49	S-30 to iC4 Reactants	10.66	1	5.548e+005
E-124	Process to Process	iC4 Products to S-31	S-43 to S-44	187.3	2	5.114e+006
E-122	Cooler	Cooling Water	S-31 to S-32	518.1	2	2.115e+007
E-130	Heater	Reboiler@COL3 to S-30	LP Steam	4384	10	1.796e+008
E-119	Process to Process	S-48 to S-49	S-30 to iC4 Reactants	44.31	1	2.463e+006
E-121	Process to Process	iC4 Products to S-31	S-35 to S-36	394.3	1	1.419e+007
E-137	Cooler	Reboiler@COL5 to S-31	S-43 to S-44	36.46	1	9.927e+005
E-133	Process to Process	iC4 Products to S-31	S-35 to S-36	20.47	1	1.206e+006
E-135	Cooler	Cooling Water	Condenser@COL5 to S-28	75.17	1	7.881e+006
E-129	Heater	Reboiler@COL4 to S-34	MP Steam	73.95	1	9.215e+006
E-120	Process to Process	iC4 Products to S-31	Condenser@COL4 to S-26	691.3	2	1.069e+007
E-136	Cooler	Cooling Water	Condenser@COL3 to S-28	2639	6	2.325e+008
E-138	Heater	Reboiler@COL4 to S-34	LP Steam	77.57	1	1.797e+007
E-126	Process to Process	S-48 to S-49	S-31 to S-32	605.7	2	9.798e+006
E-128	Heater	Reboiler@COL3 to S-30	MP Steam	235.0	1	4.962e+007
E-132	Process to Process	S-48 to S-49	S-30 to iC4 Reactants	181.3	1	8.114e+006
E-115	Process to Process	iC4 Products to S-31	S-43 to S-44	99.80	1	3.476e+006
E-117	Heater	Reboiler@COL3 to S-30	MP Steam	241.4	1	2.298e+007
E-123	Cooler	Cooling Water	S-30 to iC4 Reactants	472.2	1	1.747e+007
E-127	Process to Process	S-48 to S-49	S-30 to iC4 Reactants	127.2	1	3.184e+006
E-125	Process to Process	iC4 Products to S-31	S-31 to S-32	60.03	1	4.491e+006
E-131	Process to Process	S-48 to S-49	S-43 to S-44	227.2	3	2.691e+006
E-116	Process to Process	S-48 to S-49	S-31 to S-32	87.10	1	4.980e+006
E-118	Process to Process	iC4 Products to S-31	S-43 to S-44	17.24	1	4.715e+005

Tables 8.18 outlines the target values that the following tables will follow when calculating the % of Target.

Table 8.18: ISOALKY Light Target Values for the Cost Indices and Network Performance.

Heating (kJ/h)	Cooling (kJ/h)	# of Units	Total Area (m ²)	Operating Cost Index (Cost/s)	Capital Cost Index (Cost/s)	Total Cost Index (Cost/s)
2.826e+008	2.832e+008	16	3.410e+004	0.1651	6.759e+006	0.2216

Tables 8.19-8.20 detail the ISOALKY Light train cost indices for both the simulation base case and the simulation with heat integration. As seen from the % of Target values, they seem to converge closer to 100% for the heating, cooling, operating, capital, and total costs. This is anticipated and a quick check that the costs of the added heat integration were helpful.

Table 8.19: ISOALKY Light Aspen Energy Analyzer File Network Cost Indexes for Simulation Base Case.

	Cost Index	% of Target
Heating (Cost/s)	0.1902	123.1
Cooling (Cost/s)	5.194e-002	486.9
Operating (Cost/s)	0.2421	146.6
Capital (Cost)	2.108e+006	31.18
Total Cost (Cost/s)	0.2597	117.2

Table 8.20: ISOALKY Light Aspen Energy Analyzer File Network Cost Indexes with Heat Integration.

	Cost Index	% of Target
Heating (Cost/s)	0.1543	99.98
Cooling (Cost/s)	1.722e-002	161.4
Operating (Cost/s)	0.1715	103.9
Capital (Cost)	3.137e+006	46.42
Total Cost (Cost/s)	0.1977	89.21

Tables 8.21-8.22 detail the network performance of the simulation base case and the simulation with heat integration comparing the values from their HENs for heating, cooling, number of units and shells, as well as the total area. Similarly as above, each of the categories get closer and closer to 100% except for the number of shells, which increase to over 100%. This is overall a good sign that the heat integration has improved the HEN, although these details will need to be explored further to determine which is best.

Table 8.21: ISOALKY Light Aspen Energy Analyzer File Network Performance for Simulation Base Case.

	HEN	% of Target
Heating (kJ/s)	3.190e+008	112.9
Cooling (kJ/s)	3.196e+008	112.9
Number of Units	13.00	59.09
Number of Shells	24.00	88.89
Total Area (m ²)	8071	23.67

Table 8.22: ISOALKY Light Aspen Energy Analyzer File Network Performance with heat integration.

	HEN	% of Target
Heating (kJ/s)	2.794e+008	98.85
Cooling (kJ/s)	2.800e+008	98.85
Number of Units	24.00	109.1
Number of Shells	44.00	163.0
Total Area (m ²)	1.151e+004	33.75

Figures 8.3 and 8.4 below show the HENs of the simulation base case and the heat integration added, respectively. As with the Dimersol process, the horizontal and vertical blue and red lines represent the same aspects of the HEN, although the stream values are different and those source and target temperatures are detailed below in **Table 8.23**. One thing to note is that there is already 1 heat integration unit included in **Figure 8.3**, the simulation base case. This is due to the simulation having a heat integration unit included before having run the Aspen Energy Analyzer file.

Table 8.23: ISOALKY Light temperatures from Figures 8.1 and 8.2 for their respective streams..

Stream	T ^s (°C) (source temperature)	T ^t (°C) (target temperature)
S-43 to S-44	89.7	-15.9
CondenserCOL4 to 26-COL4	61.1	54.8
S-31 to S-32	59.1	17.5
S-35 to S-36	55.1	38.5
CondenserCOL5 to 28-COL5	54.9	47.9
S-30 to iC4 ISOALKY Reactants	51.9	15.2
CondenserCOL3 to 8 COL3	43.1	40.3
ReboilerCOL5 to BoilupCOL5	139.7	152.5
ReboilerCOL3 to 30-COL3	85.6	125.9
ReboilerCOL4 to 34-COL4	87.6	889.7
iC4 ISOALKY Products to S-31	12.8	59.1
S-48 to S-49	-10.6	31.1

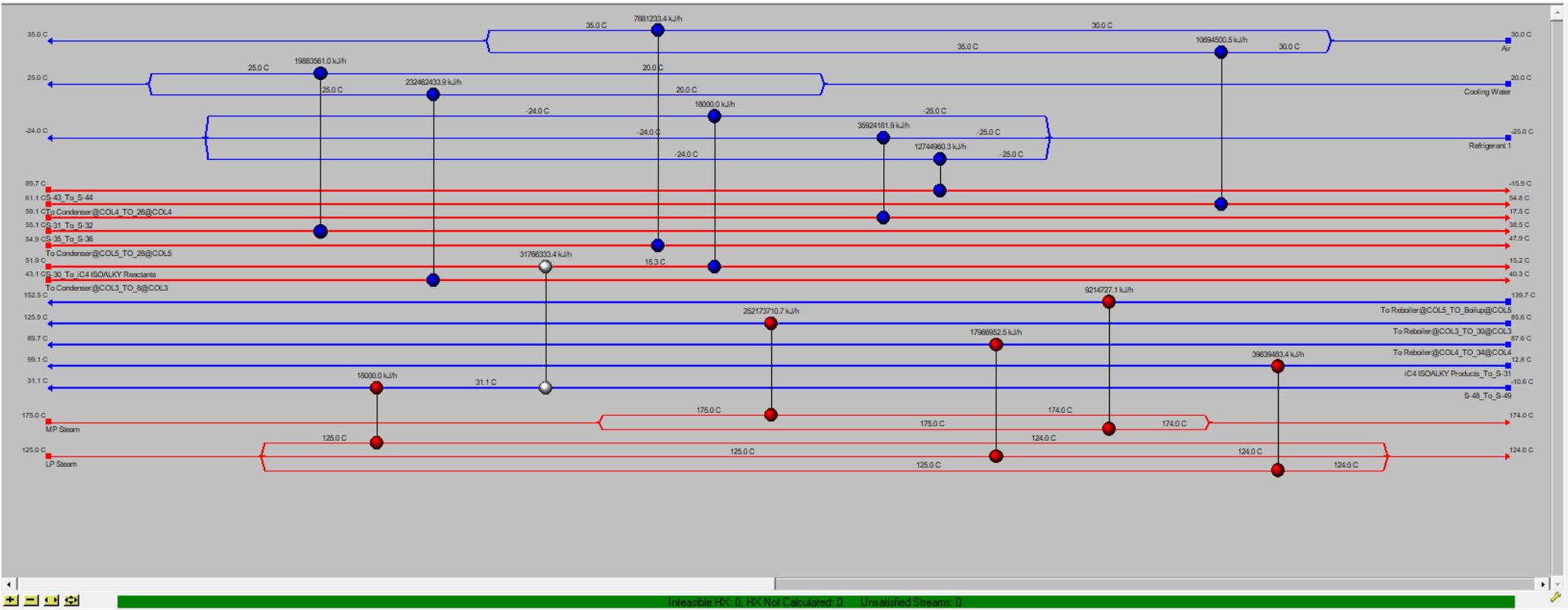


Figure 8.3: HEN diagram for ISOALKY Light train Simulation Base Case from Aspen Energy Analyzer.

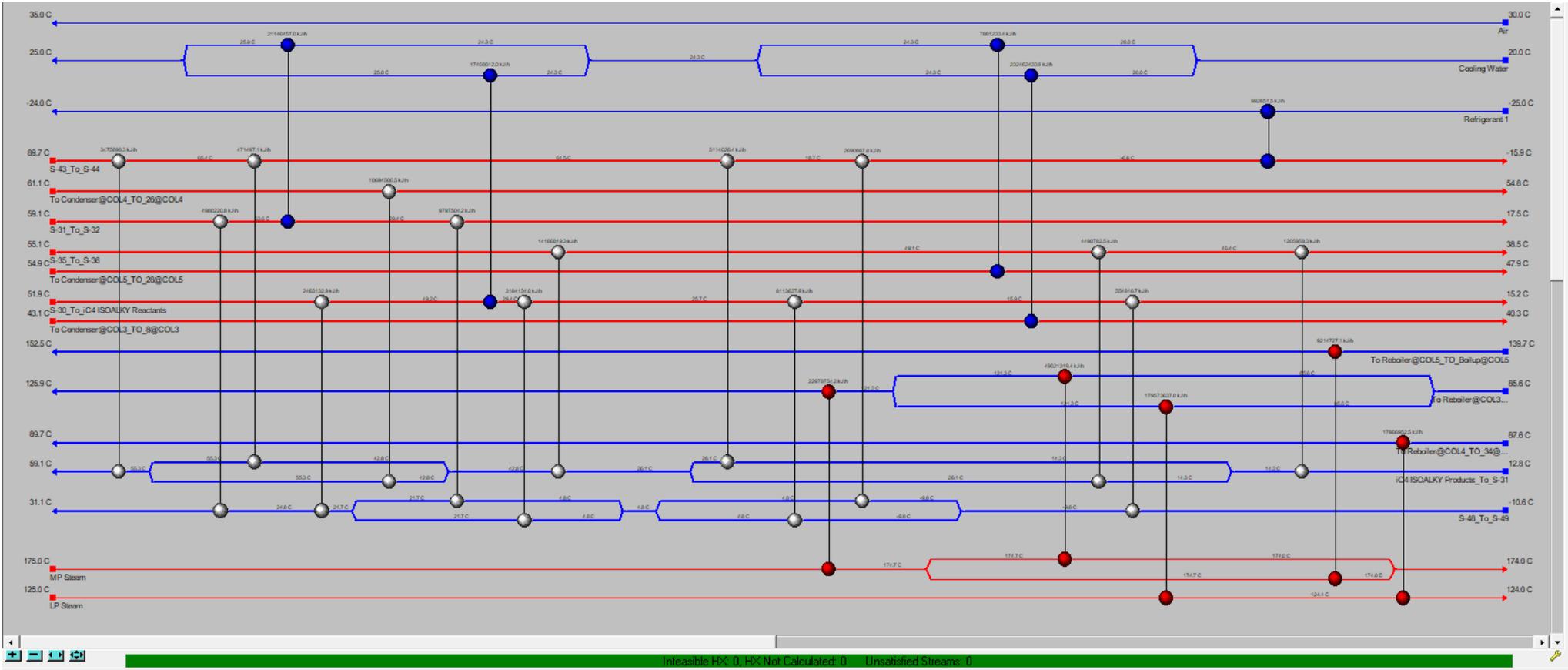


Figure 8.4: HEN diagram for ISOALKY Light train with heat integration from Aspen Energy Analyzer.

As explained with both the Dimersol and the ISOALKY Light train, the ISOALKY heavy train will be detailed similarly. In **Table 8.24** below, the utility targets for the Aspen HYSYS simulation are calculated by Aspen Energy Analyzer for the following utilities: refrigerant 1, air, HP Steam, LP Steam, MP Steam, and cooling water.

Table 8.24: Utility targets for ISOALKY Heavy Aspen HYSYS Simulation.

Utility	Target Load (kJ/h)	Target Flow Rate (kg/h)
Refrigerant 1	6.119e+006	1529867.54
Air	2.564e+008	51271628.96
HP Steam	2.184e+007	12822.30
LP Steam	1.872e+008	85223.94
MP Steam	5.419e+007	27347.48
Cooling Water	4.167e+005	19922.10

From the values in **Table 8.24** above, % of Target values were obtained for both the simulation without heat integration and with heat integration added, shown below in **Tables 8.25** and **8.26**. There are some major differences, such as the simulation base case not requiring Cooling Water as a utility, and the simulation with heat integration instead not requiring air and requiring a large amount of cooling water. The other % of Target values for the simulation with heat integration are closer to 100%, which means they are most similar to the Target values detailed in **Table 8.24**. This is expected and a large amount of cooling water is considered okay since it is easily found and inexpensive, as mentioned previously in this section.

Table 8.25: Utility needs for ISOALKY Heavy Aspen HYSYS Simulation without heat integration.

Utility	Cost Index (Cost/s)	Load (kJ/h)	% of Target
Refrigerant 1	3.343e-002	4.394e+007	718.0
Air	7.127e-005	2.566e+008	100.1
HP Steam	1.517e-002	2.184e+007	100.0
LP Steam	2.008e-002	3.806e+007	20.33
MP Steam	0.1472	2.409e+008	444.6
Cooling Water	0	0	0

Table 8.26: Utility needs for ISOALKY Heavy Aspen HYSYS Simulation with heat integration.

Utility	Cost Index (Cost/s)	Load (kJ/h)	% of Target
Refrigerant 1	1.883e-003	2.475e+006	40.45
Air	0	0	0
HP Steam	1.517e-002	2.184e+007	100.0
LP Steam	0.1016	1.925e+008	102.9
MP Steam	2.959e-002	4.841e+007	89.34
Cooling Water	1.534e-002	2.600e+008	6.240e+004

Tables 8.27 and **8.28**, respectively, go through the heat exchanger areas, number of shells, and load that is needed for each unit. Similar to in the Dimersol and the ISOALKY Light processes, the areas and

number of shells tend to decrease per unit when looking at the system with heat integration vs the simulation base case. While this is a positive, there are also a lot more units to have to compare than the few that are in the simulation base case. This is something to be considered when deciding which configuration is most optimal.

Table 8.27: Heat Exchangers for ISOALKY Heavy Aspen HYSYS Simulation without heat integration.

	Cost Index	Area (m ²)	Shells	Load (kJ/h)
Reboiler@COL7	4.128e+004	97.78	1	2.184e+007
C-06@Main	8.731e+004	303.0	1	4.394e008
Condenser@COL6	6.126e+006	2.649e+004	53	2.398e+008
Condenser@COL7	4.177e+005	1712	4	1.675e+007
HeatofRxn@Main	5.144e+004	139.0	1	3.806e+007
Reboiler@COL6	3.897e+005	1567	4	2.409e+008
H@Main	1.569e+004	11.62	1	9652

Table 8.28: Heat Exchangers for ISOALKY Heavy Aspen HYSYS Simulation with heat integration.

Label	Type	Cold Stream	Hot Stream	Area (m ²)	Shells	Load (kJ/h)
E-113	Cooler	Cooling Water	Condenser@COL6 to Reflux	1146	3	2.398e+008
E-115	Process to Process	iC5 Products to S-67	S-66 to iC5 Reactants	1806	5	9.887e+006
E-109	Cooler	Cooling Water	S-66 to iC5 Reactants	31.60	1	4.188e+006
E-116	Cooler	Refrigerant 1	S-68 to S-69	4.560	1	9652
E-114	Cooler	Cooling Water	S-66 to iC5 Reactants	257.0	1	1.598e+007
E-106	Cooler	Refrigerant 1	S-66 to iC5 Reactants	1.626	1	3.682e+005
E-108	Process to Process	iC5 Products to S-67	Condenser@COL7 to S-9	1069	3	1.625e+007
E-110	Process to Process	iC5 Products to S-67	Condenser@COL7 to S-9	9.831	1	4.921e+005
E-112	Heater	Reboiler@COL6 to BoilUp	MP Steam	769.7	2	4.841e+007
E-107	Process to Process	iC5 Products to S-67	S-66 to iC5 Reactants	461.8	3	1.142e+007
E-111	Heater	Reboiler@COL7 to S-10	MP Steam	97.78	1	2.184e+008
E-118	Heater	Reboiler@COL6 to BoilUp	LP Steam	2903	6	1.925e+008
E-117	Cooler	Refrigerant 1	S-66 to iC5	24.4	1	2.097e+006

			Reactants			
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Table 8.29 below outlines the target values for the heating, cooling, number of units, total area, operating cost index, capital cost index, and total cost index. These will be the target values that will be considered in the following tables when considering the % of target hit for each.

Table 8.29: ISOALKY Heavy Target values for the cost indexes and network performance.

Heating (kJ/h)	Cooling (kJ/h)	# of Units	Total Area (m ²)	Operating Cost Index (Cost/s)	Capital Cost Index (Cost/s)	Total Cost Index (Cost/s)
2.699e+000	2.629e+008	12	3.419e+004	0.1518	6.115e+006	0.2030

As seen down below, **Tables 8.30** and **8.31** detail the cost index and the % of target obtained for each of the values as previously mentioned. While the values do approach a % of target closer to 100% for the system with heat integration added, there are still some costs that are still quite off from this goal, especially when looking at the cooling costs.

Table 8.30: ISOALKY Heavy Aspen Energy Analyzer File Network Cost Indexes for Simulation Base Case.

	Cost Index	% of Target
Heating (Cost/s)	0.1825	124.1
Cooling (Cost/s)	3.350e-002	705.1
Operating (Cost/s)	0.2160	142.3
Capital (Cost)	7.129e+006	116.6
Total Cost (Cost/s)	0.2756	135.8

Table 8.31: ISOALKY Heavy Aspen Energy Analyzer File Network Cost Indexes with Heat Integration.

	Cost Index	% of Target
Heating (Cost/s)	0.1464	99.52
Cooling (Cost/s)	1.723e-002	363.6
Operating (Cost/s)	0.1636	107.7
Capital (Cost)	2.246e+006	36.72
Total Cost (Cost/s)	0.1824	89.85

Tables 8.32 and **8.33** below detail the values as previously mentioned along with the number of units and the number of shells in the HEN and how close they were to the target values highlighted in **Table 8.29**. Both tables show the values for the simulation base case and the simulation with heat integration added, respectively. Simply looking at the % of target values, it is apparent that the simulation with the heat integration included nears closer to 100%, which is what is anticipated.

Table 8.32: ISOALKY Heavy Aspen Energy Analyzer File Network Performance for Simulation Base Case.

	HEN	% of Target
Heating (kJ/h)	3.008e+008	114.3
Cooling (kJ/h)	3.005e+008	114.3
Number of Units	7.00	50.00
Number of Shells	65.00	382.4
Total Area (m ²)	3.032e+004	88.67

Table 8.33: ISOALKY Heavy Aspen Energy Analyzer File Network Performance with heat integration.

	HEN	% of Target
Heating (kJ/h)	2.628e+008	99.84
Cooling (kJ/h)	2.625e+008	99.83
Number of Units	13.00	92.86
Number of Shells	29.00	170.6
Total Area (m ²)	8582	25.10

Figures 8.5 and **8.6** below display the HEN of the simulation base case and the simulation with heat integration added, respectively. As described in the Dimersol section when looking at **Figures 8.1** and **8.2**, the horizontal and vertical lines are represented the same. This simulation had the least amount of heat integration units added as compared to the Dimersol and the ISOALKY Light section. The values correlating to each HENs source and target temperatures are outlined below in **Table 8.34**.

Table 8.34: ISOALKY Heavy temperatures from Figures 8.1 and 8.2 for their respective streams..

Stream	T ^s (°C) (source temperature)	T ^t (°C) (target temperature)
Condenser COL7 to 9-COL7	83.4	48.8
S-66 to iC5 ISOALKY Reactants	80	12.9
S-68 to S-69	72.5	72
Condenser COL6 to Reflux COL6	56.3	55.6
Reboiler COL7 to 10-COL7	195.6	205.6
Reboiler COL6 to Boil Up COL6	85.4	134.6
iC5 ISOALKY Products to S-67	12.8	72.5

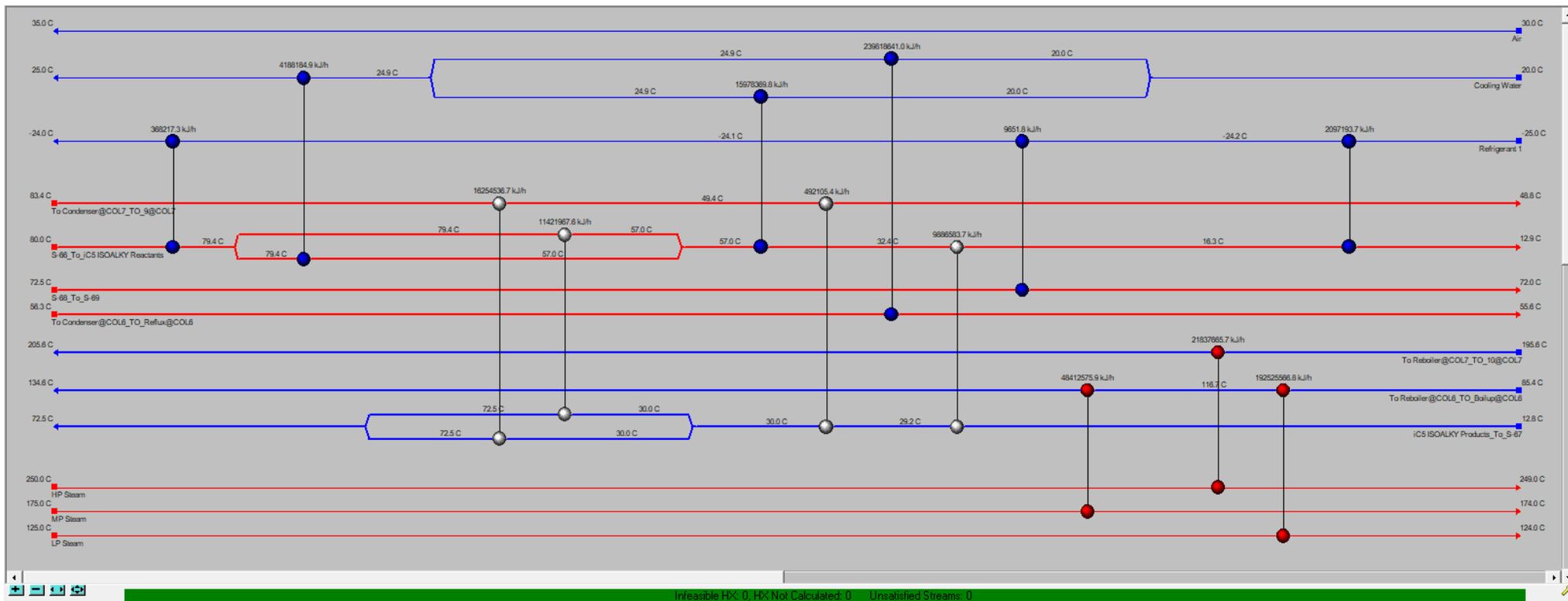


Figure 6: HEN diagram of ISOALKY Heavy train with heat integration from Aspen Energy Analyzer.

9 - Capital Investment, Operating Costs, and Profitability Analysis

Total capital investment (TCI) includes fixed capital investment (FCI) from equipment and working capital from inventory. For pricing equipment, the factored estimate method was used to obtain a FCI estimate. Prices of equipment were input into the Economics Excel spreadsheet which then estimated the additional cost of related factors including installation, piping, control, and other considerations. The initial base price of all equipment was \$10,545,000. After the spreadsheet estimated the additional costs revolving around the equipment, the intermediate FCI was calculated as \$53,146,000. More adjustments were made to factor in inflation, set to 4%, and site location, which for the west coast multiplied the FCI by 125%. The final FCI was set at \$84,100,000. The only inventory consideration was the static cost of the catalyst to be used in the ISOALKY reactors, which was listed at a base cost of \$1,000,000 with a yearly \$10,000 cost on top of the base price. The overall TCI calculated by the spreadsheet was \$85,100,000

Operating costs include variable costs contributed by the cost of reacting materials, utilities, and catalysts, profit made from byproducts, and fixed costs from operator wages and maintenance costs. To cover the variable costs, many of the chemical prices are listed in the economic premises in **Section 4**. In order to get a yearly total of all variable costs, they were all put in terms of cost per unit of product, which was then multiplied by the yearly capacity of the plant to obtain a yearly variable cost. An example calculation using the FCC Propene/Propylene cost is illustrated below. Because the process produces four total products and jet fuel was the main product, the other products, propane, butane, and motor alkylate, were treated as byproducts. Their price per unit of product was calculated in the same manner as the other materials, but was subtracted from the total to represent the profit they contributed as opposed to the other materials' costs. Jet fuel selling price was not accounted for on this tab, but instead set in the "Cash Flow" tab of the spreadsheet. The yearly \$10,000 cost of the ISOALKY catalyst was accounted for here, as well as the cost of the Dimersol catalyst. The cost of the Dimersol catalyst was listed as \$0.4/bbl in 1977 (Andrews & Bonnifay, 1977). This was adjusted for inflation using C.E. indices for 2024, 831, and 1977, 205. Thus the adjusted cost of the Dimersol catalyst was \$1.62/bbl. Because the amount of catalyst used per unit of product was not specified, it was assumed that the flow rate of the catalyst was 10% that of the FCC propane/propylene flow rate, as little catalyst is necessary to promote the reaction (Andrews & Bonnifay, 1977). **Table 9.1** lists all the variable costs and gains and the unit to unit of product ratio used to calculate the product basis price for each material. **Table 9.2** and **Table 9.3** detail the cost of utilities per piece of equipment. Note that neither table contains the consumption of cooling water, as the price per gal was so insignificant as to not contribute to the cost. The final variable cost in terms of jet fuel was \$1.61/gal of jet fuel produced. This was multiplied by yearly plant capacity to obtain a yearly variable cost of \$714,575,000/year.

Sample Variable Cost Calculation for FCC Propane/Propylene:

Known values:

FCC PP Price: \$91.84/bbl

FCC PP Flow Rate: 205 GPM

Jet Flow Rate: 442923120 gal/year

Gallon Basis Price:

$$\text{Price} = \$91.84/\text{bbl} \left(\frac{1 \text{ bbl}}{42 \text{ gal}} \right) = \$2.19/\text{gal Reactant}$$

Yearly flow of FCC PP:

$$\text{Flow Rate} = 205 \text{ GPM} \left(\frac{60 \text{ min}}{\text{hr}} \right) \left(\frac{24 \text{ hr}}{\text{day}} \right) \left(\frac{365 \text{ days}}{\text{year}} \right) = 107746989 \text{ gal Reactant / year}$$

$$\text{Reactant : Product Ratio} = \frac{107746989 \text{ gal Reactant / year}}{442923120 \text{ gal Product / year}} = 0.24 \text{ gal Reactant / gal Product}$$

Product Basis Price:

$$\text{Price} = \$2.19/\text{gal Reactant} * 0.24 \text{ gal Reactant / gal Product} = \$0.53 / \text{gal Product}$$

Table 9.1: Given Costs, Unit Ratios, and Product Basis Costs for Each Material.

Name	Type	Unit	Price (\$) per Unit	Unit Ratio	Price (\$) per Gal Product
PP Stream	Reactant	gal	2.19	0.24	0.53
C4 Mix		gal	2.43	0.25	1.10
iC4 Stream		gal	2.64	0.002	0.01
C5 Mix		gal	2.12	0.21	0.44
iC5 Stream		gal	2.67	0.21	0.56
Cooling Water	Utility	ft ³	1.42E-04	0.72	0.00
Electricity		kWh	0.42	0.80	0.34
HP Steam		klb	30.03	0.007	0.20
LP Steam		klb	27.78	0.01	0.14
ISOALKY Ionic Liquid	Catalyst	gal	10000	2.43E-02	0.23
Dimersol Catalyst		gal	0.04	2.25E-05	0.00
Sales Propane	Byproduct	gal	-2.11	0.03	-0.07
Sales Butane		gal	-2.13	0.07	-0.15

Sales Motor Alkylate		gal	-3.01	0.56	-1.70
Total Product Basis Cost (\$ per gal Product)					1.61

*Note that costs were converted from \$/bbl as in **Section 4** to \$/gal.

Table 9.2: Total Electrical Costs for Pumps, Heat Exchanger, and Compressor

Equipment - ##	Duty (Btu/hr) (via Aspen)	Duty (kW)	Energy (kWh = kW * Op. Hrs per year)	Yearly Utility Cost (\$) = kWh * \$0.42/kWh
P-01	20341	5.96	4.79E+04	2.01E+04
P-02	6258	1.83	1.47E+04	6.19E+03
P-03	13557	3.97	3.19E+04	1.34E+04
P-04	31888	9.35	7.51E+04	3.16E+04
P-05	2059	0.60	4.85E+03	2.04E+03
P-06	39984	11.7	9.42E+04	3.96E+04
P-07	1239	0.36	2.92E+03	1.23E+03
P-08	71463	20.9	1.68E+05	7.07E+04
P-09	11043	3.24	2.60E+04	1.09E+04
P-10	104782	30.7	2.47E+05	1.04E+05
P-11	8103	2.37	1.91E+04	8.02E+03
P-12	495041	145	1.17E+06	4.90E+05
P-13	629682	185	1.48E+06	6.23E+05
P-14	6203	1.82	1.46E+04	6.14E+03
P-15	7244	2.12	1.71E+04	7.17E+03
P-16	23595	6.91	5.56E+04	2.34E+04
P-17	45210	13.2	1.07E+05	4.47E+04
P-18	38417	11.3	9.05E+04	3.80E+04
P-19	521624	153	1.23E+06	5.16E+05
P-20	10474	3.07	2.47E+04	1.04E+04
P-21	13910	4.08	3.28E+04	1.38E+04
P-22	38141	11.2	8.99E+04	3.77E+04
HX-01	4.59E+07	13443	1.08E+08	4.54E+07

HX-02	3.01E+07	8829	7.10E+07	2.98E+07
HX-03	3.40E+07	9979	8.02E+07	3.37E+07
HX-04	1.88E+07	5523	4.44E+07	1.87E+07
HX-05	1.21E+07	3540	2.85E+07	1.20E+07
HX-06	4.17E+07	12206	9.81E+07	4.12E+07
C-01	5.10E+06	1495	1.20E+07	5.05E+06

Table 9.3: Total Steam Costs for Columns and Compressor

Equipment Name	Utility Type	Utility Usage (lb/hr)	Yearly Usage (klb)	Steam Cost (\$)
LPG Sep	LP Steam	96945	77945	2.17E+06
C3 Sep		18034	144995	2.07E+06
iC4 Sep Lyt		253118	2035068	4.03E+06
Hvy Sep	HP Steam	8568	68884	5.65E+07
C4 Sep Lyt		11928	95901	2.88E+06
iC5 Sep		311889	2507586	7.53E+07
Jet Splitter		28268	227278	6.83E+06
Compressor		6274	50441	1.51E+06

*Steam Cost calculated by multiplying yearly usage by \$27.78/klb for LP Steam and \$30.03/klb for HP Steam

Fixed costs were mostly assumed and are detailed in **Section 4**. To summarize, the plant assumes 5 operators, as suggested by Chevron, with a yearly wage of \$112k including benefits. The figure for yearly wage comes from the standard assumption of a \$70k wage with an added 60% to account for benefits.. This comes to \$560,000/year for operator wages. Maintenance costs were estimated to be 5% of investment, adding another \$4,205,000/year to the fixed cost total. These were the only considerations for fixed costs, so the final yearly fixed cost was \$4,765,000/year. The final step in setting up the Economics spreadsheet was to set up the “Cash Flow” tab. Income tax was assumed to be 24%, and an accounts receivable of 30 days was input. Cost of capital was set as 10%, and the capacity of the plant was assumed to be 100% throughout its operation, since it is a plant add-on rather than an entirely new plant. Annual inflation was once again set as 4%.

In determining economic feasibility for this addition project, return on investment (ROI) is a major consideration. For this plant, the ROI was calculated at a value of 273%. This is great but ultimately unrealistic and is likely related to the fact that the Economics with Macros spreadsheet tool treated total product flow rate as jet fuel despite inputting byproduct credits for motor alkylate, butane, and propane as percentages of the overall products. The ROI was calculated by the Economics Excel sheet by dividing net income by capital investment and converting this value to a percentage. By letting the macros sheet adjust the selling price to meet the target ROI of 15%, it calculated an ideal selling price of \$1.88/gal. Realistically,

this is likely a weighted average of all sales products. The payback period (PBP) was also calculated by the excel sheet and found to be 0.4 years. This is very short primarily because the capital costs consisted of new equipment only and the utilities calculated for these new pieces of equipment are relatively low. Another reason is that the plant is operating at full capacity right from the beginning, so there is no ramp up period to take into account. Looking at **Figure 9.1**, the first bar on the far left is the design period for the plan, which aligns with the timeline of this project: from Jan 2024 to May 2024. The spreadsheet only accounts in full calendar years, so the design period is accounted to take all of 2024 in this model. The next two bars represent the construction period, which the Economics Sheet with Macros anticipates to take 2 years which accounts for the years 2025-26 having a negative cash flow. Assuming the plant is able to start up in 2027, the negative cash flow from the previous years are swiftly accounted for and the plant breaks even shortly after it resumes production. Similarly, **Figure 9.2** shows projected cumulative cash flow for the lifetime of the plant. Projected cumulative takeaway earnings reach a maximum of roughly 4.6 million.

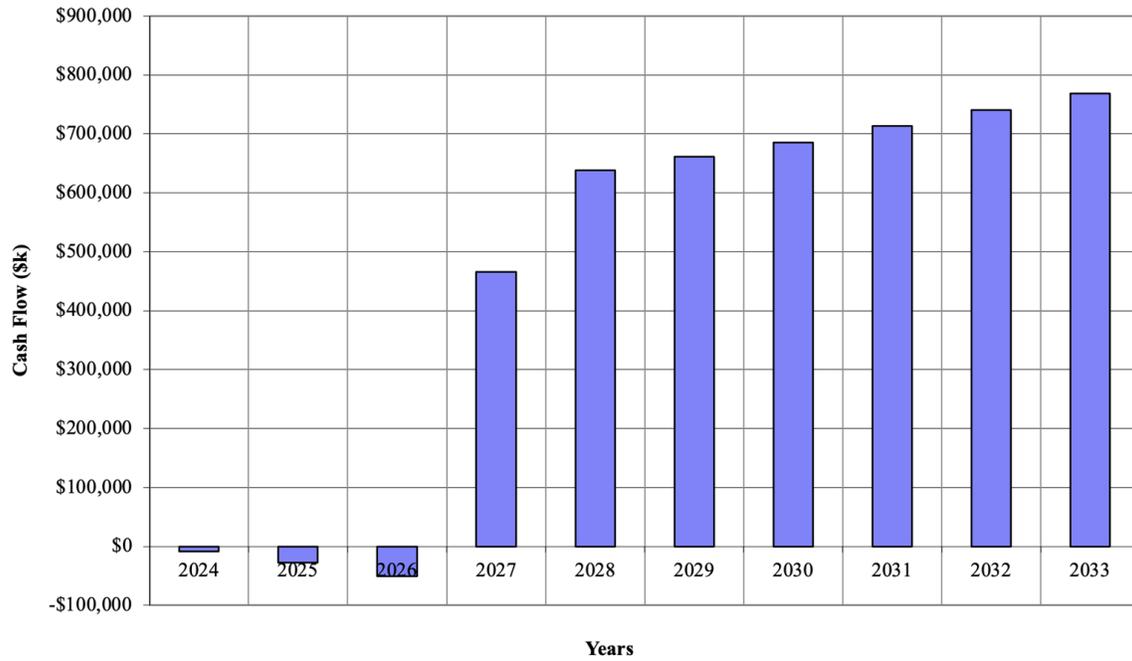


Figure 9.1: Cash Flow Chart Projected for Lifetime of the Plant

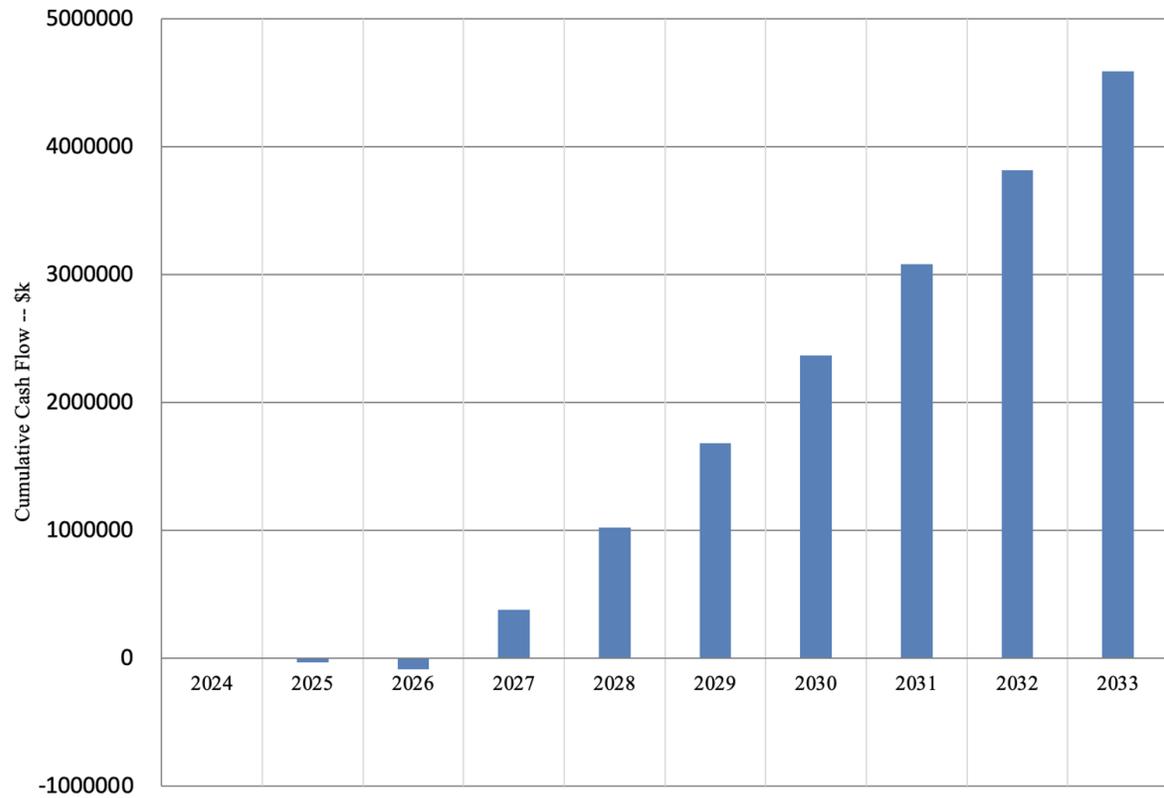


Figure 9.2: Cumulative Cash Flow Projected over the Lifetime of the Plant

The Net Present Value (NPV), or the difference between cash inflow and outflow was calculated via a user-defined function in the Excel sheet. It was found to be \$2,467,010, although compared to IRR and ROI this value was less important for the economic analysis. A hurdle rate of 15% was set in order for the process to be viable, meaning the internal rate of return (IRR) must be greater than 15% for the gains to be worth the cost. To this end, the sell price of the jet fuel was set to \$142.29/bbl, and converted to \$3.55/gal. An Excel spreadsheet tool was used to determine the IRR, as well as other economic values based on the equipment costs calculated below and via assumptions and calculations made in **Appendix H**. Ultimately the IRR, calculated via a macro in Excel with net cash flow as the input, was found to be a rather desirable 226%. This number is well above the hurdle rate set at the beginning of the project's design, however it should be noted that the estimates made throughout determining the costs of the project were conservative, and it is therefore likely the true IRR would be much lower. The spreadsheet tool does, however, enable the ability to find the minimum sell price of jet fuel in order to meet the hurdle rate. This sell price comes out to \$1.84/gal, or \$77.15 /bbl of jet fuel. Additionally, a 0% IRR is achieved when the sell price of jet fuel is at \$1.79/gal or \$75.38/bbl. **Figure 9.3** below shows a sensitivity analysis performed on the influence jet fuel's selling price has on IRR. The sale price of jet fuel was varied by $\pm 50\%$ in increments of 5% from its initial set sell price of \$3.55 per gallon. Any variability greater than 50% would cause an error in the calculation of IRR.

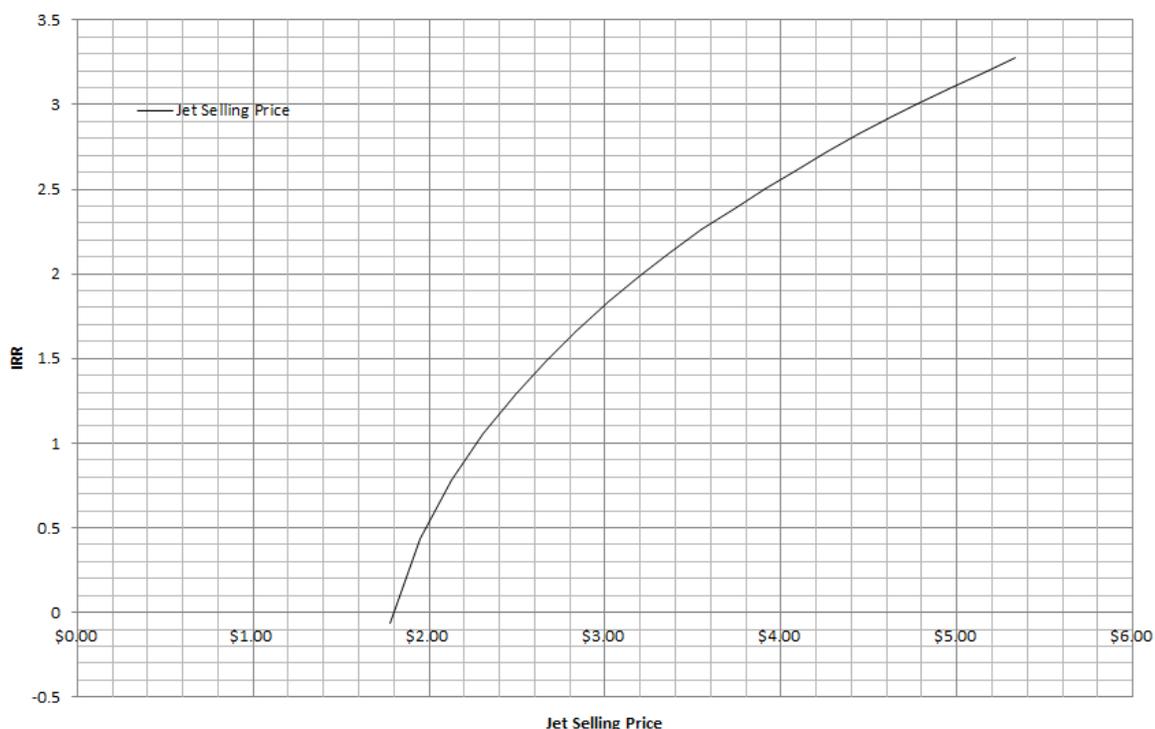


Figure 9.3: Sensitivity Analysis of Jet Fuel Selling Price on IRR

Additionally, because the motor alkylate comes from both the light and heavy ISOALKY processes, this is another major product of the process. **Figure 9.4** shows a sensitivity analysis done on the influence motor alkylate's sell price has on the IRR, keeping the initial jet sell price of \$3.55/gal. Motor alkylate sell price was varied by $\pm 100\%$ in increments of 10%.

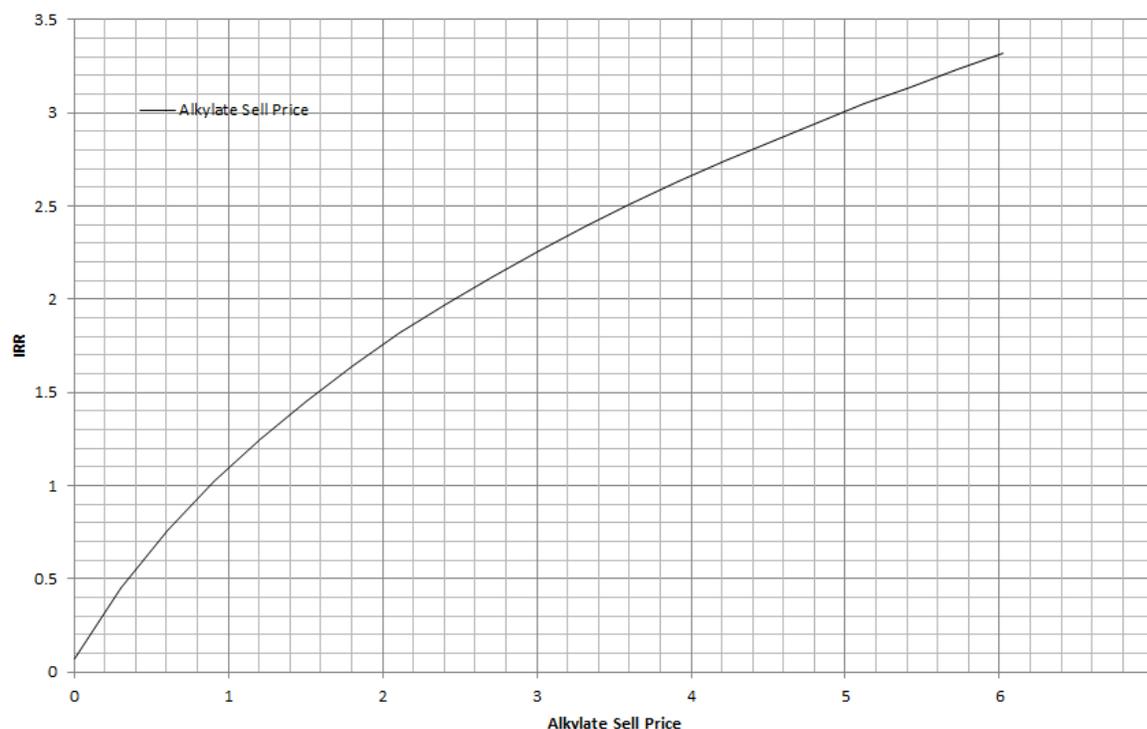


Figure 9.4: Sensitivity Analysis of Motor Alkylate Sell Price on IRR.

IRR is still positive even with motor alkylate being sold for \$0. This fact combined with the sensitivity analysis on the jet fuel sell price implies that the jet fuel is by far contributing the most to the overall profit of the plant. To draw a main conclusion from this analysis, based on the estimates of cost of equipment and materials as well as profit from the products, the plant theoretically surpasses the required 15% hurdle rate with a majority of the profit being made as a result of the jet production. Therefore, the conversion of one of the alkylation trains from motor alkylate to jet fuel production is an economically feasible opportunity. It should be noted, however, that the economic analysis has an inherent skew as a result of the tools used to calculate it, so the practical profitability is likely to be lower than that which has been calculated and documented in this report. To better understand the estimates made in calculating the costs of the plant conversion, methodology on pricing the new equipment for the plant's conversion and the final price used in the economic analysis is detailed in the following subsections.

9.1 - Pumps

Pumps were priced using Matche.com's centrifugal pump cost estimates. The required inputs include the pumps' pipe diameters, material of construction, pump type, and seal type. Since pumps of a large capacity were required in the process, these were deconstructed into several pumps in series totaling to 72 pumps. There are two different diameters used amongst the pumps: 2 in and 2.5 in. Pumps with pipe diameter of 2 in were priced at \$12,300, and pumps with 2.5 in diameter were priced at \$14,400. Then, in order to price the original amount of pumps, the six-tenths rule was applied as in the equation below.

$$\text{Adjusted Cost} = \text{Base Cost} * \left(\frac{\text{Required Size}}{\text{Base Size}} \right)^{0.6}$$

Table 9.1.1 below details the price estimates for each of the pumps, and **Table 9.1.2** shows the final summed 2024 price estimate for all of the pumps.

Table 9.1.1: Price estimates for each individual pump in 2014 USD

Pump #	Base Cost	Adjusted Cost
P-01	\$14,400.00	\$21,826.32
P-02	\$14,400.00	\$14,400.00
P-03	\$12,300.00	\$18,643.31
P-04	\$12,300.00	\$18,643.31
P-05	\$12,300.00	\$12,300.00
P-06	\$12,300.00	\$23,778.28
P-07	\$12,300.00	\$18,643.08
P-08	\$14,400.00	\$21,826.52
P-09	\$12,300.00	\$18,643.31
P-10	\$14,400.00	\$21,826.32
P-11	\$12,300.00	\$18,643.55
P-12	\$14,400.00	\$59,648.42
P-13	\$14,400.00	\$65,659.52
P-14	\$12,300.00	\$12,300.00
P-15	\$12,300.00	\$18,643.07
P-16	\$14,400.00	\$14,400.00
P-17	\$14,400.00	\$21,826.15
P-18	\$14,400.00	\$21,826.32
P-19	\$14,400.00	\$60,920.08
P-20	\$12,300.00	\$12,300.00
P-21	\$12,300.00	\$18,643.31
P-22	\$12,300.00	\$18,643.06

Table 9.1.2: Summed price estimated for 2014 and 2024 USD.

Total (2014 USD)	\$533,983.92
Total (2024 USD)	\$770,249.33

9.2 - Compressors

The compressor was priced using Matche.com's compressor cost estimates. The required inputs include the compressor's total power in *HP*, and the type of compressor being used. The material of construction is carbon steel. The single compressor was split into a set of 14 compressors in parallel and two in series. The calculated horse power of these compressors, 7 HP, was used as power input, and the

type of compressor was selected to be a rotary screw air compressor. The resulting cost estimate was a base cost of \$6,900. The price of this compressor assumes a pressure change that is half of that required by the designed compressor and a volumetric flow rate, so an adjustment was made to account for the higher pressure requirements using the equation above. Price adjustments were done on the compressor in terms of pressure change and volumetric flow rate, and the two prices were summed to obtain the final 2014 USD price, \$44,072.89, which was then adjusted to 2024 USD using the appropriate C.E. indices resulting in a final pricing of \$63,573.28

9.3 - Heat Exchangers

Heat exchangers were priced using Matche.com's heat exchanger cost estimates. Necessary inputs included the type of exchanger, total area in square feet, construction material, and internal pressure rating. Across all exchangers, type was chosen as a large shell/tube exchanger with fixed tubes, and material was chosen to be carbon steel as suggested. Due to the large areas calculated for some heat exchangers being far outside the accepted range in Matche, the cost of these exchangers was estimated as the sum of several exchangers' costs, with the area of the original exchanger divided evenly between the smaller exchangers. Exchangers were given a pressure rating above that of the internal pressure estimated using the PFD. **Table 9.3.1** details the required specifications and resulting price for each heat exchanger. **Table 9.3.2** totals the estimated cost and adjusts cost based on C.E. index. With Matche prices being estimated for 2014, the C.E. index for 2014 was found to be 576.1 (Maxwell, 2020), and the 2024 C.E. index was estimated as 831.

Table 9.3.1: Heat Exchanger Pricing in 2014 USD

Name	Area (sqft)	Divided Area : # HXs	Internal Pressure Rating (psi)	Individual Price (2014 USD)	Total Price (2014 USD)
HX-01	6700	6700 : 1	300	\$134,400	\$134,400.00
HX-02	24338	6085 : 4	300	\$130,100	\$520,400.00
HX-03	9525	9525 : 1	300	\$151,300	\$151,300.00
HX-04	19760	4090 : 4	150	\$105,500	\$422,000.00
HX-05	20081	5020 : 4	300	\$122,000	\$488,000.00
HX-06	8349	8349 : 1	300	\$144,800	\$144,800.00

Table 9.3.2: Total Price of all Heat Exchangers

Total (2014 USD)	\$1,860,900.00
Total (2024 USD)	\$2,684,269.92

9.4 - Flash Drums

Flash Drum price was estimated using Matche.com's vessel cost estimates. Using the given residence time of five minutes and a volumetric flow rate of 2613 GPM, a volume of 13065 gal was calculated for the tank and used as input in Matche, returning a 2014 cost estimate of \$46,800.00. This was adjusted by multiplying the price by the ratio of C.E. indices for 2024 (831) to 2014 (576.1), resulting in a 2024 cost estimate of \$67,507.03.

9.5 - Filters, Dryers, and Chlorine Absorbers

As mentioned in **Section 7.5.1**, sizing of the filters was determined based on the inlet flow rate and **Figure 7.5.1.1**. From this, an area was obtained and pricing could be determined from the Matche Cost Reference website. The pricing is listed in **Table 9.5.1** in 2008 USD. This price was later converted to 2024 USD using a C.E. index for 2014 of 576.1 and an assumed C.E. index for April 2024 of 831. The individual filter pricing is listed in **Table 9.5.1** and the cumulative cost is listed in **Table 9.5.2**.

Table 9.5.1: Filter & Dryer Pricing in 2014 USD

Equipment Name	Area (ft^2)	Price (2014 USD)
Dryer-1	40.4	\$6400.00
Dryer-2	37.1	\$6000.00
Wash-NaOH	15.0	\$3000.00
Wash-H ₂ O	12.6	\$2600.00

Table 9.5.2: Total Price of all Filters & Dryers

Total (2014 USD)	\$18,000.00
Total (2024 USD)	\$25,964.24

The chlorine absorber columns are priced in two parts. As mentioned in **Section 7.5.2**, the absorbent used was molecular sieves. The cost for volume of absorbents required was obtained from the Cost Formulas Excel spreadsheet provided on the CHEN 4530 Canvas page. This spreadsheet has a built in capability to input C.E. index, as such it adjusts pricing to the current year automatically. For the vessel, the same volume was used and input into the Matche Cost Reference website, which output a cost in 2014 USD. The individual chlorine absorber pricing is listed in **Table 9.5.3** as well as the cumulative cost of all required equipment in **Table 9.5.4**.

Table 9.5.3: Chlorine Absorber Pricing

Equipment Name	Volume (ft^2)	Absorbent Price (2024 USD)	Vessel Price (2014 USD)
CL-1	59.0	\$7,466.33	\$4,600.00
CL-2	44.0	\$5,568.11	\$3,900.00
CL-3	192	\$24,297.22	\$9,100.00
CL-4	83.0	\$10,503.48	\$5,600.00

Table 9.5.4: Total Price of all Chlorine Absorbers & Vessels

Total (2024 USD)	\$81,300.16
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9.6 - Distillation Columns

The equation below was used to price the columns. This equation was provided in the design report document (Design Report v3b, 2023) where the height of the column in meters is the input. In **Table 9.6.1** the results of these calculations are collected. Likewise, in **Table 9.6.2**, the sum of these prices are presented and converted into 2024 USD assuming a C.E. index for April 2024 of 831, given the C.E. index for April

2023 was found to be 803.3 (Maxwell, 2020). The C.E. index for 2008 was found to be 575.4 (Maxwell, 2020).

$$\text{Cost per Unit (2008 USD)} = [\$600,000 + 17.72 * m^{2.392}] * 1.41$$

Table 9.6.1: Column Pricing in 2008 USD

Column Name	Height (m)	Price (2008 USD)
LPG Sep	38.56	\$1,001,470.20
Heavy Sep	16.00	\$864,970.02
C3 Sep	42.67	\$1,044,145.81
iC4 Sep Lyt	59.74	\$1,289,121.83
C4 Sep Lyt	23.04	\$891,380.65
iC5 Sep	71.32	\$1,523,034.74
Jet Splitter	30.94	\$937,814.95

Table 9.6.2: Total Price of all Distillation Columns

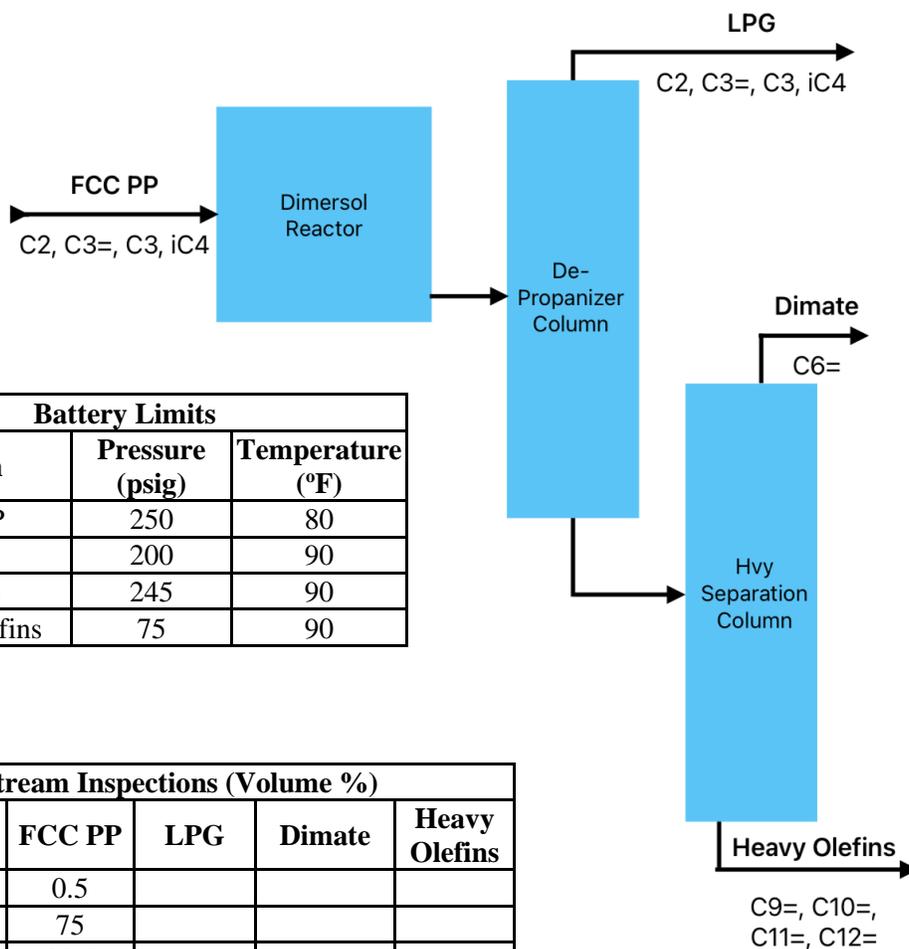
Total (2008 USD)	\$7,551,938.19
Total (2024 USD)	\$10,906,605.20

9.7 - Reactors

The Dimersol reactor was priced using a method very similar to the flash drum. Using the given residence time of five minutes and a volumetric flow rate of 205 GPM, a volume of 1025 gal was calculated and input into Matche. Because the reactor's internals were considered "black box", the reactor was priced as a simple mixer constructed from carbon steel with an internal pressure rating of 300 psi. This returned a 2014 cost estimate of \$273,800.00, which was adjusted into 2024 value using the C.E. index for 2024, 831, and the C.E. index for 2014, 576.1. The final price was found to be \$394,944.97.

10 - Homework Problem

(50 pts) You have been tasked by Chevron to simulate the Dimersol Process in HYSYS, see flow diagram below. From the information gained by simulating the process, equipment will be designed. Pieces of equipment that will need to be designed include the reactor, heat exchangers, columns and pumps. Given the volume of feed in barrels per day, you will need to create a material balance around the reactor and determine the heat of reaction. Once your material and energy balances are complete you will simulate the reactor and separation train in Aspen HYSYS to determine the distribution of products. Finally using the simulation you will design the desired pieces of equipment.



Battery Limits		
Stream	Pressure (psig)	Temperature (°F)
FCC PP	250	80
LPG	200	90
Dimate	245	90
Heavy Olefins	75	90

Stream Inspections (Volume %)				
Component	FCC PP	LPG	Dimate	Heavy Olefins
C2	0.5			
C3=	75			
C3	23.5			
iC4	1			
C6=	—	0	99.99	
C9=	—			
C10=	—			
C11=	—			
C12=	—			
Flow (BPD)	7000			

Dimersol Product Distribution by Mass % (C3= → Products)	
C6=	92
C9=	6.5
C10=	0.5
C11=	0.5
C12=	0.5

Assumptions:

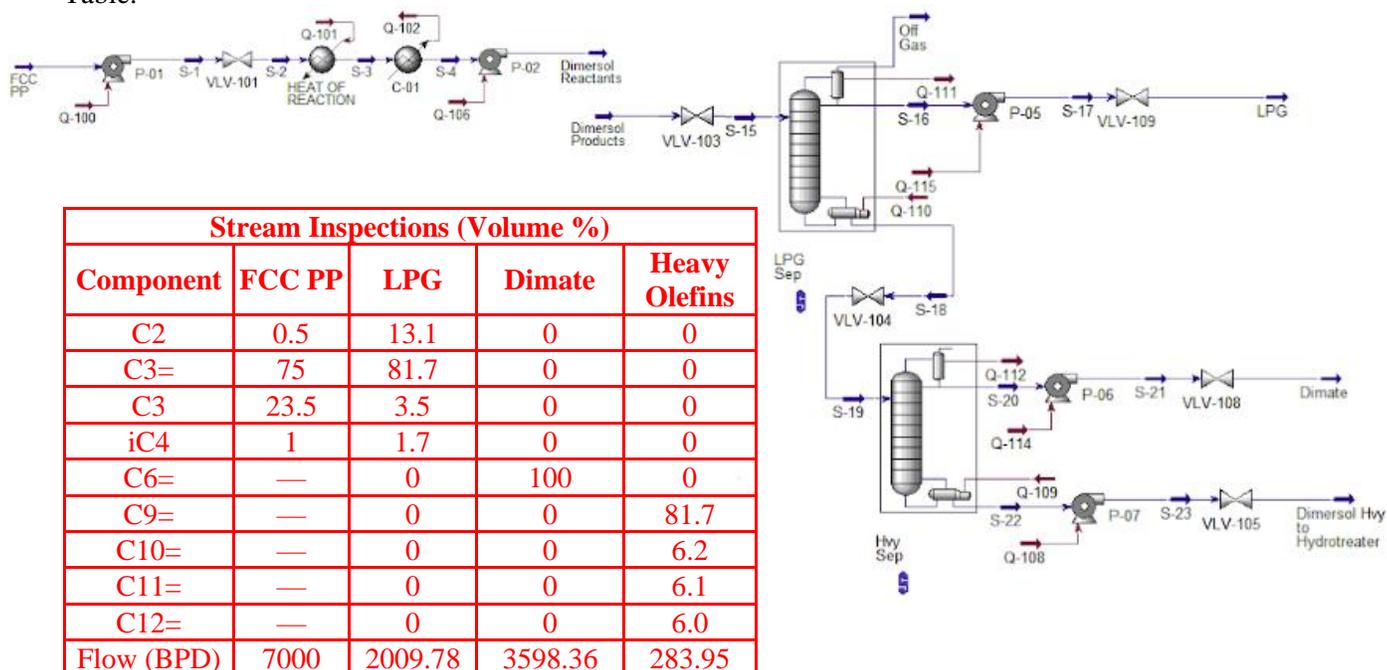
- Dimersol reactor operates at 300 psig and 100°F, heat of reaction is -113.8 kJ/mol, the amount of propane consumed is equal to the amount produced by mass, the reactor has a 5 minute residence time and 95% conversion of propene by mass.
- Dimersol Process will be modeled as a black box reactor. The reactants will be heated to model heat of reaction and cooled to emulate the actual process using a CSTR. This stream will end as the Dimersol Reactants Stream and a new Dimersol Products Stream will be added using the mass balances.

(5 pts) Part 1: Create a table for the material balances around the reactor and determine heat flow from the heat of reaction.

Dimersol Reactor						
In	Flow Rate (GPM)	Flow Rate (lbs/hr)	Flow Rate (mol/min)	Out	Flow Rates (lbs/hr)	Flow Rates (mol/min)
Propylene	153.14	40153.31	7087.99	Propylene	2007.7	354.40
Propane	47.98	12177.32	2159.10	Propane	12177.3	2159.10
Isobutane	2.04	574.06	74.74	Isohexene	35094.0	6194.90
Ethane	1.02	183.60	46.21	Nonene	2479.5	437.68
				Heavier	572.2	101.00
				Isobutane	574.06	74.74
				Ethane	183.60	46.21
Sum	204.18	53088.29	9368.04		53088.29	9368.04

Heat of Reaction: Approx. -806613 kJ/min

(25 pts) Part 2: Take a screenshot of your completed HYSYS flowsheet and fill in the Stream Inspections Table.



(20 pts) Part 3: Design the reactor giving the total volume required for the unit. For the columns, please report the reflux ratio, height from tangent to tangent, the diameter and the number of stages. When designing the heat exchanger please report the required heat exchange area, U of the unit, configuration and material. Reporting the pump design you should include the capacity, head required and NPSH_A.

Reactor Specs:

- CSTR
 - Volume: 1025 gal

Column Specs:

- LPG Column
 - Reflux: 1.5, H: 126.5 ft, D: 10 ft, #Stages: 55
- Dimate Column
 - Reflux: 2.0, H: 52.5 ft, D: 8.3 ft, #Stages: 35

HX Specs:

- Cooler 1
 - Area: 6700 ft², U: 20 Btu/(hr*°F*ft²), Passes (s:t): 1:2, Material: Carbon Steel

Pump Specs:

- Pump 1
 - Capacity: 207.86 GPM, Head: 481.3 ft, NPSH_A: 1432.5 ft
- Pump 2
 - Capacity: 207.86 GPM, Head: 275.16 ft, NPSH_A: 566.5 ft
- Pump 3
 - Capacity: 54.71 GPM, Head: 330.45 ft, NPSH_A: 6.53 ft
- Pump 4
 - Capacity: 110.54 GPM, Head: 1031.7 ft, NPSH_A: 92.58 ft
- Pump 5
 - Capacity: 10.28 GPM, Head: 473.29 ft, NPSH_A: 5.21 ft

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<https://www.fishersci.com/store/msds?partNumber=AC610361000&productDescription=N-HEPTANE+ANHYD&vendorId=VN00033901&countryCode=US&language=en>

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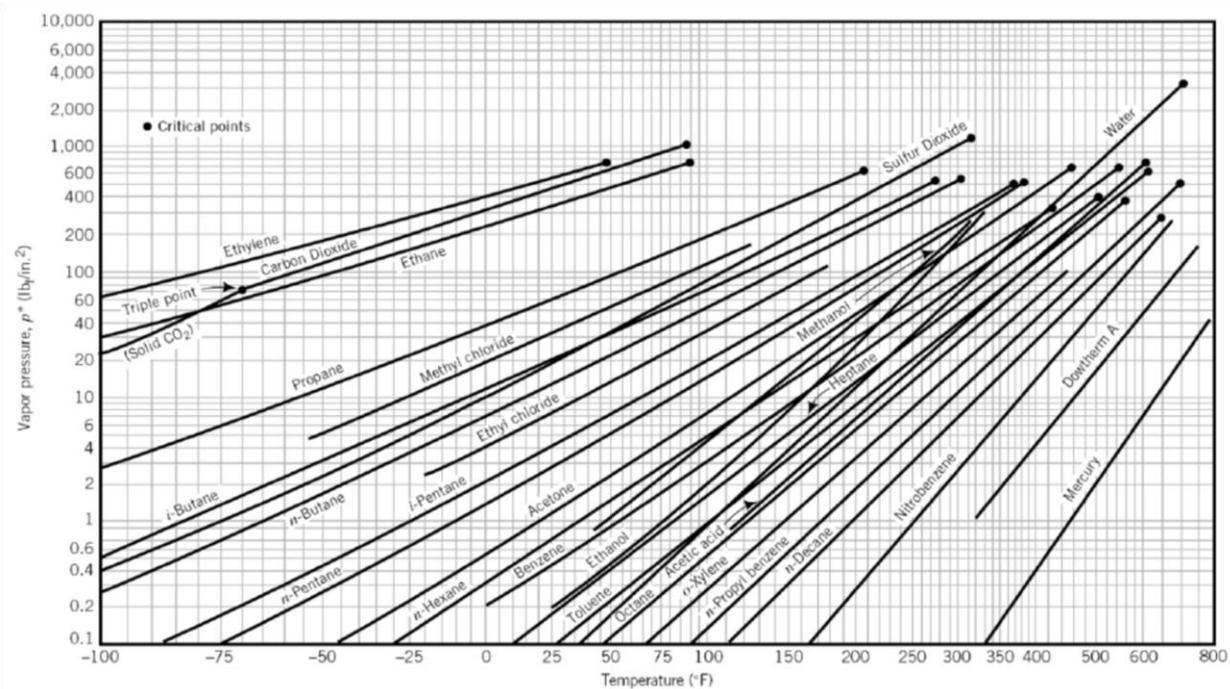
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Appendices

Appendix A : Cox Chart



Appendix B : PDF Links to SDS

Chemical	Link
Ethane (C2)	https://www.airgas.com/msds/001024.pdf
Propane (C3)	https://www.airgas.com/msds/001045.pdf
Propylene (C3=)	https://www.airgas.com/msds/001046.pdf
Butane (C4)	https://www.airgas.com/msds/001007.pdf
Butene (C4=)	https://www.airgas.com/msds/001009.pdf
Isobutane (iC4)	https://www.airgas.com/msds/001030.pdf
Pentane (C5)	https://www.airgas.com/msds/001133.pdf
Pentene (C5=)	https://www.airgas.com/msds/001119.pdf
Isopentane (iC5)	https://amp.generalair.com/MsdsDocs/PA46122S.pdf
Cyclopentane (CC5)	https://www.airgas.com/msds/001124.pdf
Hexane (C6)	https://beta-static.fishersci.com/content/dam/fishersci/en_US/documents/programs/education/regulatory-documents/sds/chemicals/chemicals-h/S25352A.pdf
Isohexane (iC6)	https://www.fishersci.com/store/msds?partNumber=AC141021000&countryCode=US&language=en
Heptane (C7)	https://www.fishersci.com/store/msds?partNumber=AC610361000&productDescription=N-HEPTANE+ANHYD&vendorId=VN00033901&countryCode=US&language=en
Octane (C8)	https://www.fishersci.com/store/msds?partNumber=AC396901000&productDescription=N-OCTANE&vendorId=VN00032119&countryCode=US&language=en
Nonene (C9)	https://www.agilent.com/cs/library/msds/WRK-100N_NAEnglish.pdf
Decane (C10)	https://www.fishersci.com/store/msds?partNumber=O2128500&productDescription=DECANE+CERT+500ML&vendorId=VN00033897&countryCode=US&language=en
Undecane (C11)	https://www.fishersci.com/msdsproxy?productName=AC140660100&productDescription=N-UNDECANE,+99%25+10LT&catNo=AC140660100&vendorId=VN00032119&storeId=10652
Dodecane (C12)	https://www.fishersci.com/msdsproxy?productName=O2666500&product
Water (H2O)	https://www.sigmaldrich.com/US/en/sds/sigma/w4502?userType=undefined
Caustic (NaOH)	https://fscimage.fishersci.com/msds/89984.htm

Appendix C : Material Balance Spreadsheet

All material balances are detailed in the following Google Sheets spreadsheet. [Mass Balances and Heat of Reactions](#)

Reaction yields from the reactor provided by Chevron are detailed in the following Excel spreadsheet. [Alkylate to Jet Conceptual Yield for CU.xlsx](#)

Appendix D : Refinery Table Spreadsheet

All closures concerning mass balances around reactors and stream purity information are detailed in the following Excel spreadsheet.

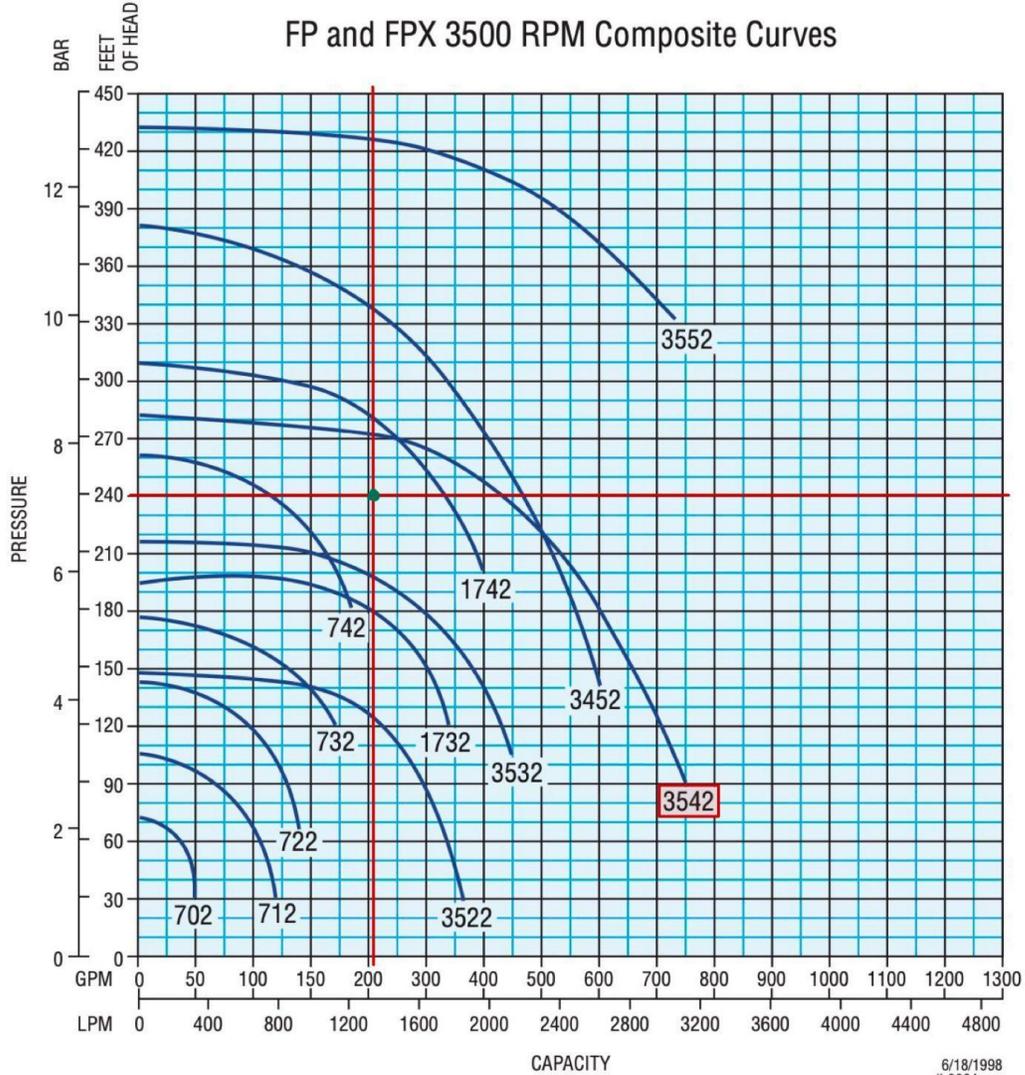
[Refinery Table.xlsx](#)

Appendix E : Pump Curves



P-01

FP/FPX Performance Curves Models: 3500 RPM (Composite)



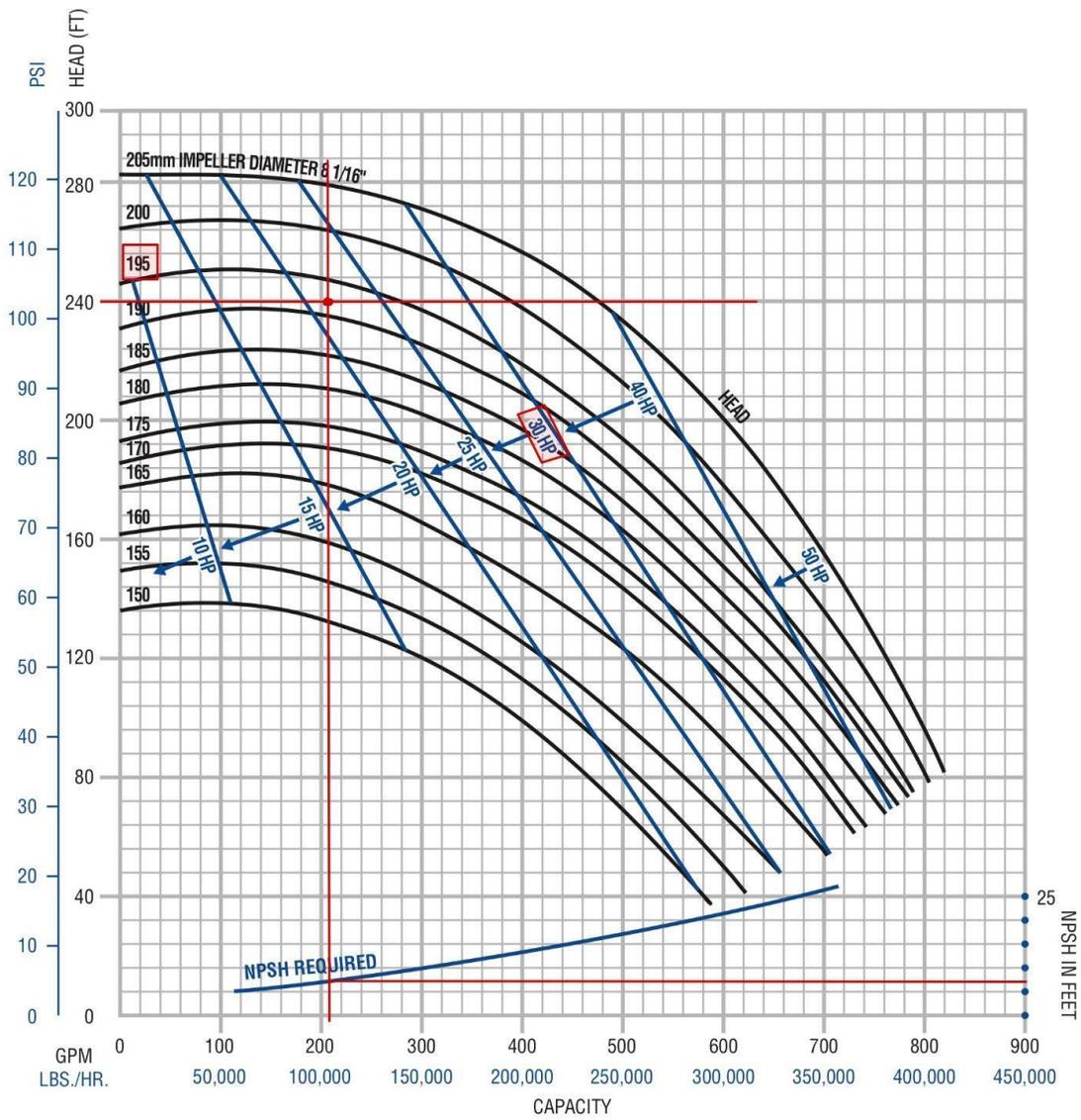
6/18/1998
il-0364.eps
RD 2/08

Performance curve based on tests using 70°F water and 0 psig inlet pressure. A tolerance of ± 5% applies to all figures. Actual performance may vary by application product. Please contact Fristam for different conditions.

P-01



FP/FPX/FPR Performance Curves Model: 3542 (3500 RPM, Inlet 3", Outlet 2.5")

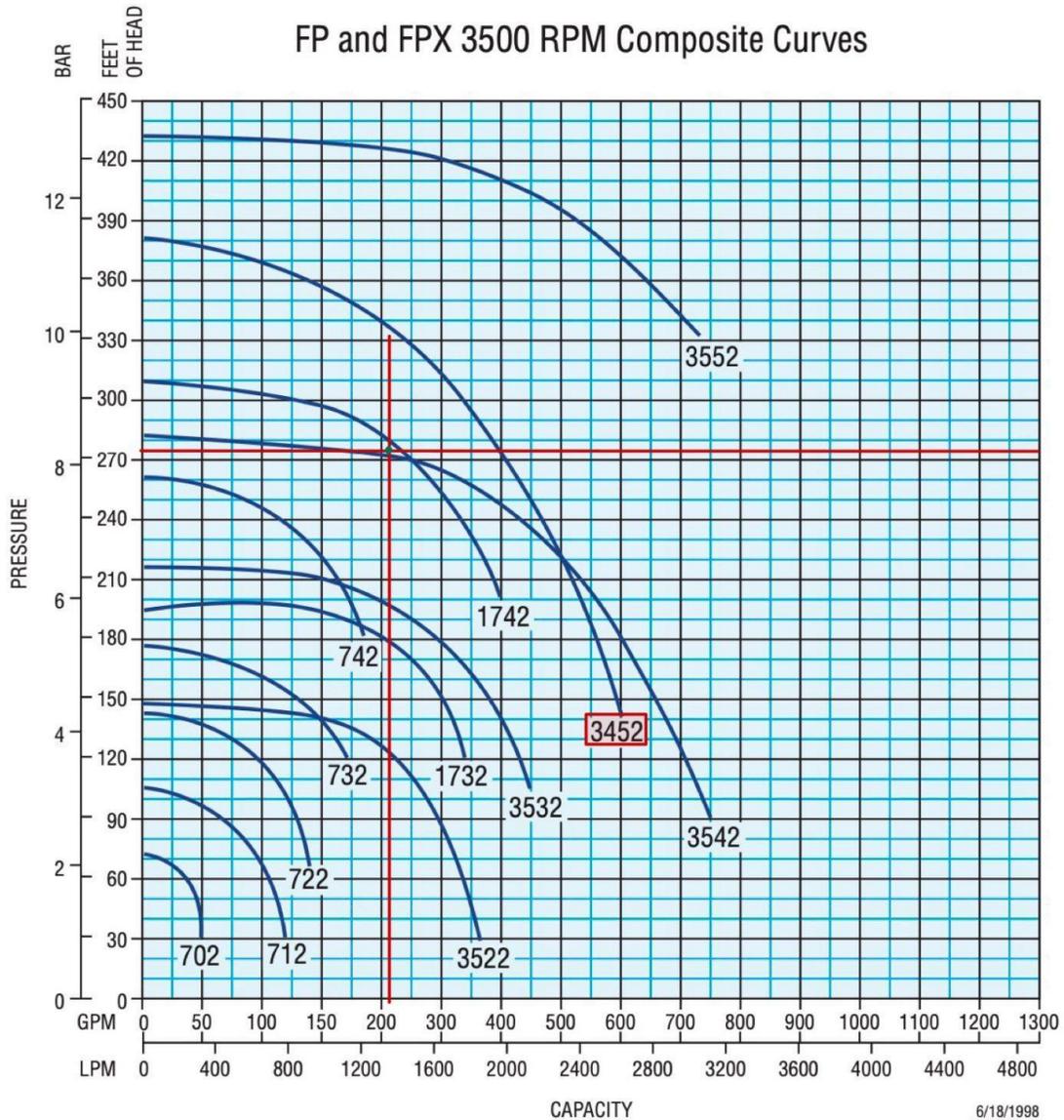


Performance curve based on tests using 70°F water and 0 psig inlet pressure. A tolerance of ± 5% applies to all figures. Actual performance may vary by application product. Please contact Fristam for different conditions.

P-02



FP/FPX Performance Curves Models: 3500 RPM (Composite)



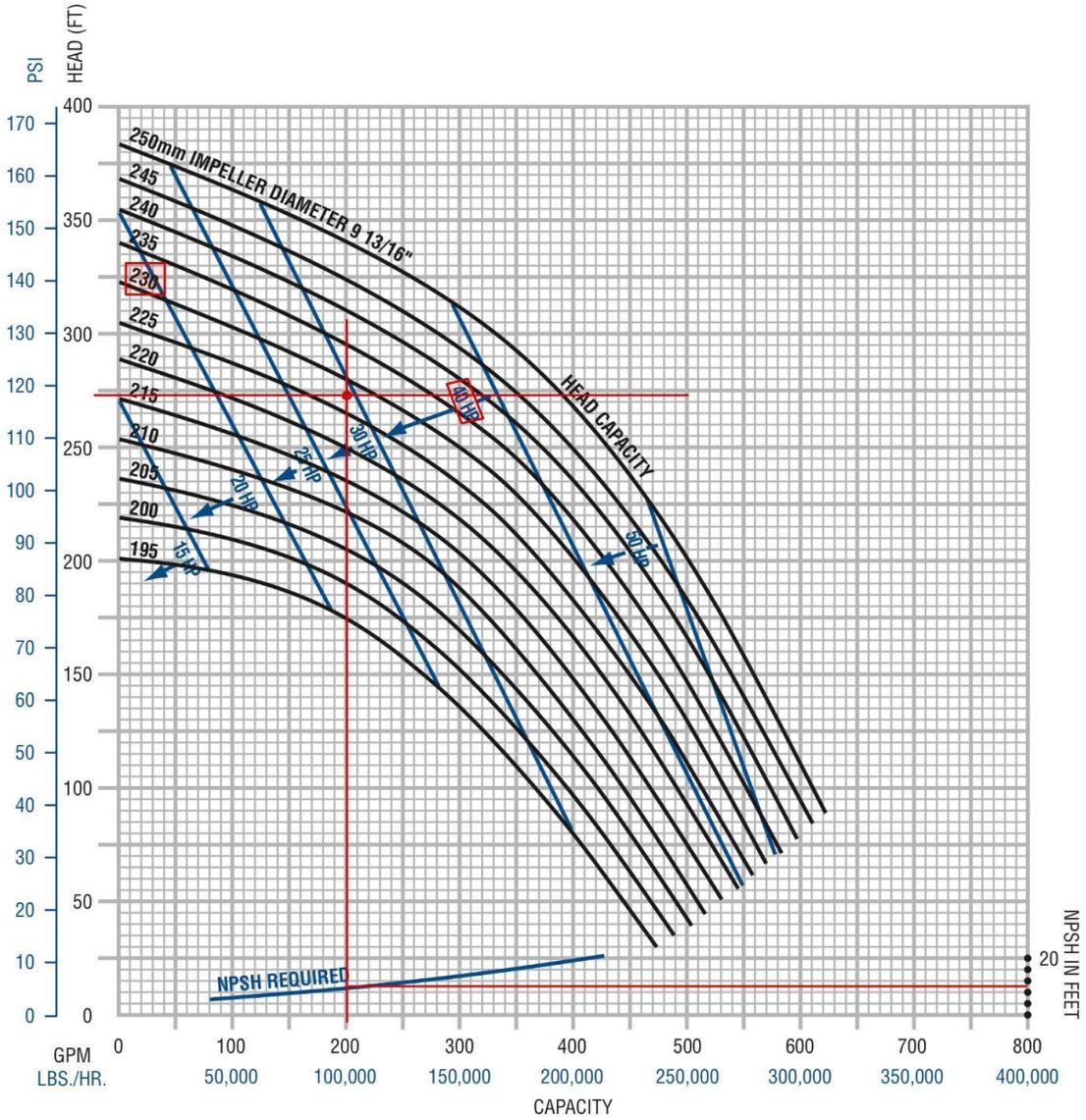
6/18/1998
il-0364.eps
RD 2/08

Performance curve based on tests using 70°F water and 0 psig inlet pressure. A tolerance of ± 5% applies to all figures. Actual performance may vary by application product. Please contact Fristam for different conditions.

P-02



FP/FPX/FPR Performance Curves Model: 3452 (3500 RPM, Inlet 3", Outlet 2")

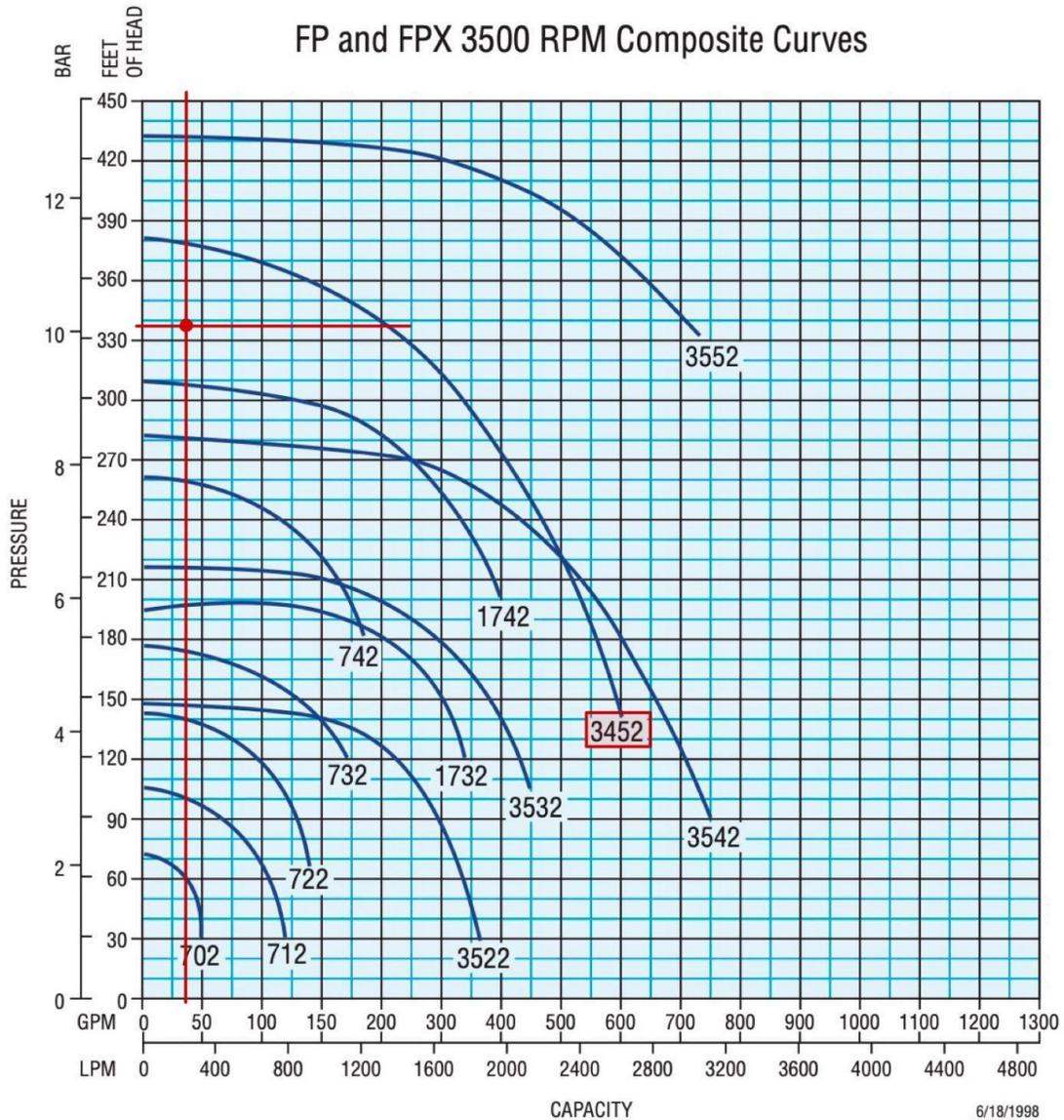


Performance curve based on tests using 70°F water and 0 psig inlet pressure. A tolerance of ± 5% applies to all figures. Actual performance may vary by application product. Please contact Fristam for different conditions.

P-03



FP/FPX Performance Curves Models: 3500 RPM (Composite)



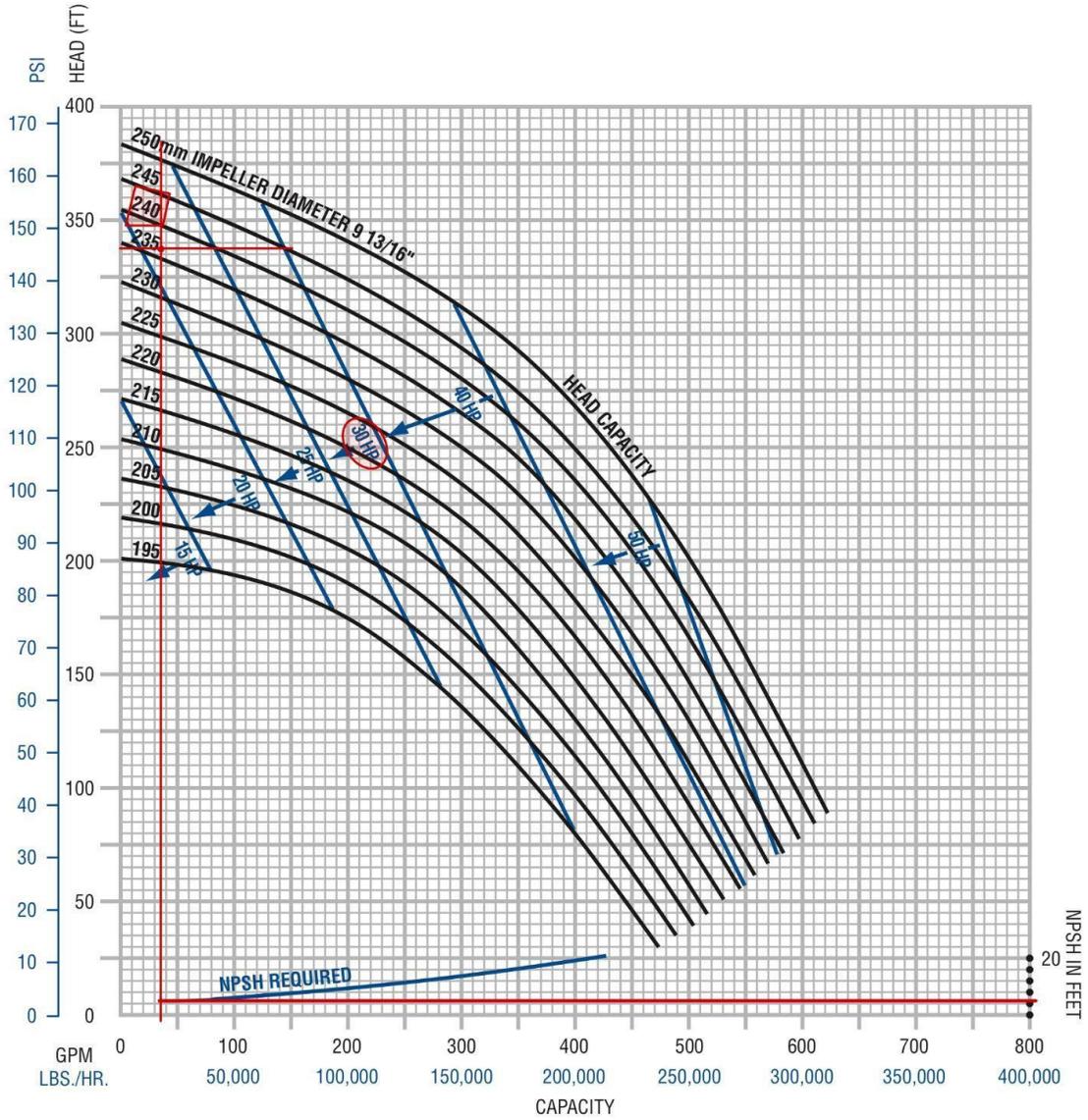
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RD 2/08

Performance curve based on tests using 70°F water and 0 psig inlet pressure. A tolerance of ± 5% applies to all figures. Actual performance may vary by application product. Please contact Fristam for different conditions.

P - 03



FP/FPX/FPR Performance Curves Model: 3452 (3500 RPM, Inlet 3", Outlet 2")

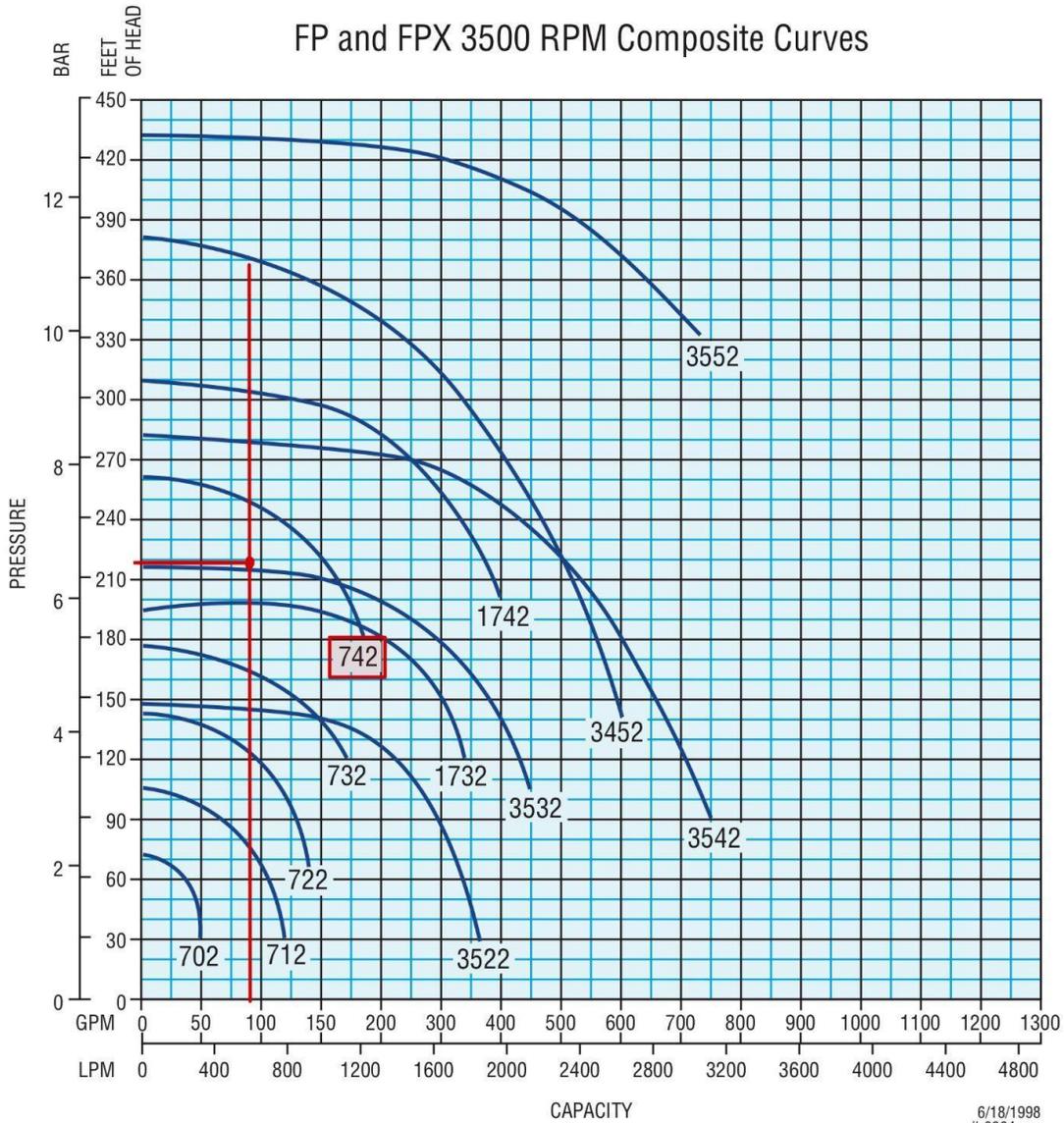


Performance curve based on tests using 70°F water and 0 psig inlet pressure. A tolerance of ± 5% applies to all figures. Actual performance may vary by application product. Please contact Fristam for different conditions.

P-04



**FP/FPX Performance Curves
Models: 3500 RPM (Composite)**



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RD 2/08

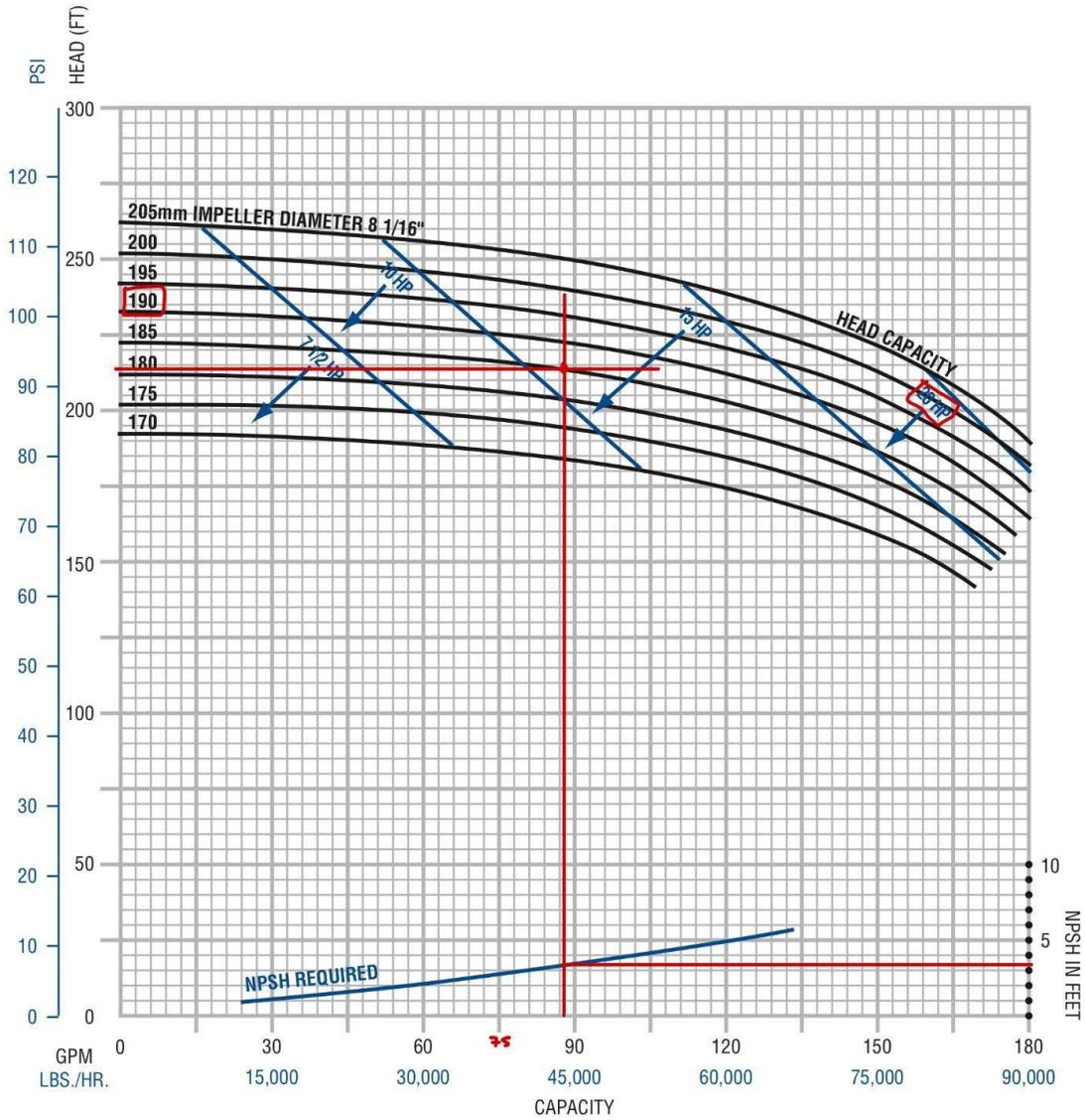
Performance curve based on tests using 70°F water and 0 psig inlet pressure. A tolerance of ± 5% applies to all figures. Actual performance may vary by application product. Please contact Fristam for different conditions.

P-04



FP/FPX Performance Curves Model: 742 (3500 RPM, Inlet 2.5", Outlet 2")

FPR model 742 covers the range of both the FP/FPX 732 and 742

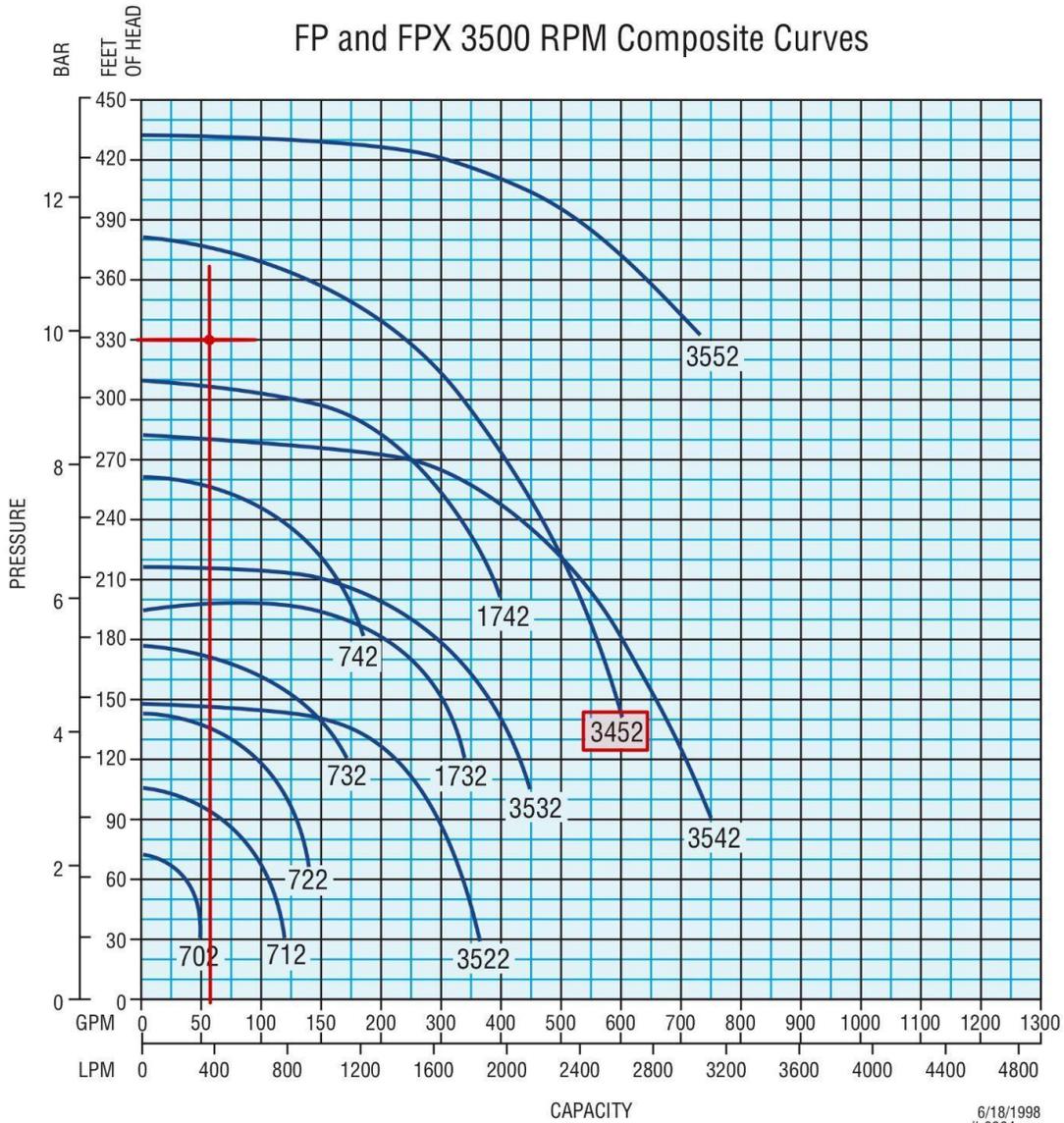


Performance curve based on tests using 70°F water and 0 psig inlet pressure. A tolerance of ± 5% applies to all figures. Actual performance may vary by application product. Please contact Fristam for different conditions.

P-05



**FP/FPX Performance Curves
Models: 3500 RPM (Composite)**

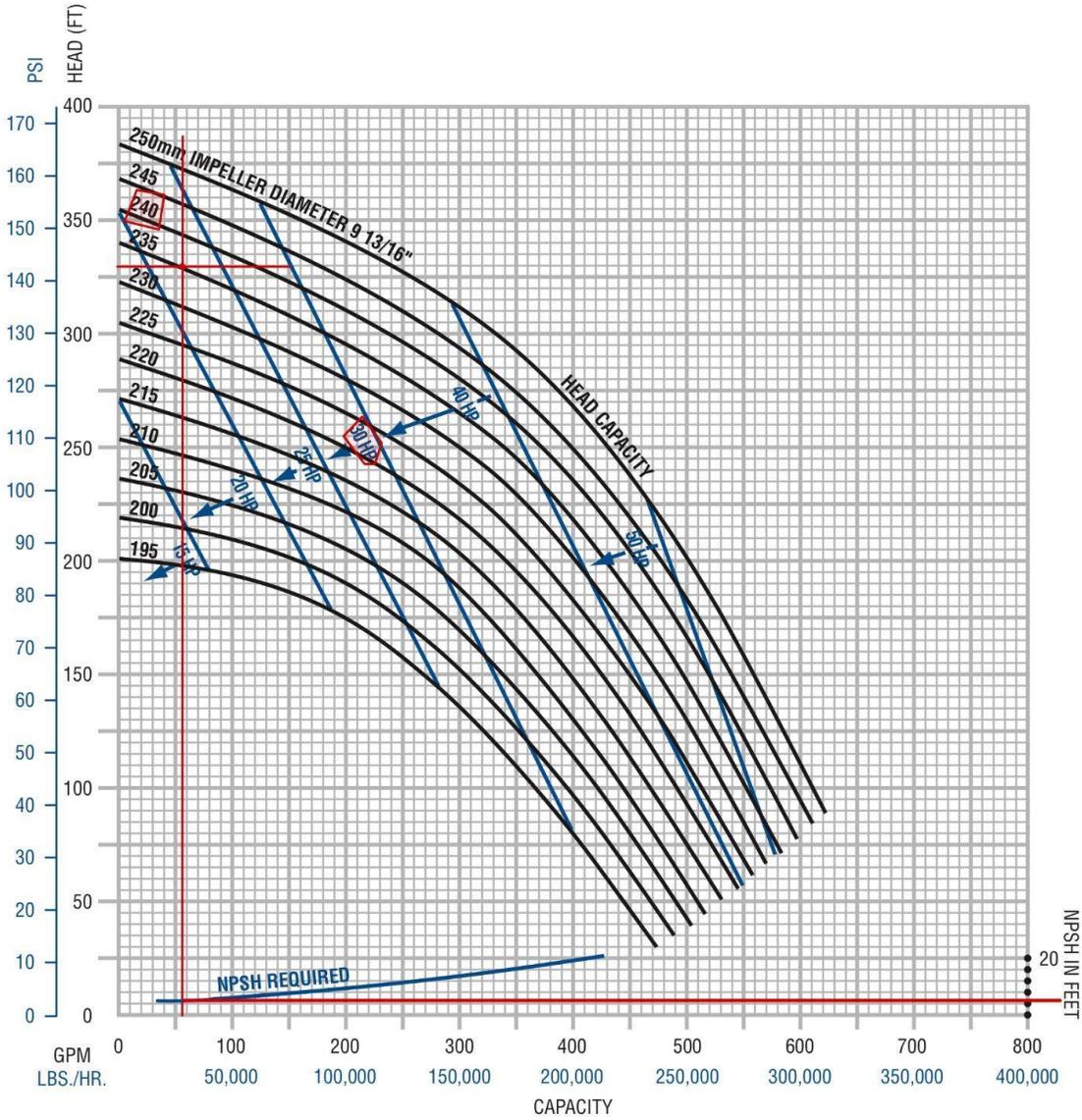


Performance curve based on tests using 70°F water and 0 psig inlet pressure. A tolerance of ± 5% applies to all figures. Actual performance may vary by application product. Please contact Fristam for different conditions.

P-05



FP/FPX/FPR Performance Curves Model: 3452 (3500 RPM, Inlet 3", Outlet 2")

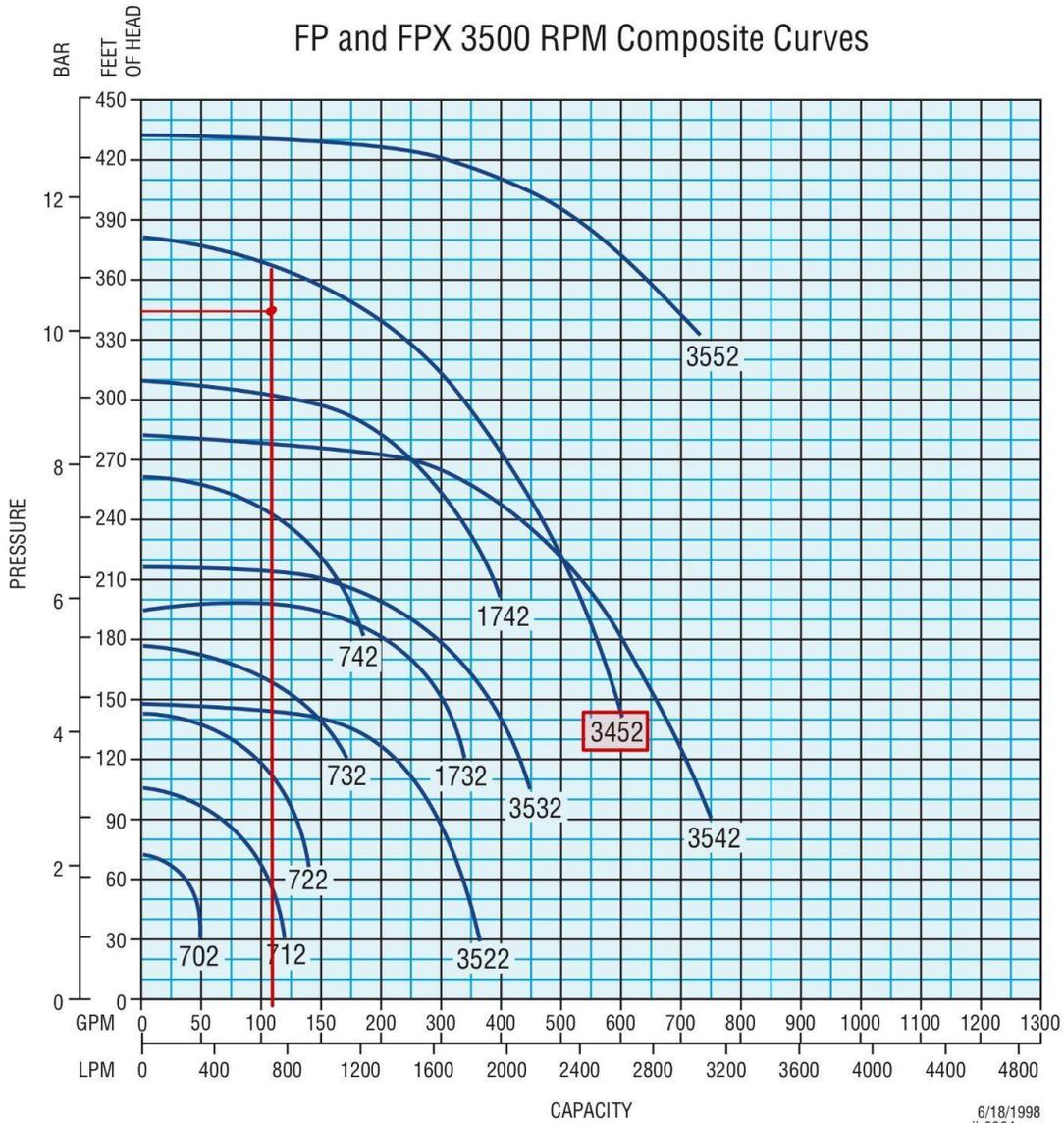


Performance curve based on tests using 70°F water and 0 psig inlet pressure. A tolerance of ± 5% applies to all figures. Actual performance may vary by application product. Please contact Fristam for different conditions.

P-06



FP/FPX Performance Curves
Models: 3500 RPM (Composite)



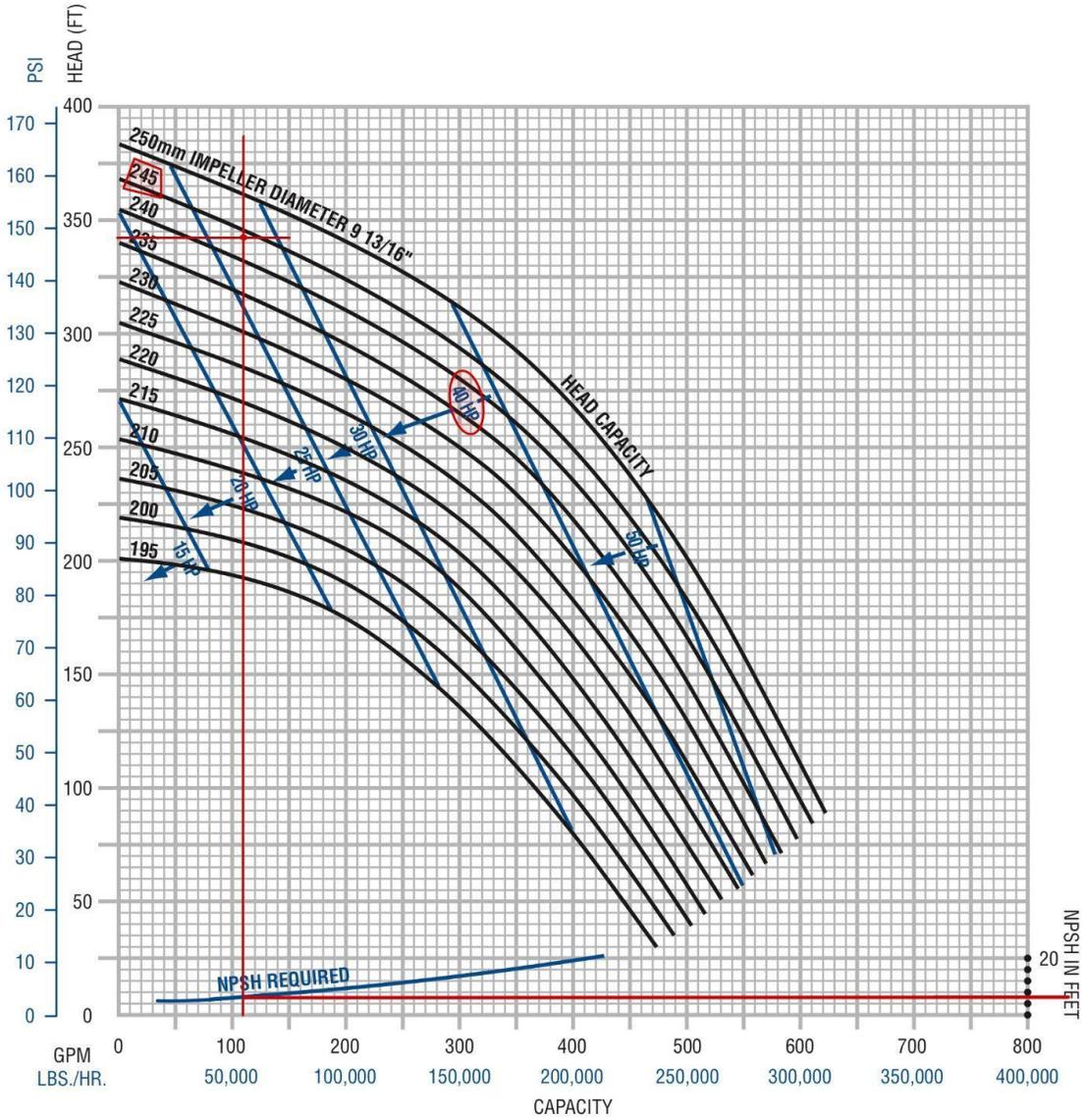
6/18/1998
 il-0364.eps
 RD 2/08

Performance curve based on tests using 70°F water and 0 psig inlet pressure. A tolerance of ± 5% applies to all figures. Actual performance may vary by application product. Please contact Fristam for different conditions.

P-06



FP/FPX/FPR Performance Curves Model: 3452 (3500 RPM, Inlet 3", Outlet 2")

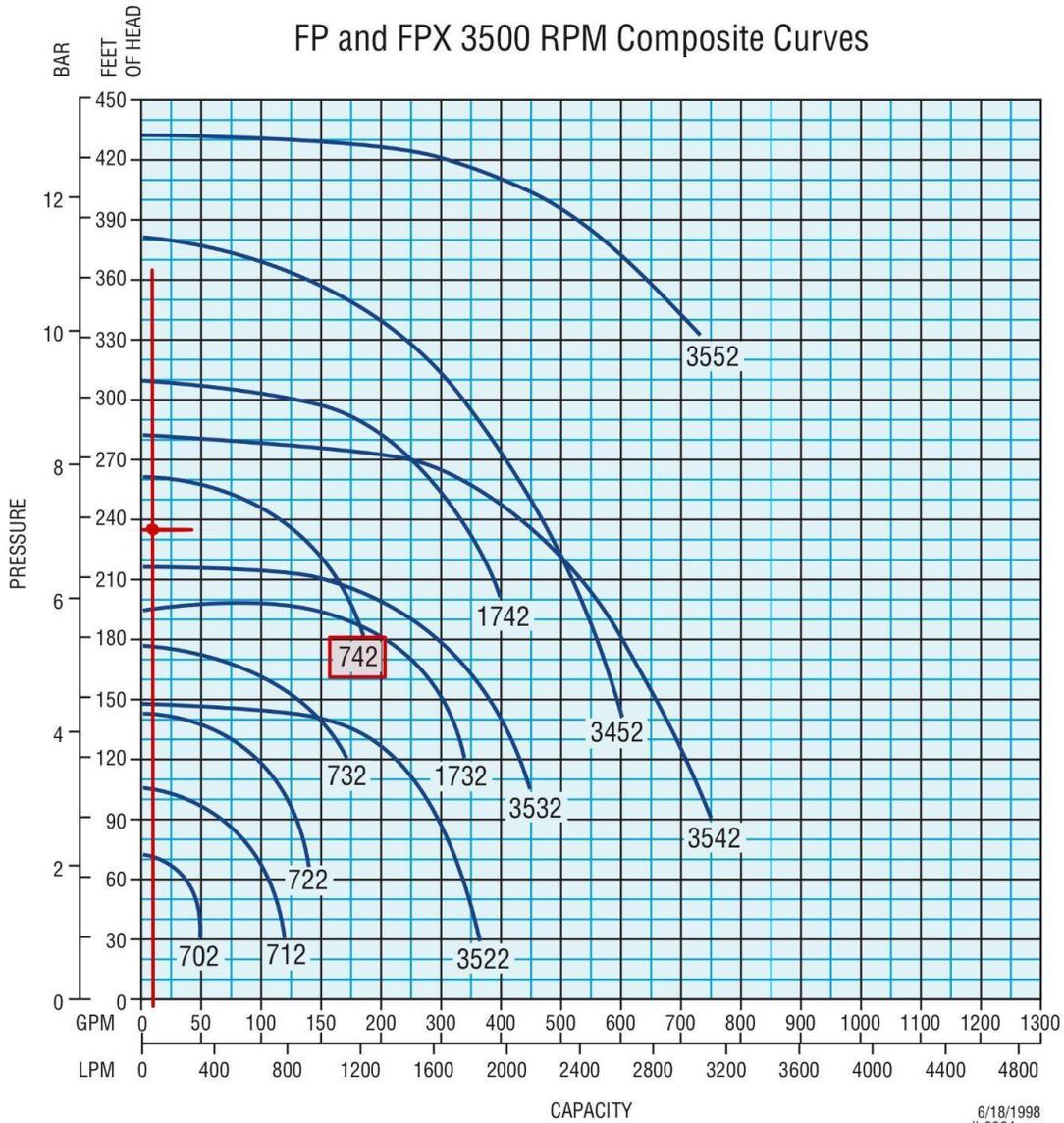


Performance curve based on tests using 70°F water and 0 psig inlet pressure. A tolerance of ± 5% applies to all figures. Actual performance may vary by application product. Please contact Fristam for different conditions.

P-07



**FP/FPX Performance Curves
Models: 3500 RPM (Composite)**



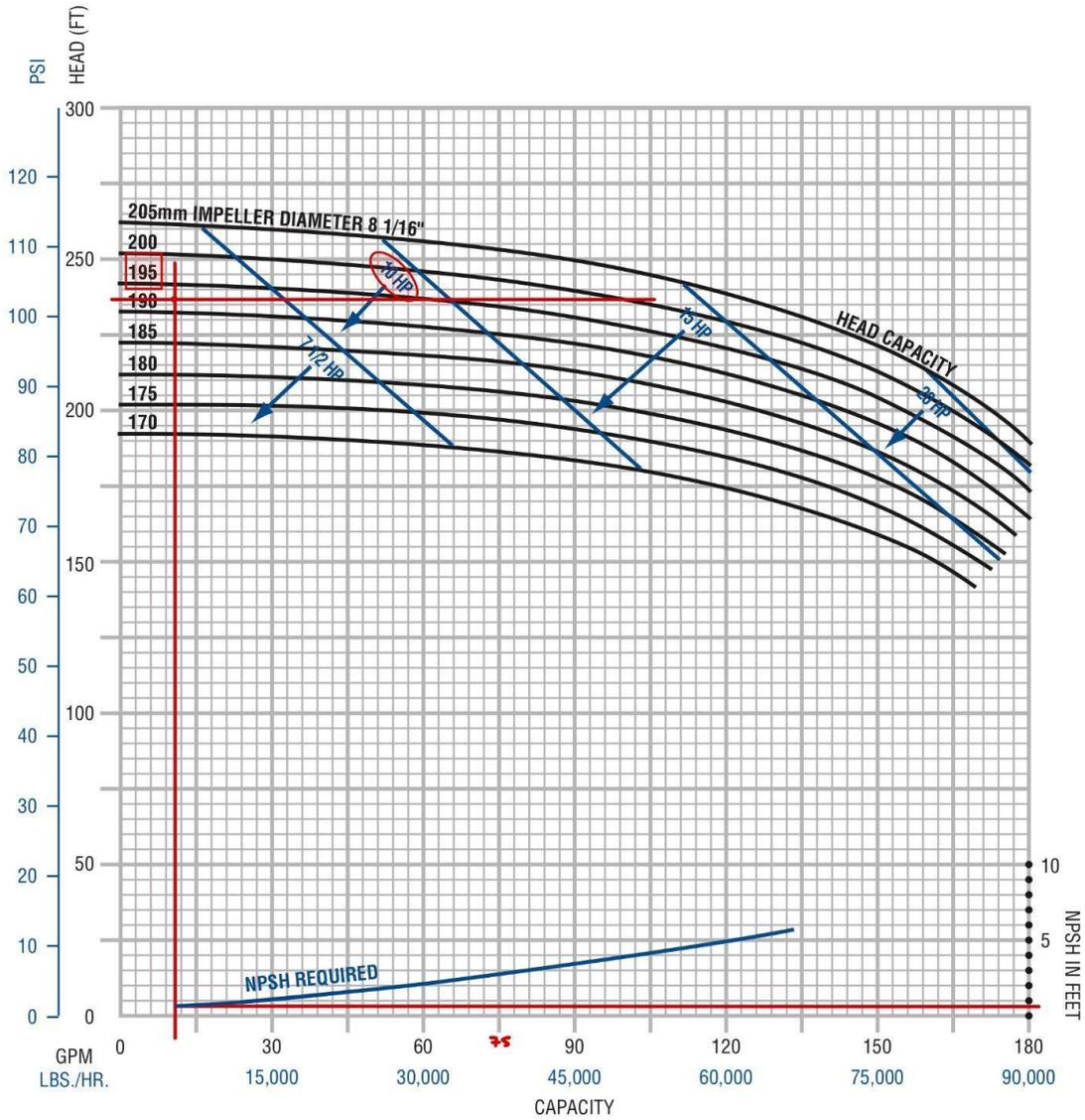
Performance curve based on tests using 70°F water and 0 psig inlet pressure. A tolerance of ± 5% applies to all figures. Actual performance may vary by application product. Please contact Fristam for different conditions.

P-07



FP/FPX Performance Curves Model: 742 (3500 RPM, Inlet 2.5", Outlet 2")

FPR model 742 covers the range of both the FP/FPX 732 and 742

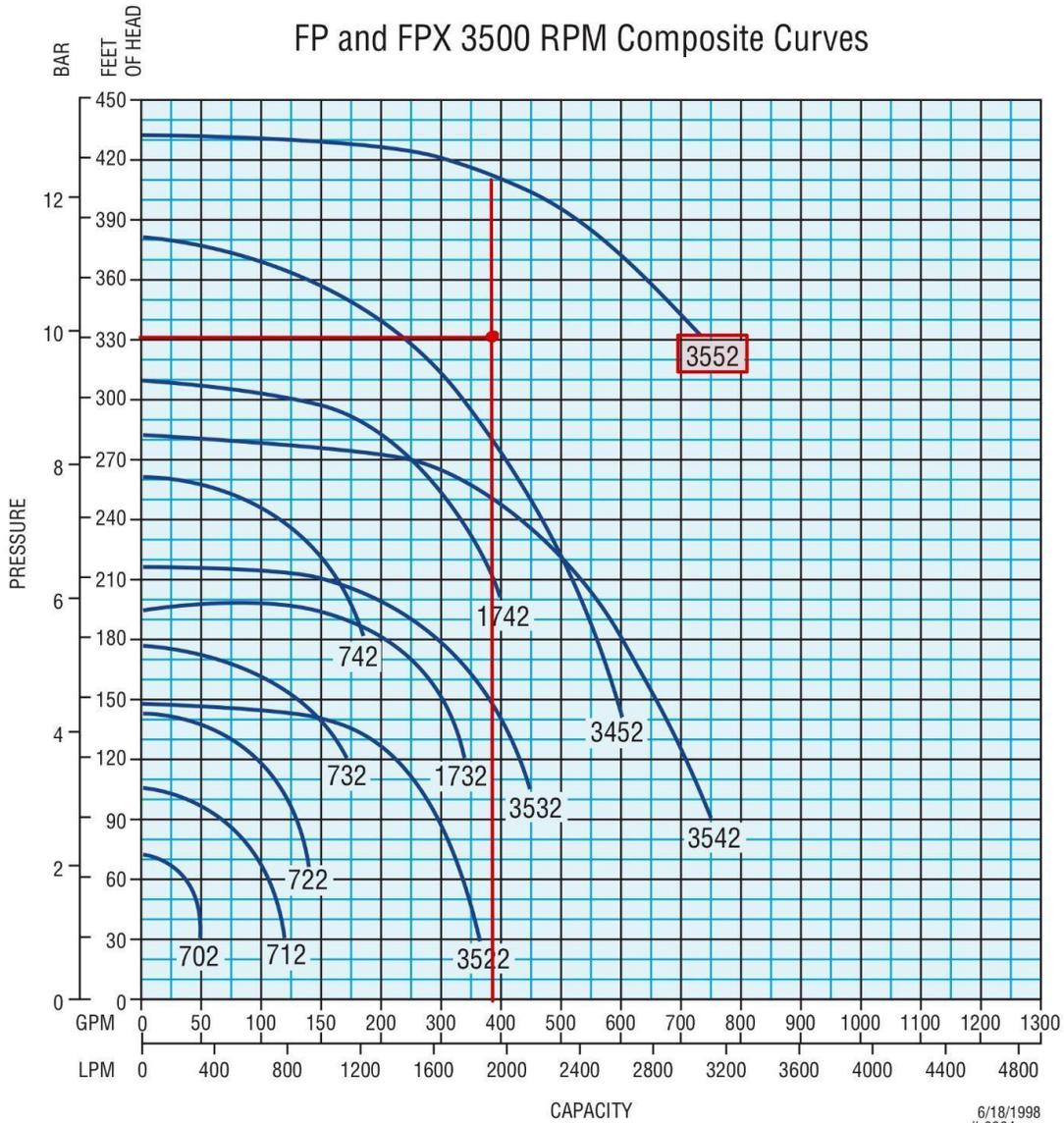


Performance curve based on tests using 70°F water and 0 psig inlet pressure. A tolerance of ± 5% applies to all figures. Actual performance may vary by application product. Please contact Fristam for different conditions.

P-08



FP/FPX Performance Curves
Models: 3500 RPM (Composite)

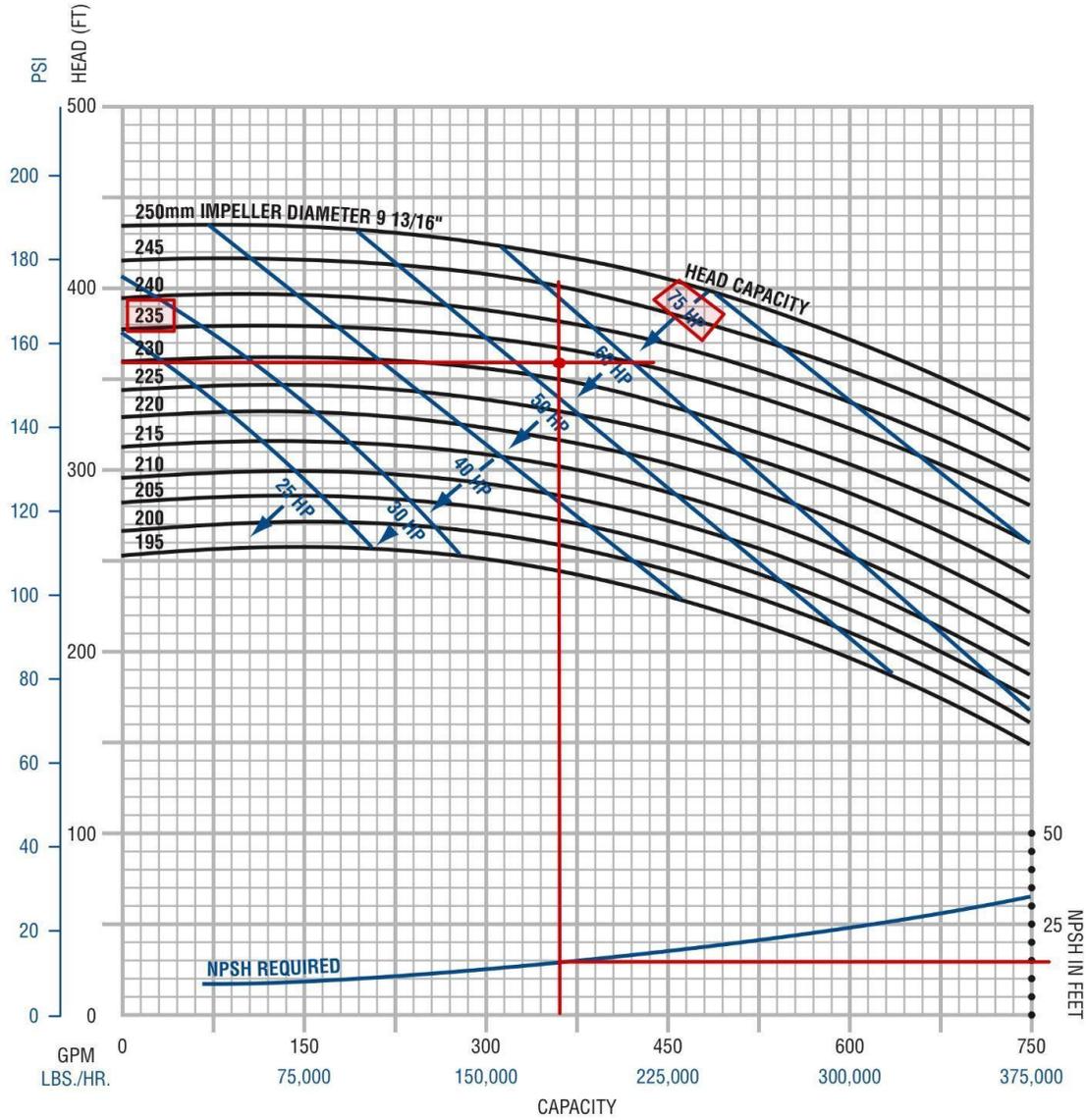


Performance curve based on tests using 70°F water and 0 psig inlet pressure. A tolerance of ± 5% applies to all figures. Actual performance may vary by application product. Please contact Fristam for different conditions.

P-08



FP/FPX/FPR Performance Curves Model: 3552 (3500 RPM, Inlet 3", Outlet 2.5")

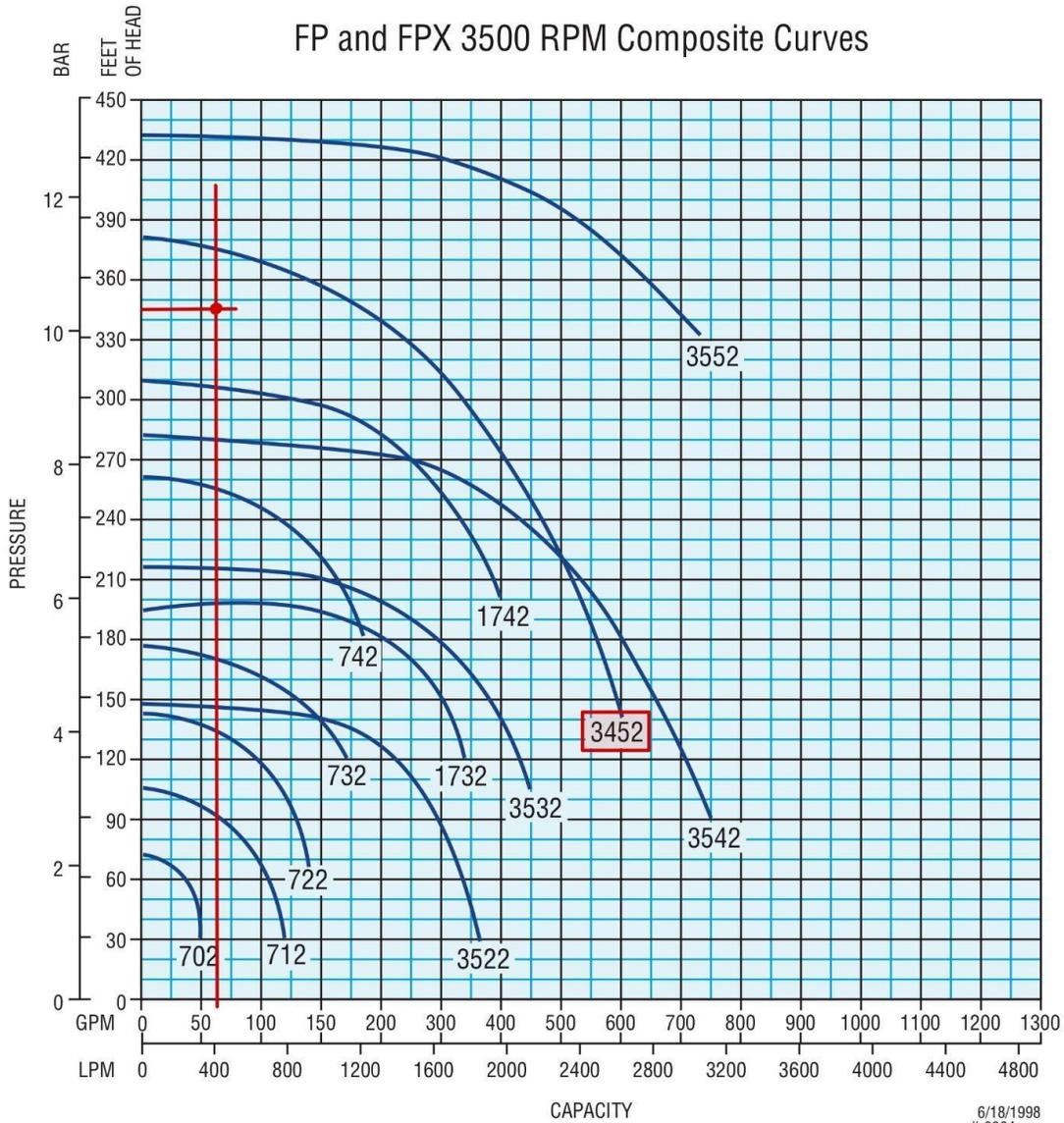


Performance curve based on tests using 70°F water and 0 psig inlet pressure. A tolerance of ± 5% applies to all figures. Actual performance may vary by application product. Please contact Fristam for different conditions.

P-09



FP/FPX Performance Curves
Models: 3500 RPM (Composite)

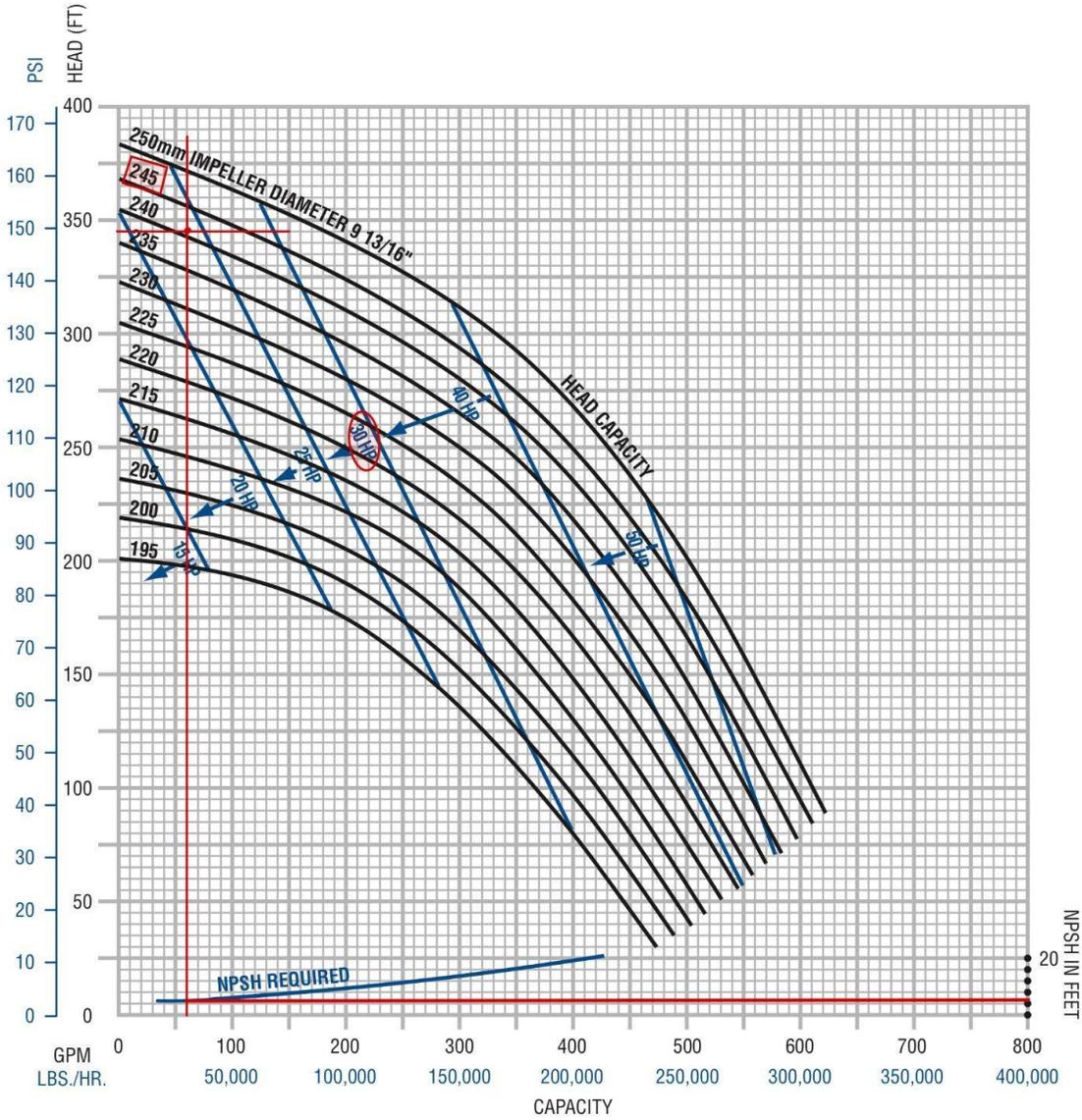


Performance curve based on tests using 70°F water and 0 psig inlet pressure. A tolerance of ± 5% applies to all figures. Actual performance may vary by application product. Please contact Fristam for different conditions.

P-09



FP/FPX/FPR Performance Curves Model: 3452 (3500 RPM, Inlet 3", Outlet 2")

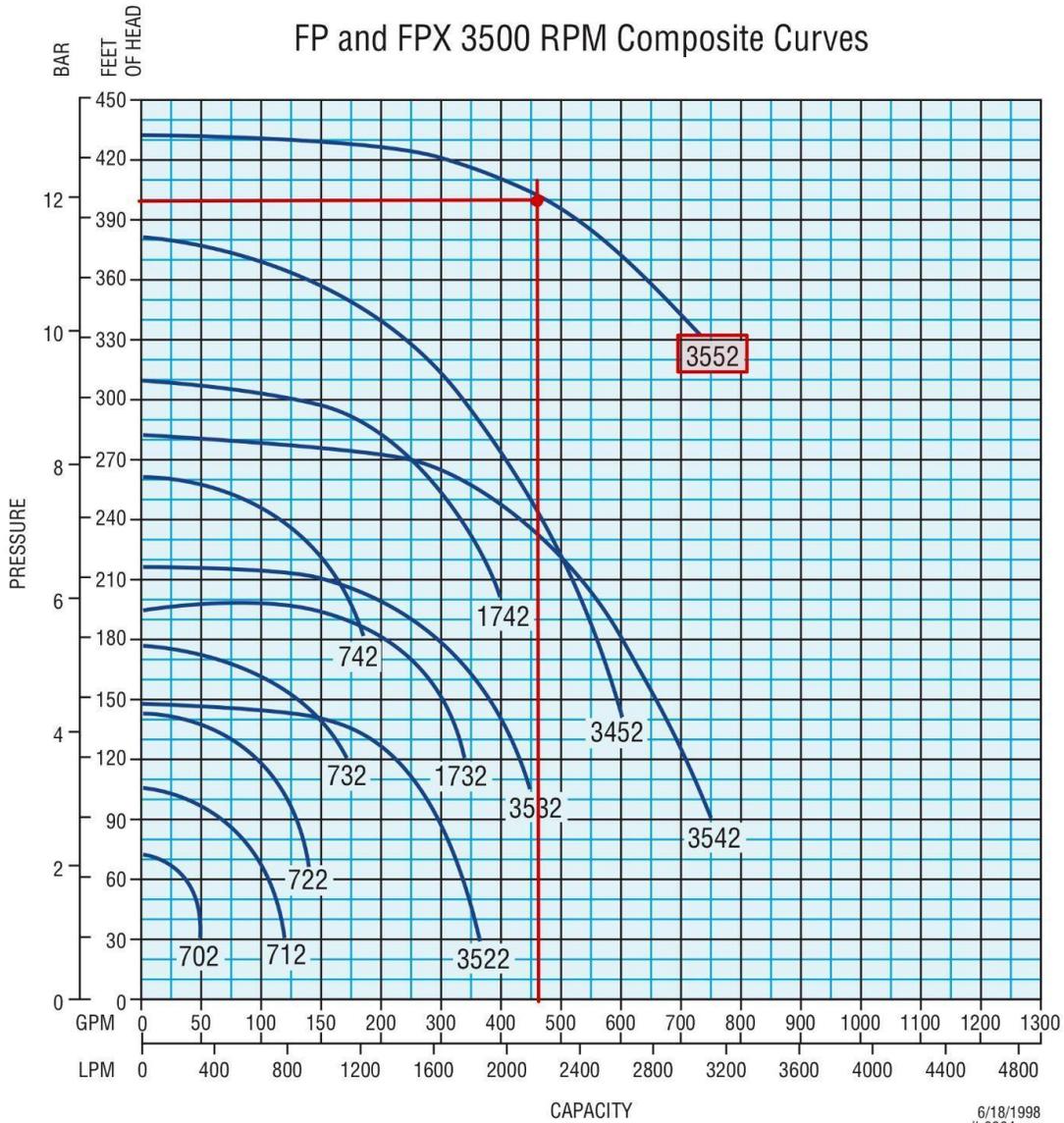


Performance curve based on tests using 70°F water and 0 psig inlet pressure. A tolerance of ± 5% applies to all figures. Actual performance may vary by application product. Please contact Fristam for different conditions.

P-10



FP/FPX Performance Curves Models: 3500 RPM (Composite)



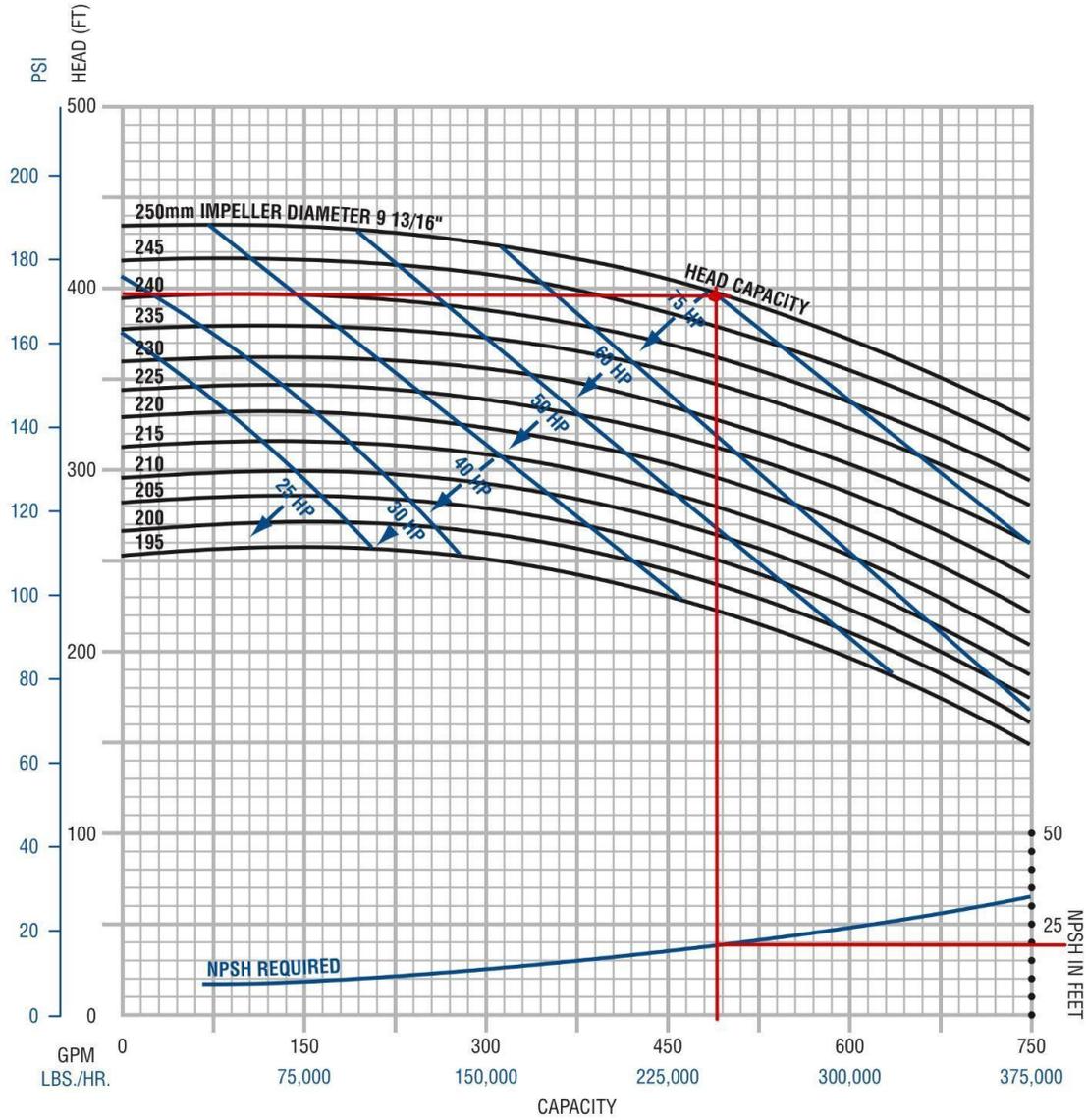
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RD 2/08

Performance curve based on tests using 70°F water and 0 psig inlet pressure. A tolerance of ± 5% applies to all figures. Actual performance may vary by application product. Please contact Fristam for different conditions.

P-10



FP/FPX/FPR Performance Curves Model: 3552 (3500 RPM, Inlet 3", Outlet 2.5")

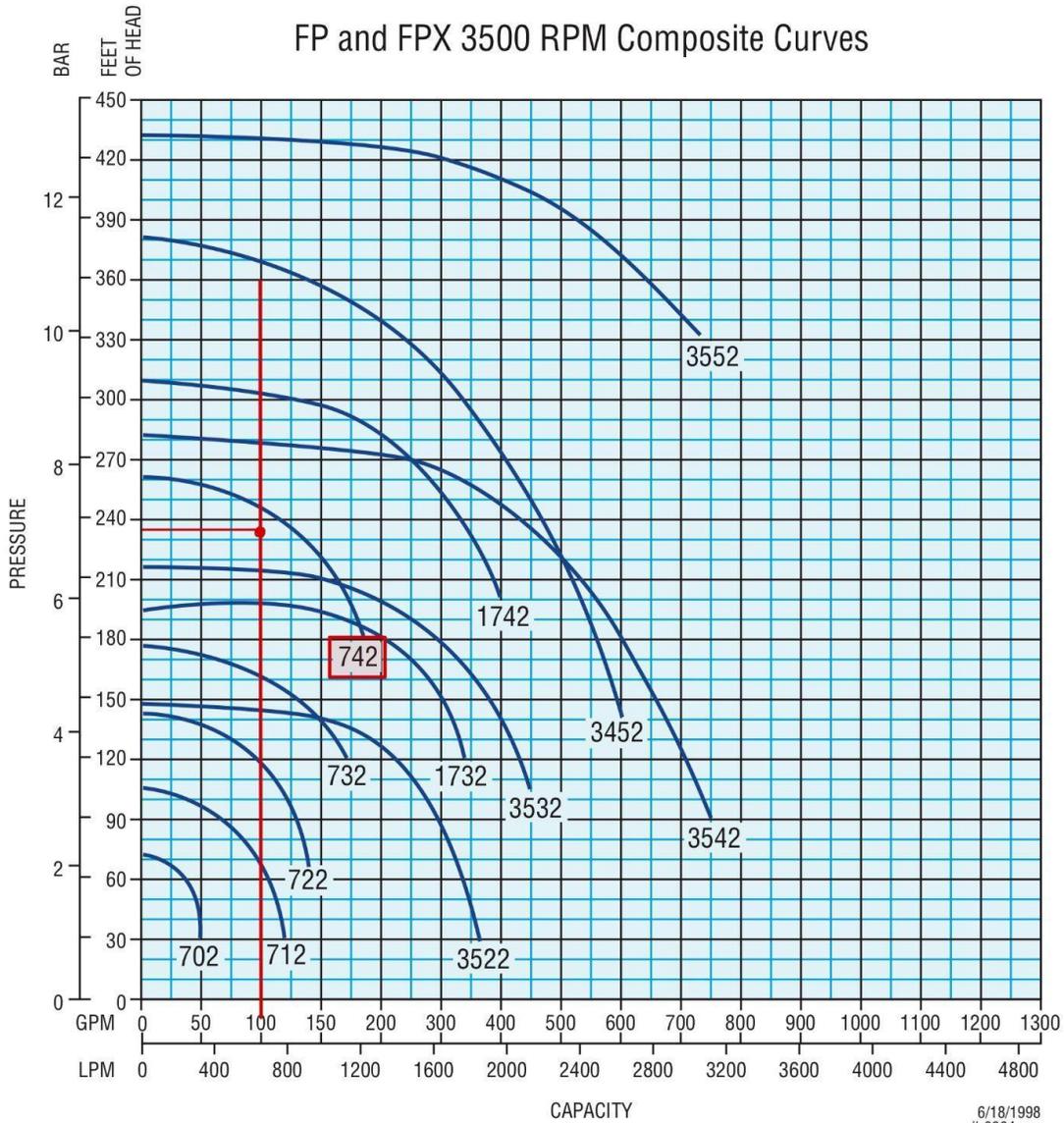


Performance curve based on tests using 70°F water and 0 psig inlet pressure. A tolerance of ± 5% applies to all figures. Actual performance may vary by application product. Please contact Fristam for different conditions.

P-11



FP/FPX Performance Curves
Models: 3500 RPM (Composite)



6/18/1998
 il-0364.eps
 RD 2/08

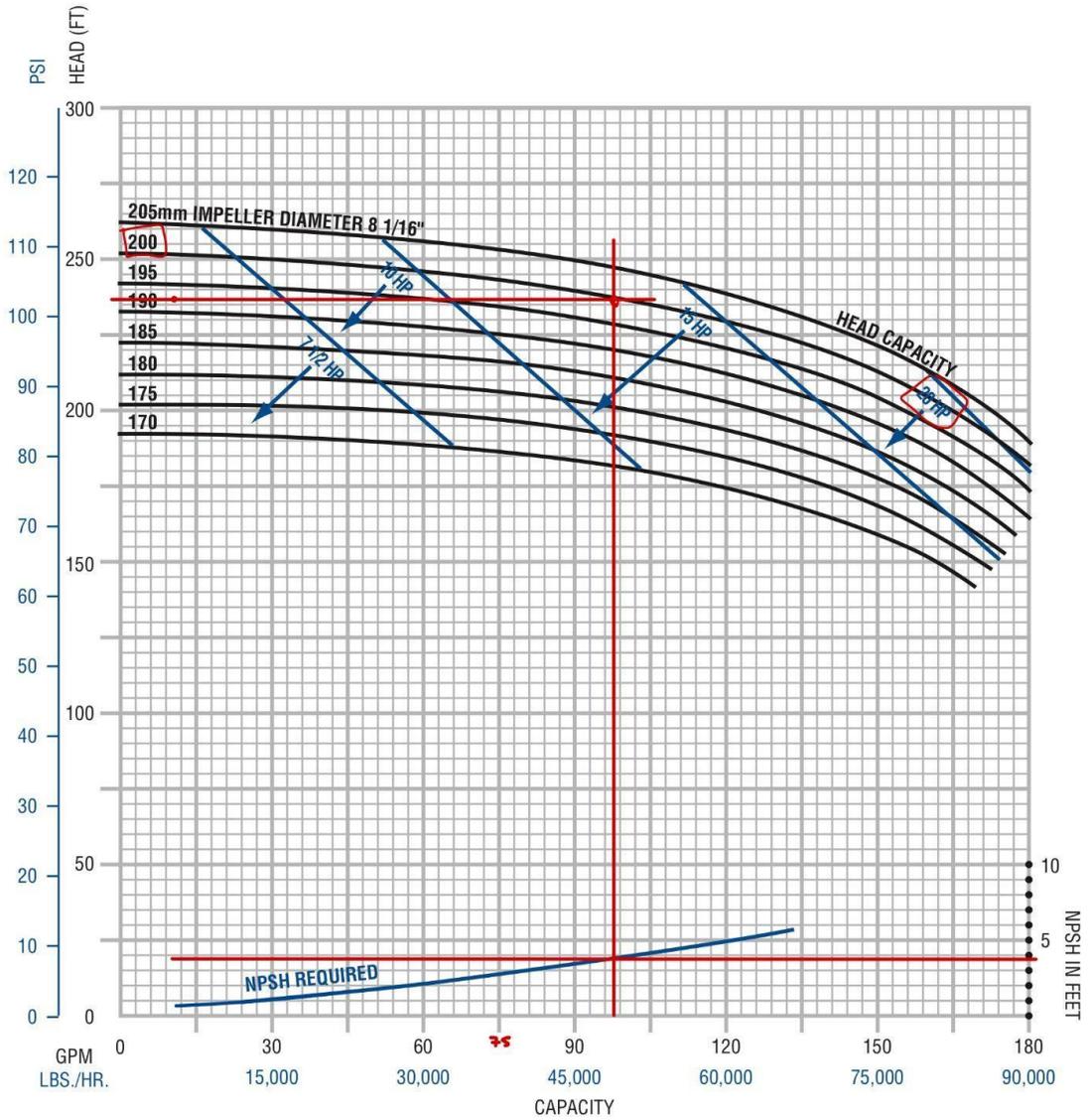
Performance curve based on tests using 70°F water and 0 psig inlet pressure. A tolerance of ± 5% applies to all figures. Actual performance may vary by application product. Please contact Fristam for different conditions.

P-11



FP/FPX Performance Curves Model: 742 (3500 RPM, Inlet 2.5", Outlet 2")

FPR model 742 covers the range of both the FP/FPX 732 and 742

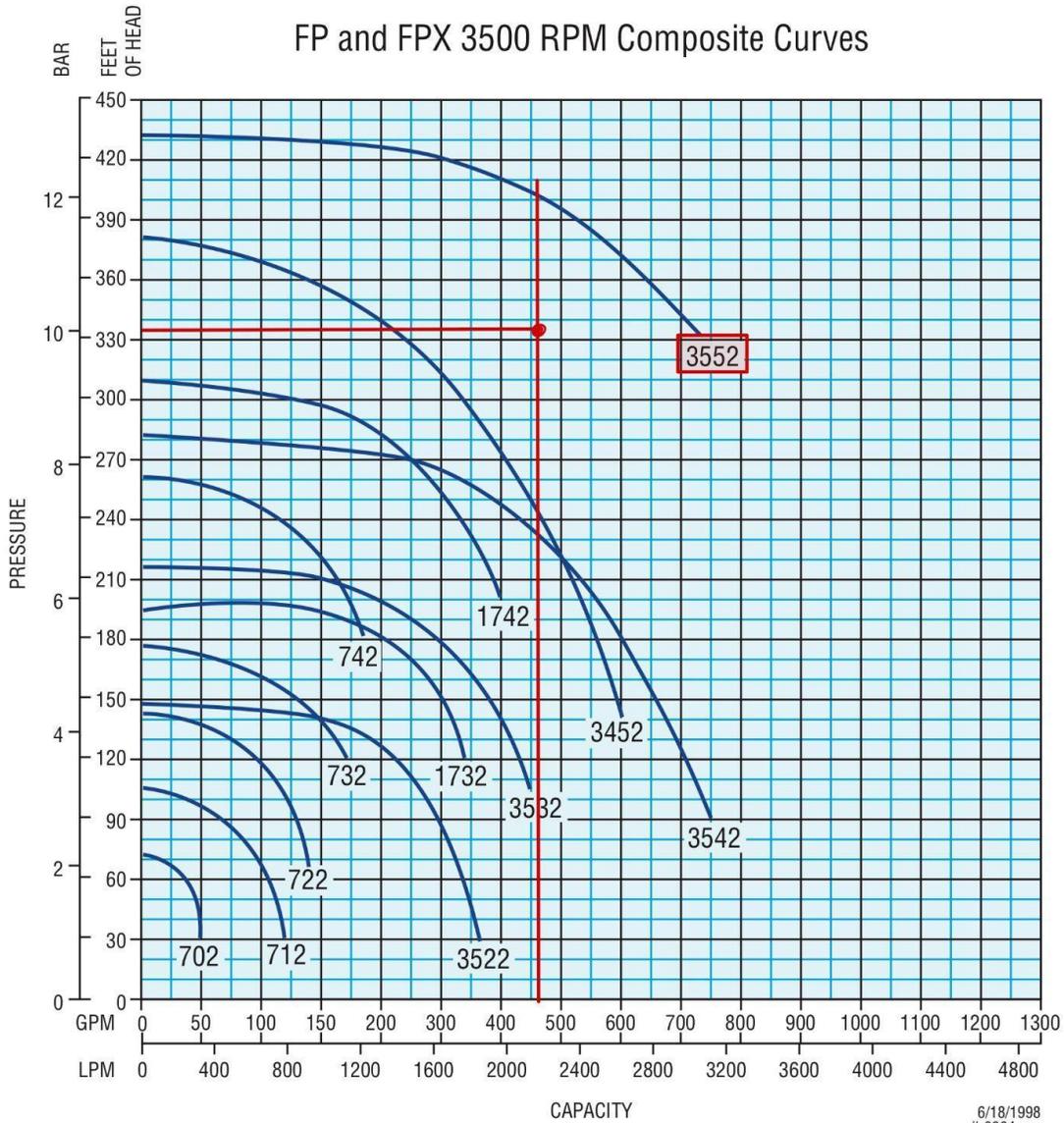


Performance curve based on tests using 70°F water and 0 psig inlet pressure. A tolerance of ± 5% applies to all figures. Actual performance may vary by application product. Please contact Fristam for different conditions.

P-12



FP/FPX Performance Curves Models: 3500 RPM (Composite)



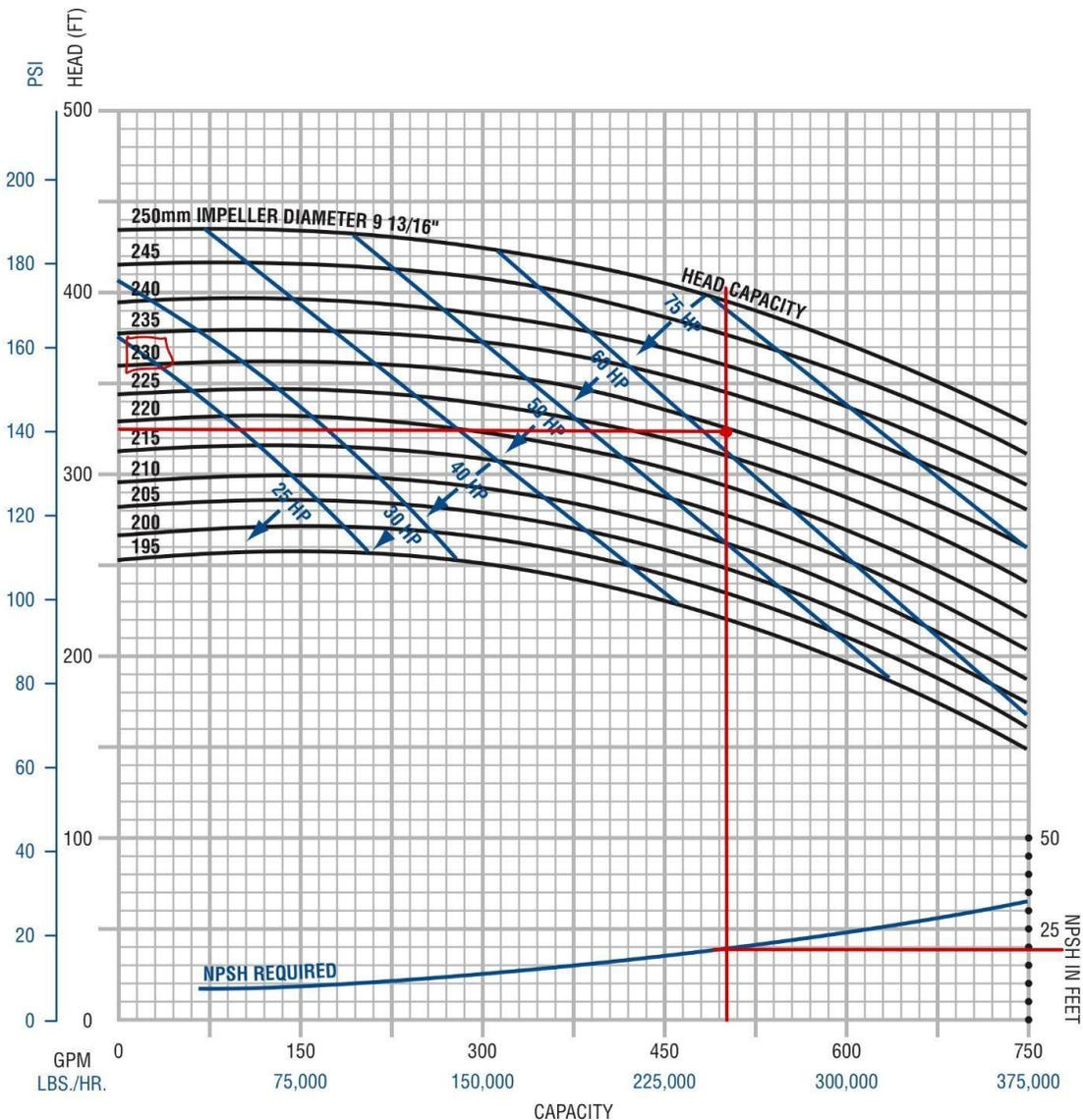
6/18/1998
il-0364.eps
RD 2/08

Performance curve based on tests using 70°F water and 0 psig inlet pressure. A tolerance of ± 5% applies to all figures. Actual performance may vary by application product. Please contact Fristam for different conditions.

P-12



FP/FPX/FPR Performance Curves Model: 3552 (3500 RPM, Inlet 3", Outlet 2.5")

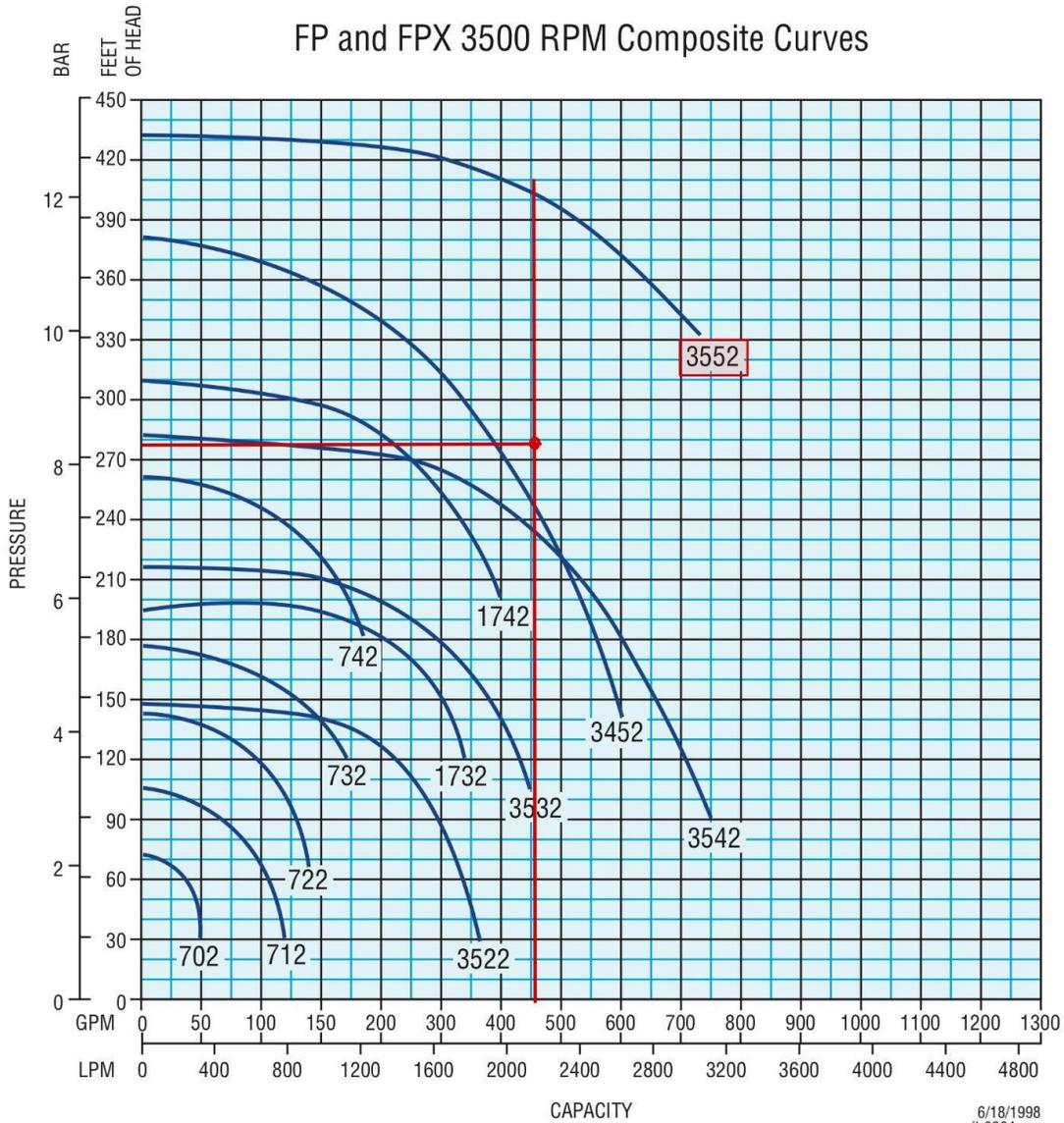


Performance curve based on tests using 70°F water and 0 psig inlet pressure. A tolerance of ± 5% applies to all figures. Actual performance may vary by application product. Please contact Fristam for different conditions.

P-13



FP/FPX Performance Curves Models: 3500 RPM (Composite)



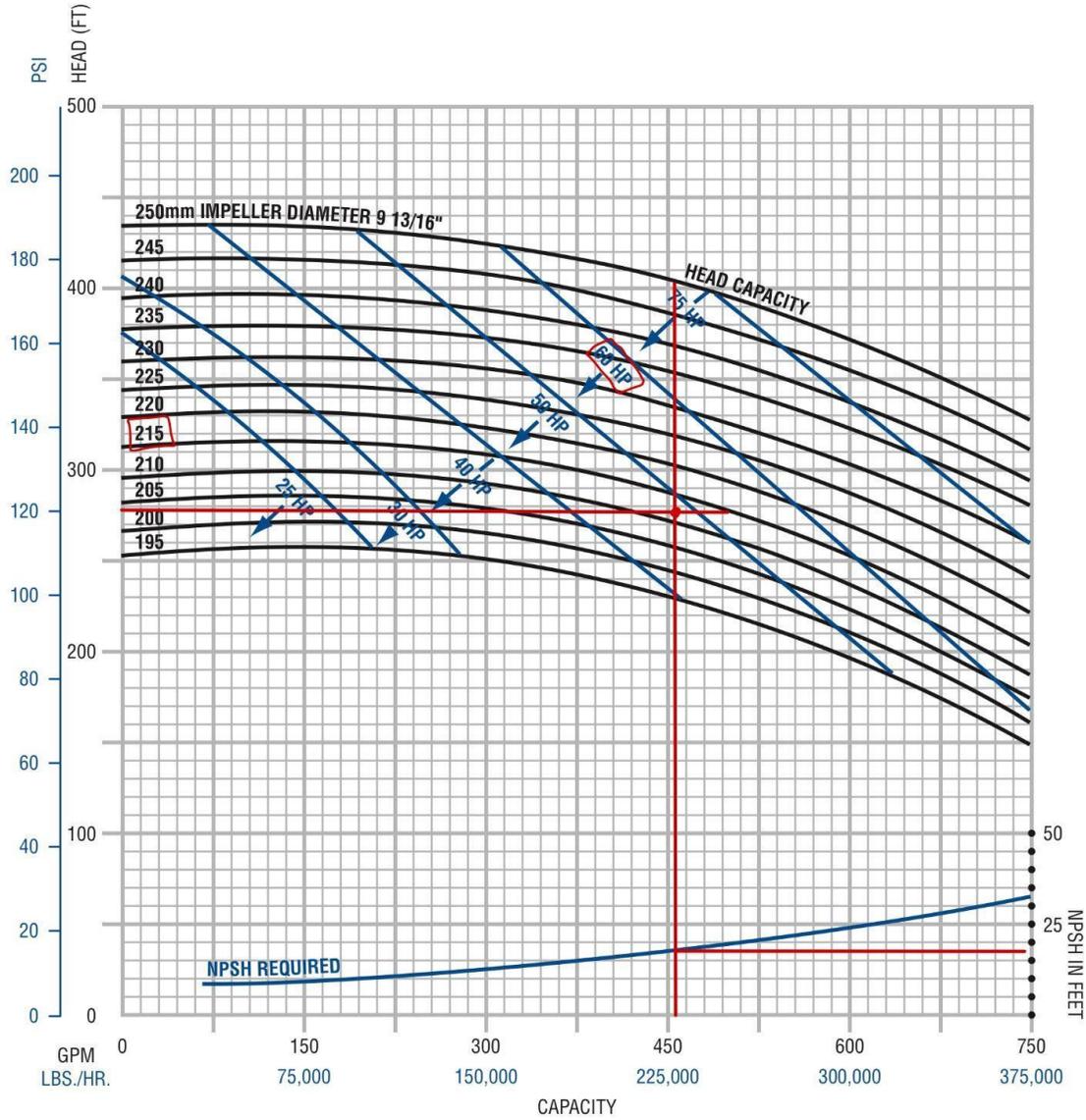
6/18/1998
il-0364.eps
RD 2/08

Performance curve based on tests using 70°F water and 0 psig inlet pressure. A tolerance of ± 5% applies to all figures. Actual performance may vary by application product. Please contact Fristam for different conditions.

P-13



FP/FPX/FPR Performance Curves Model: 3552 (3500 RPM, Inlet 3", Outlet 2.5")

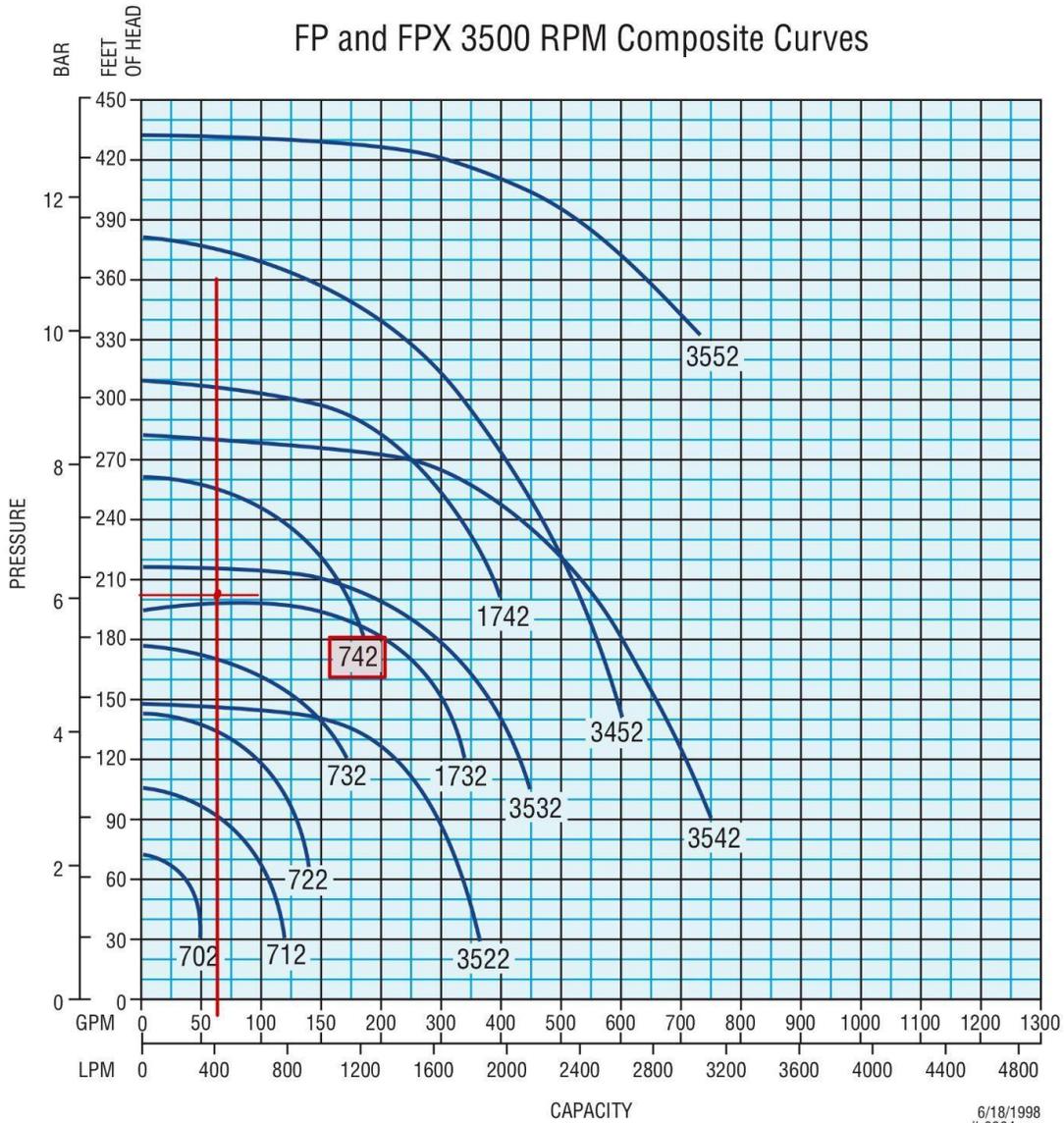


Performance curve based on tests using 70°F water and 0 psig inlet pressure. A tolerance of ± 5% applies to all figures. Actual performance may vary by application product. Please contact Fristam for different conditions.

P-14



**FP/FPX Performance Curves
Models: 3500 RPM (Composite)**



6/18/1998
il-0364.eps
RD 2/08

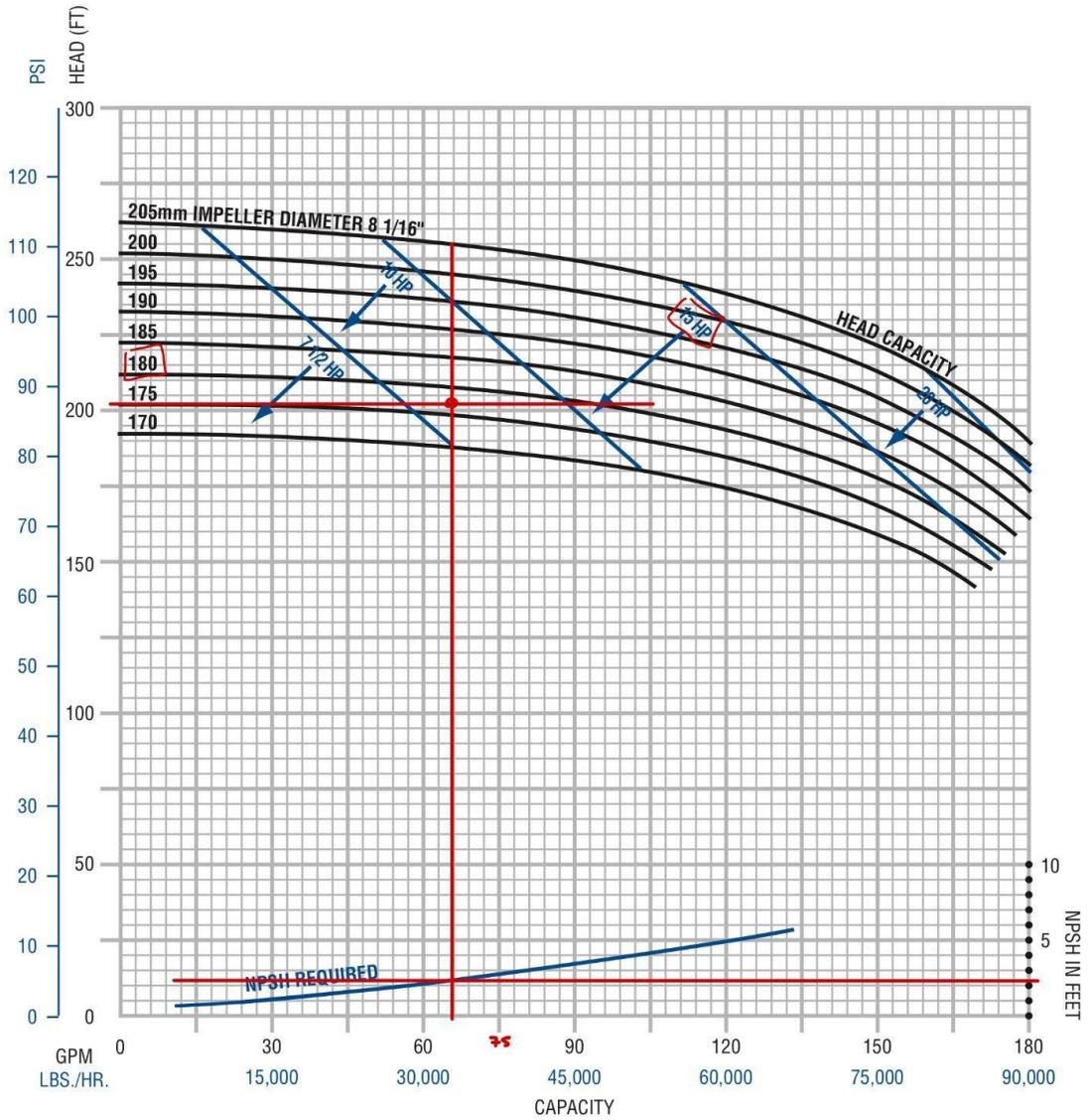
Performance curve based on tests using 70°F water and 0 psig inlet pressure. A tolerance of ± 5% applies to all figures. Actual performance may vary by application product. Please contact Fristam for different conditions.

P-14



FP/FPX Performance Curves Model: 742 (3500 RPM, Inlet 2.5", Outlet 2")

FPR model 742 covers the range of both the FP/FPX 732 and 742

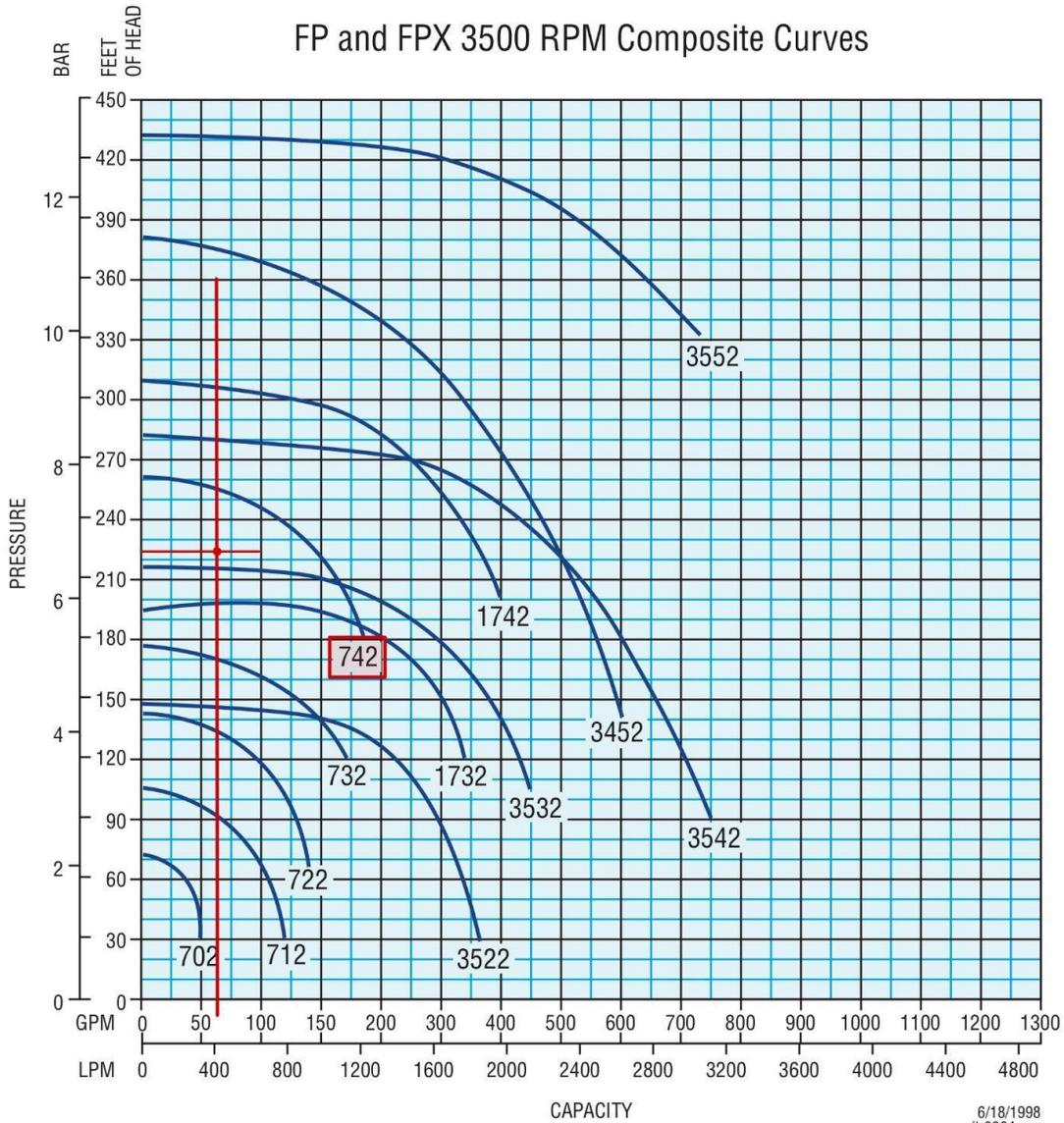


Performance curve based on tests using 70°F water and 0 psig inlet pressure. A tolerance of ± 5% applies to all figures. Actual performance may vary by application product. Please contact Fristam for different conditions.

P-15



**FP/FPX Performance Curves
Models: 3500 RPM (Composite)**



6/18/1998
il-0364.eps
RD 2/08

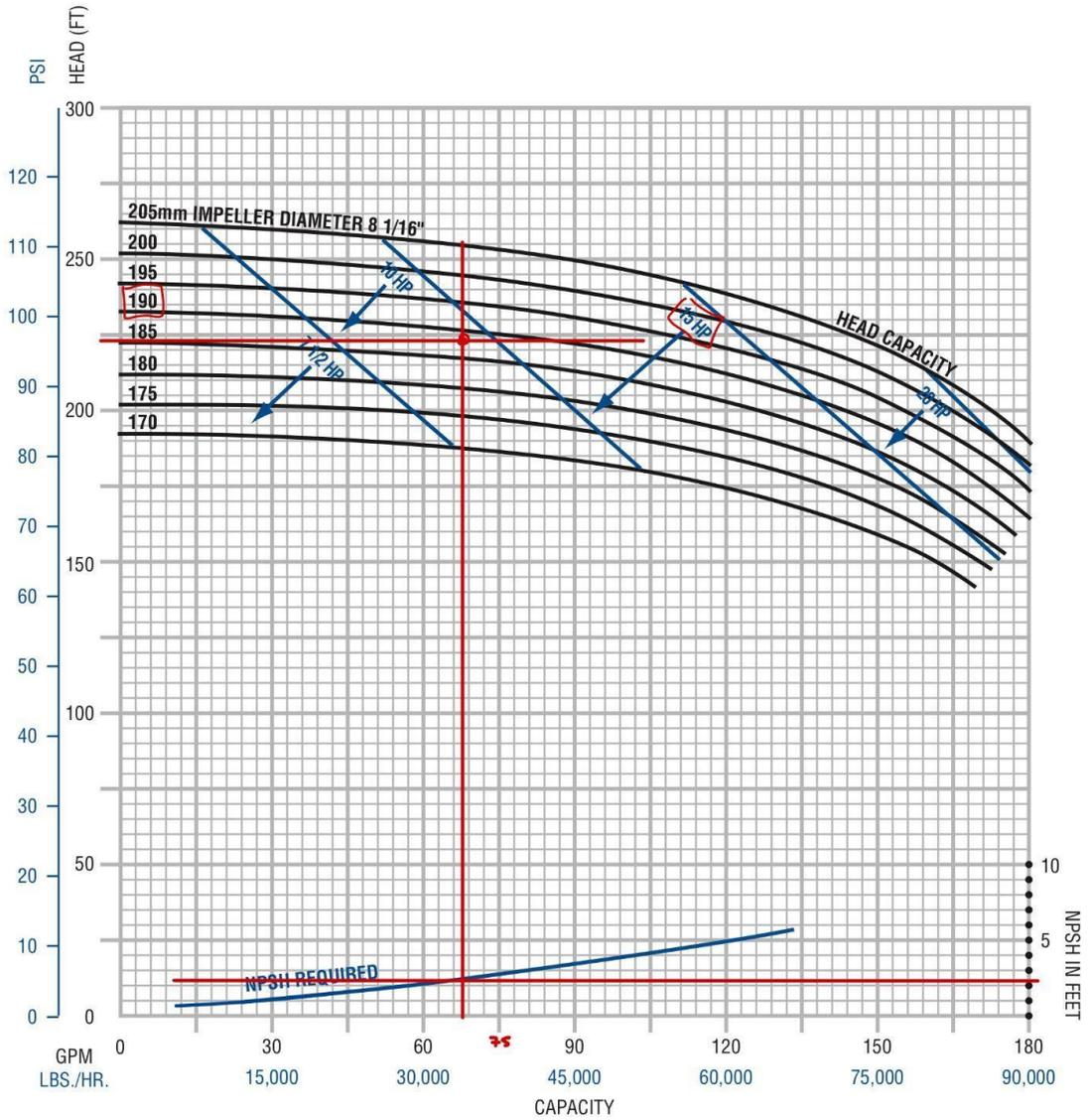
Performance curve based on tests using 70°F water and 0 psig inlet pressure. A tolerance of ± 5% applies to all figures. Actual performance may vary by application product. Please contact Fristam for different conditions.

P-15



FP/FPX Performance Curves Model: 742 (3500 RPM, Inlet 2.5", Outlet 2")

FPR model 742 covers the range of both the FP/FPX 732 and 742

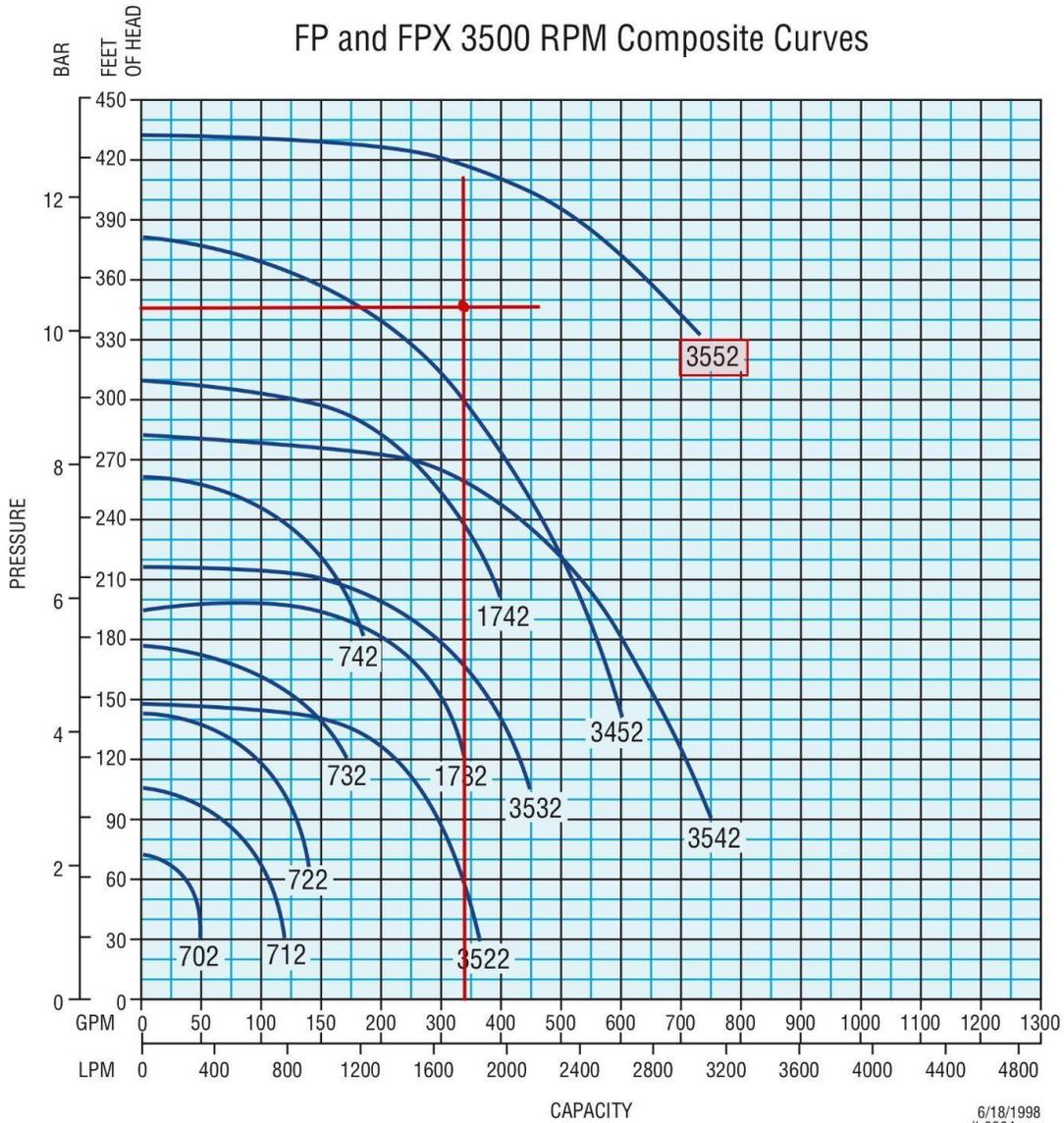


Performance curve based on tests using 70°F water and 0 psig inlet pressure. A tolerance of ± 5% applies to all figures. Actual performance may vary by application product. Please contact Fristam for different conditions.

P-16



FP/FPX Performance Curves Models: 3500 RPM (Composite)



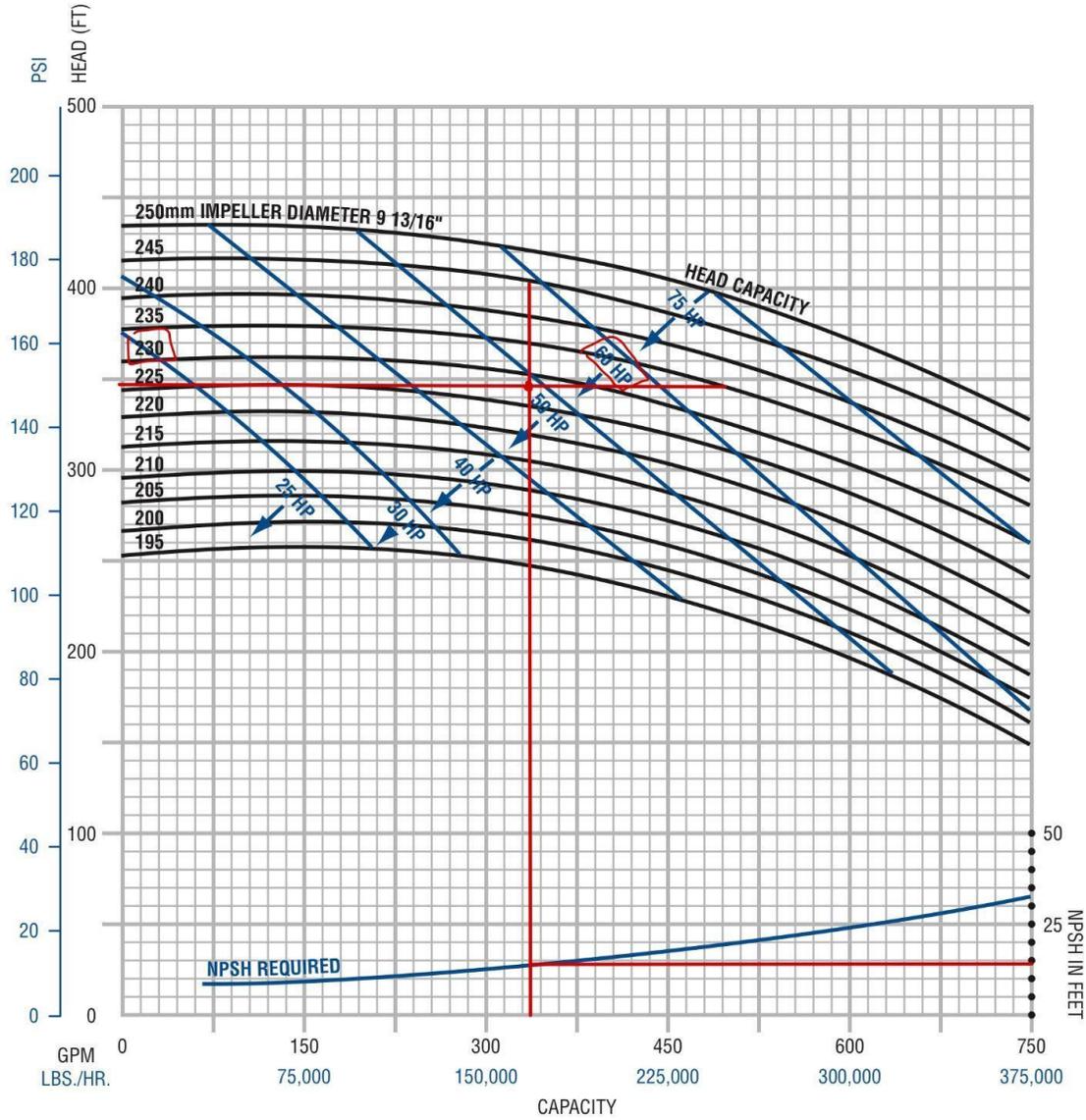
6/18/1998
il-0364.eps
RD 2/08

Performance curve based on tests using 70°F water and 0 psig inlet pressure. A tolerance of ± 5% applies to all figures. Actual performance may vary by application product. Please contact Fristam for different conditions.

P-16



FP/FPX/FPR Performance Curves Model: 3552 (3500 RPM, Inlet 3", Outlet 2.5")

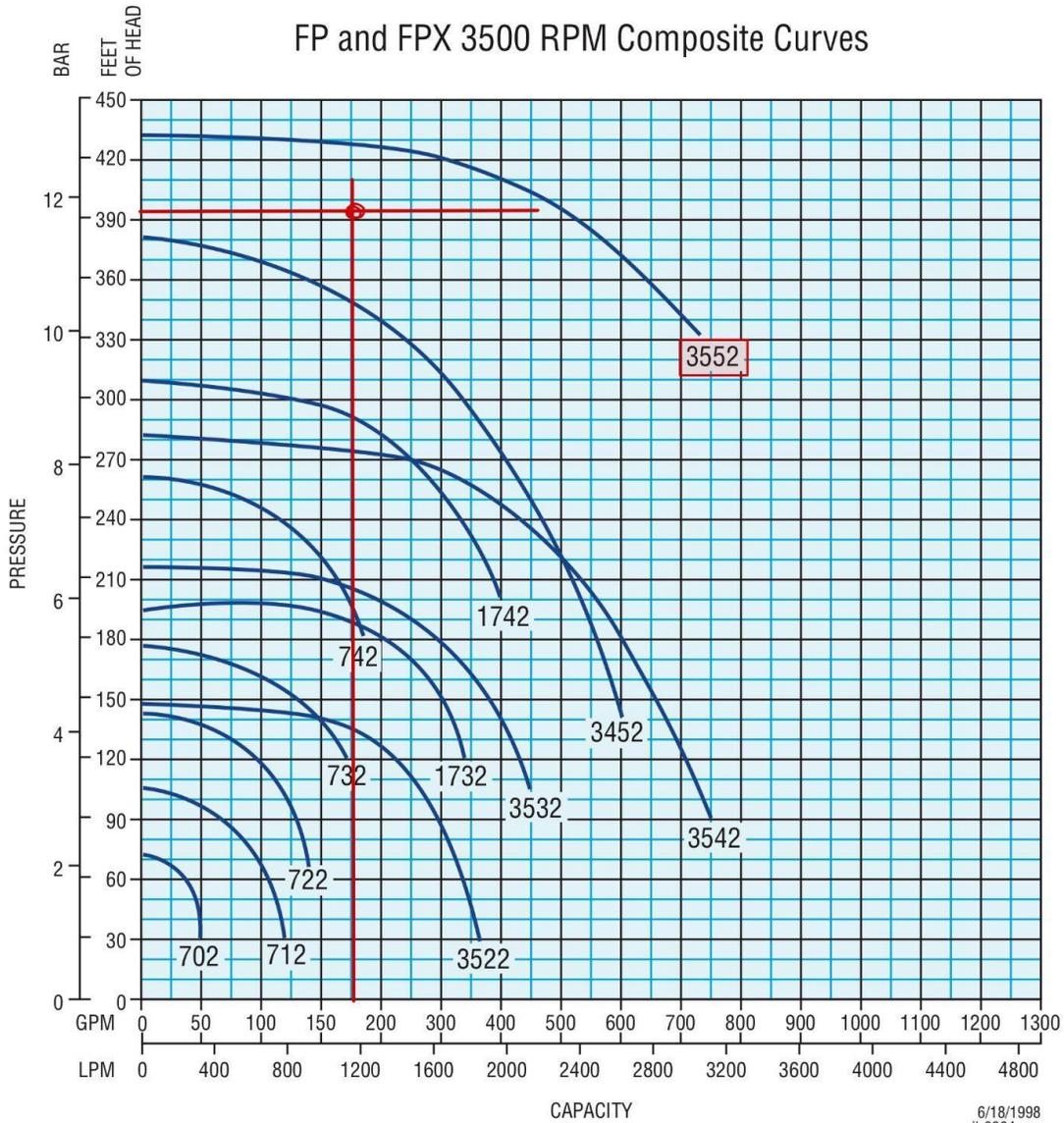


Performance curve based on tests using 70°F water and 0 psig inlet pressure. A tolerance of ± 5% applies to all figures. Actual performance may vary by application product. Please contact Fristam for different conditions.

P-17



FP/FPX Performance Curves Models: 3500 RPM (Composite)



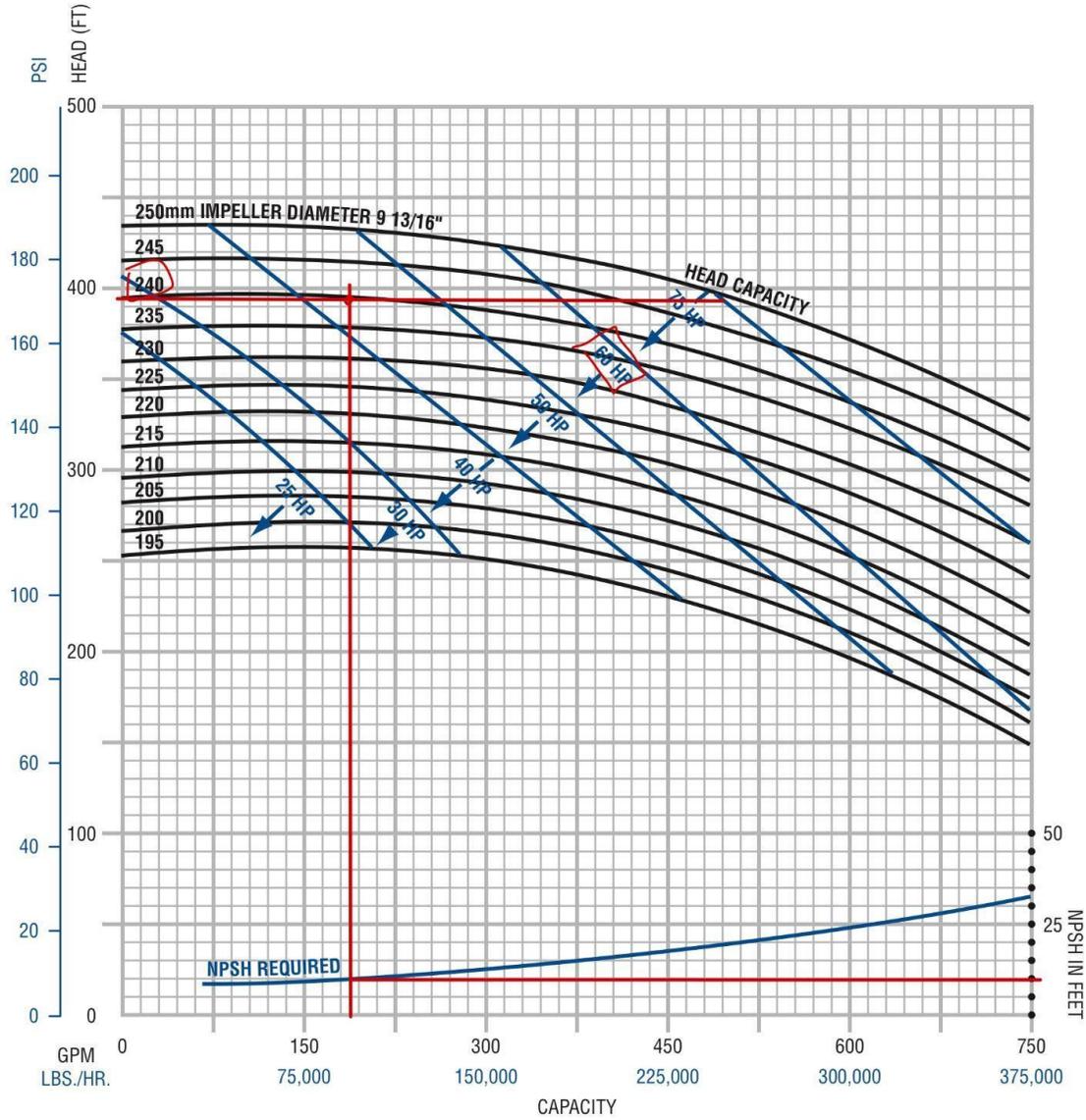
6/18/1998
il-0364.eps
RD 2/08

Performance curve based on tests using 70°F water and 0 psig inlet pressure. A tolerance of ± 5% applies to all figures. Actual performance may vary by application product. Please contact Fristam for different conditions.

P-17



FP/FPX/FPR Performance Curves Model: 3552 (3500 RPM, Inlet 3", Outlet 2.5")

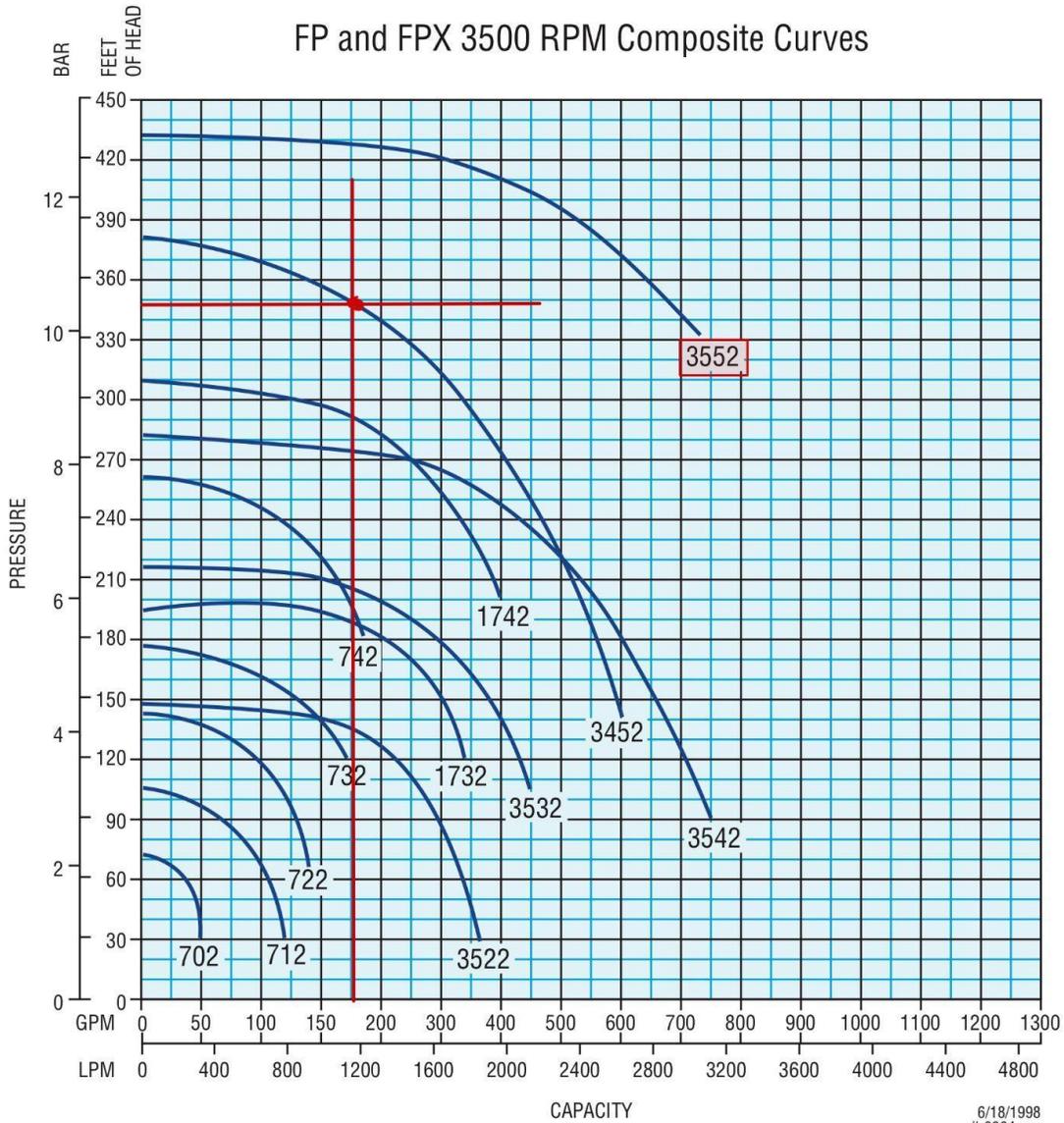


Performance curve based on tests using 70°F water and 0 psig inlet pressure. A tolerance of ± 5% applies to all figures. Actual performance may vary by application product. Please contact Fristam for different conditions.

P-18



FP/FPX Performance Curves
Models: 3500 RPM (Composite)



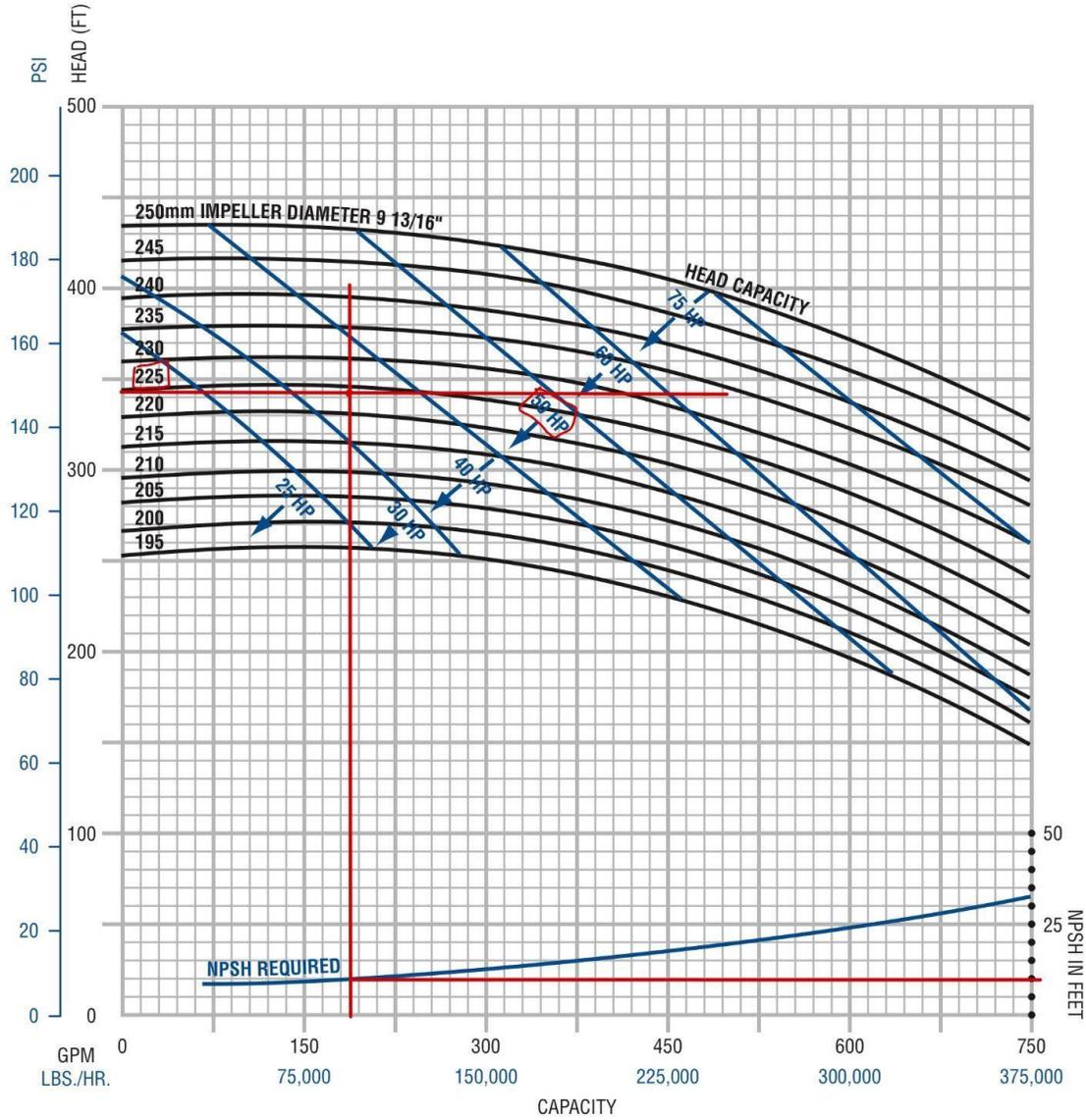
6/18/1998
 il-0364.eps
 RD 2/08

Performance curve based on tests using 70°F water and 0 psig inlet pressure. A tolerance of ± 5% applies to all figures. Actual performance may vary by application product. Please contact Fristam for different conditions.

P-18



FP/FPX/FPR Performance Curves Model: 3552 (3500 RPM, Inlet 3", Outlet 2.5")

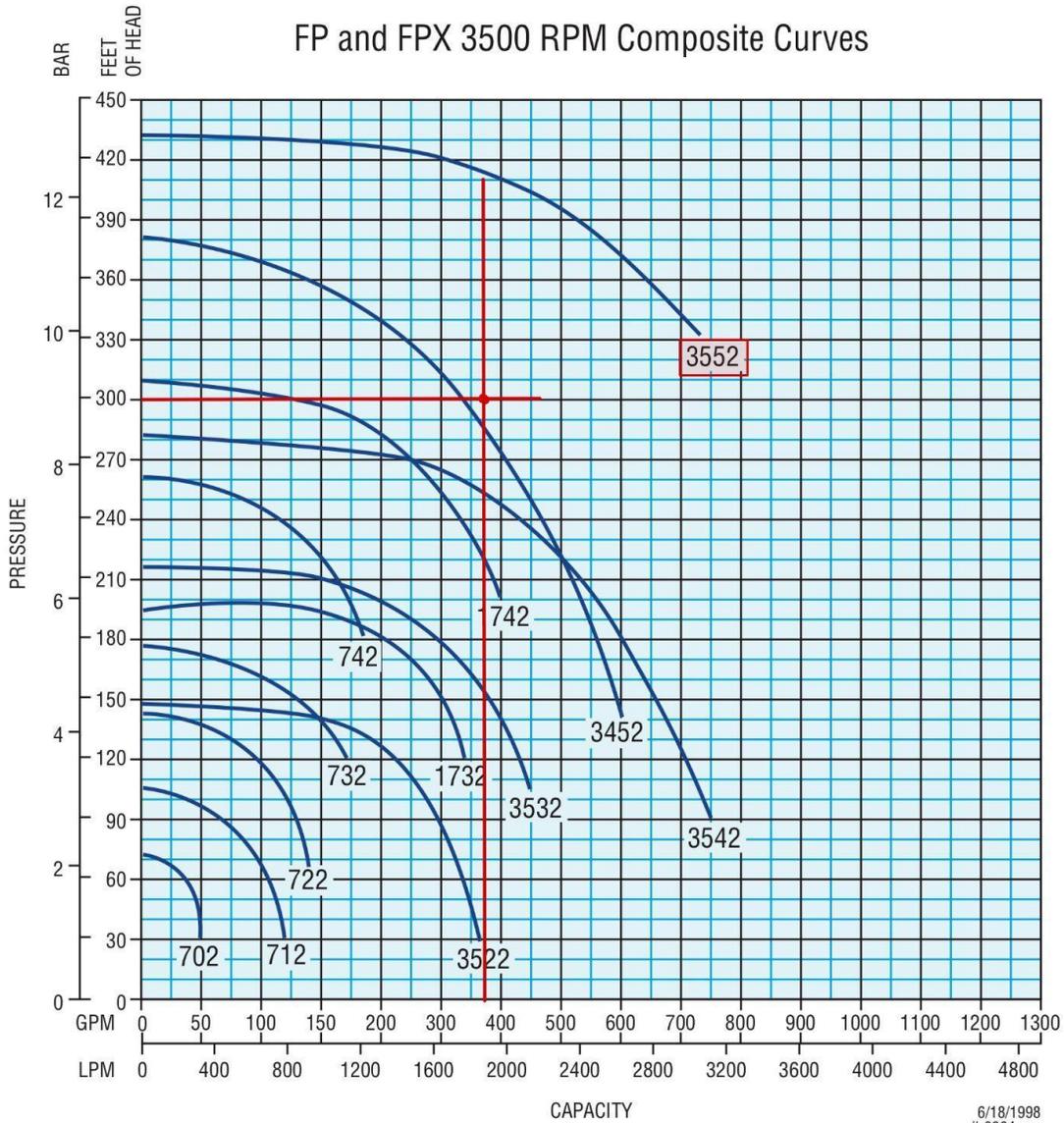


Performance curve based on tests using 70°F water and 0 psig inlet pressure. A tolerance of ± 5% applies to all figures. Actual performance may vary by application product. Please contact Fristam for different conditions.

P-19



FP/FPX Performance Curves Models: 3500 RPM (Composite)



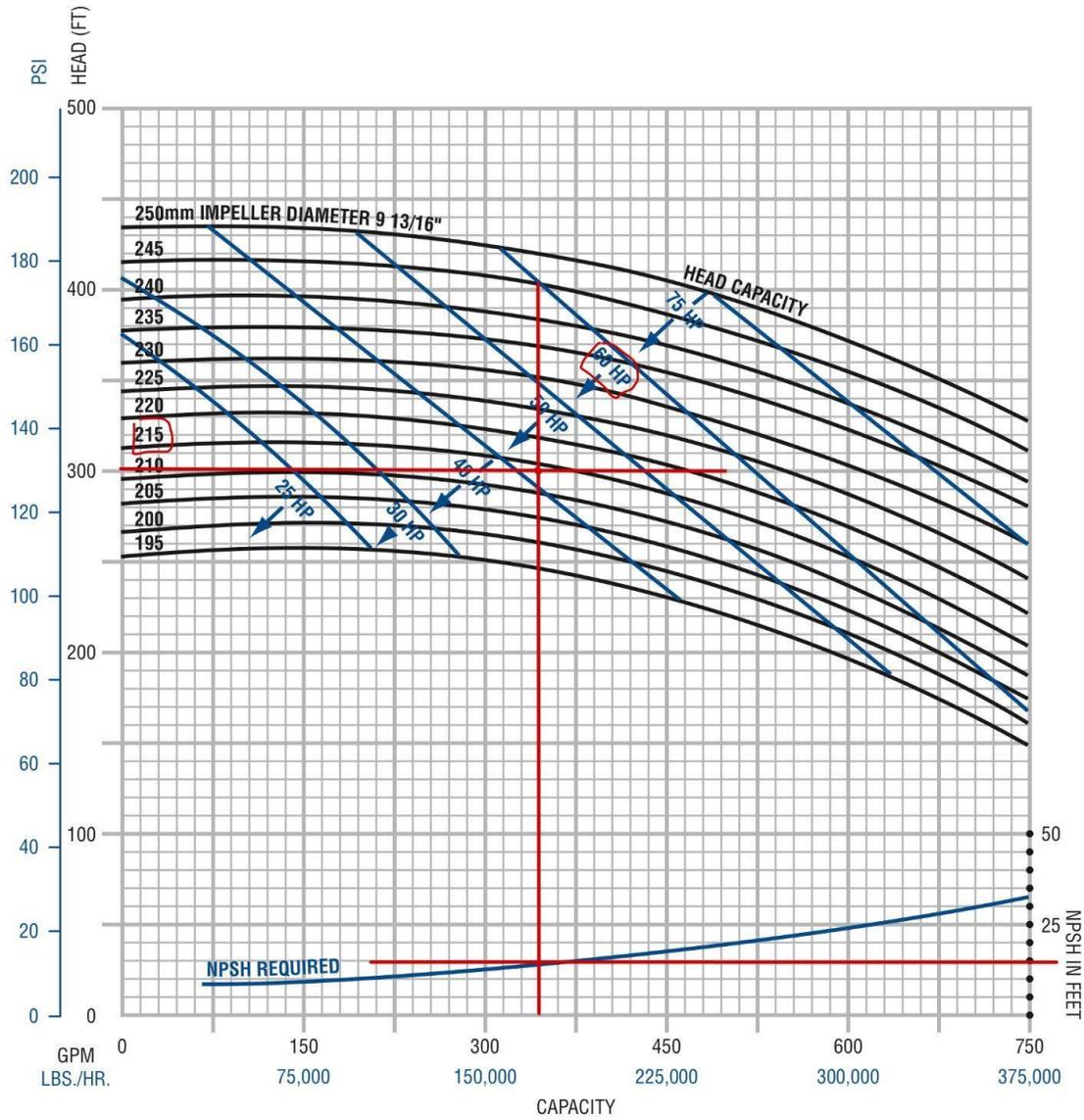
6/18/1998
il-0364.eps
RD 2/08

Performance curve based on tests using 70°F water and 0 psig inlet pressure. A tolerance of ± 5% applies to all figures. Actual performance may vary by application product. Please contact Fristam for different conditions.

P-19



FP/FPX/FPR Performance Curves
Model: 3552 (3500 RPM, Inlet 3", Outlet 2.5")

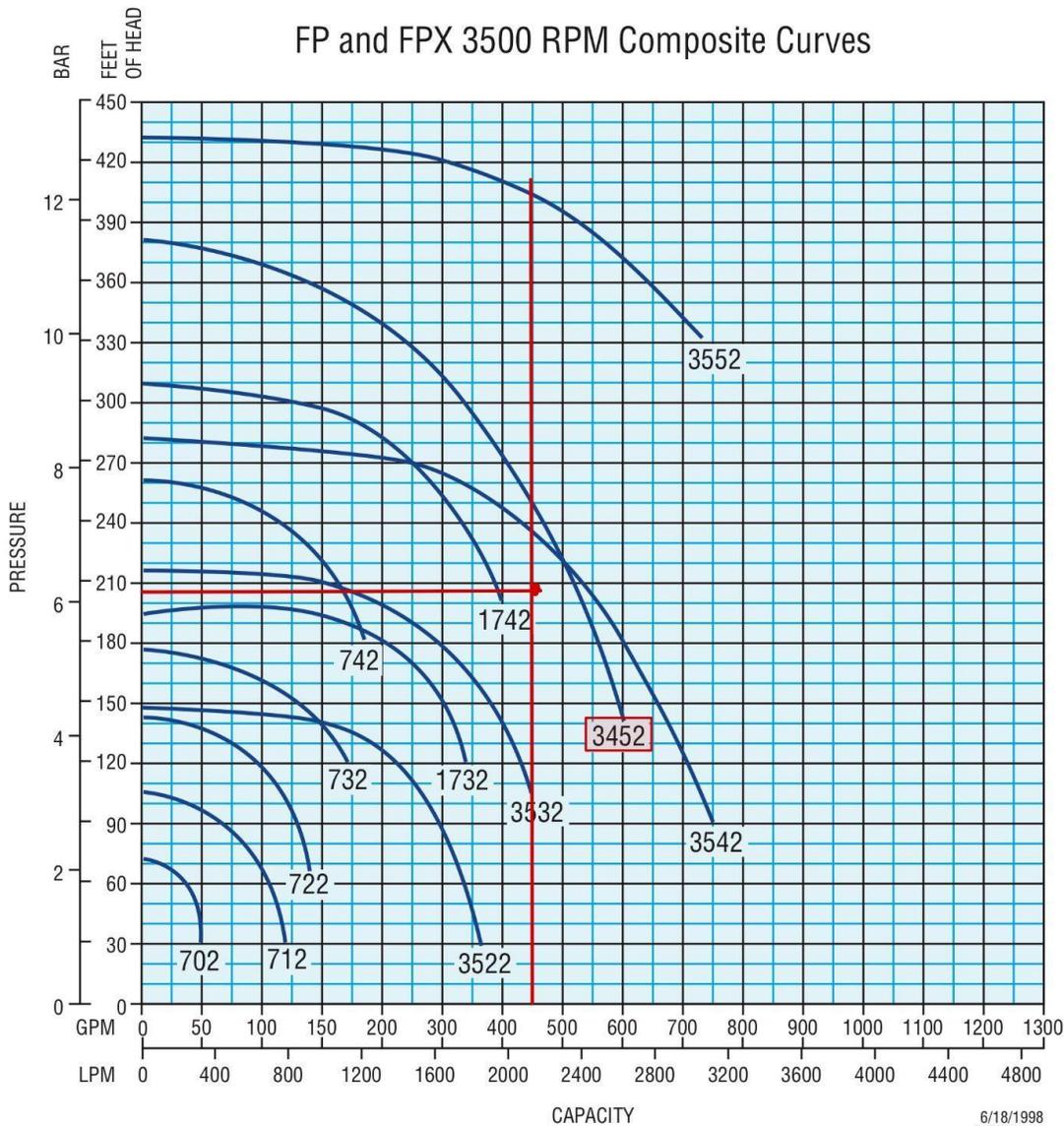


Performance curve based on tests using 70°F water and 0 psig inlet pressure. A tolerance of ± 5% applies to all figures. Actual performance may vary by application product. Please contact Fristam for different conditions.

P-20



FP/FPX Performance Curves Models: 3500 RPM (Composite)



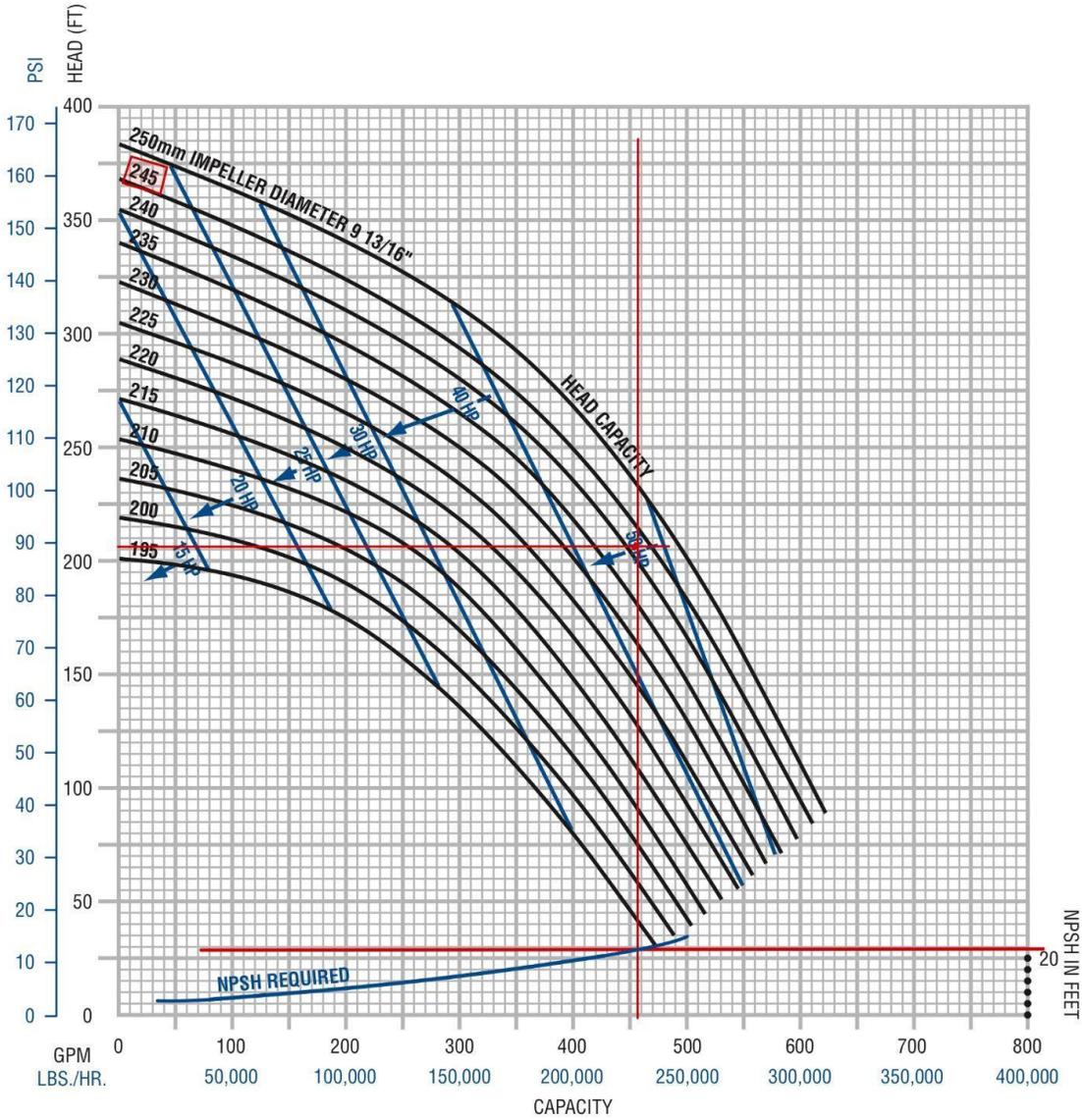
6/18/1998
il-0364.eps
RD 2/08

Performance curve based on tests using 70°F water and 0 psig inlet pressure. A tolerance of ± 5% applies to all figures. Actual performance may vary by application product. Please contact Fristam for different conditions.

P-20



FP/FPX/FPR Performance Curves Model: 3452 (3500 RPM, Inlet 3", Outlet 2")

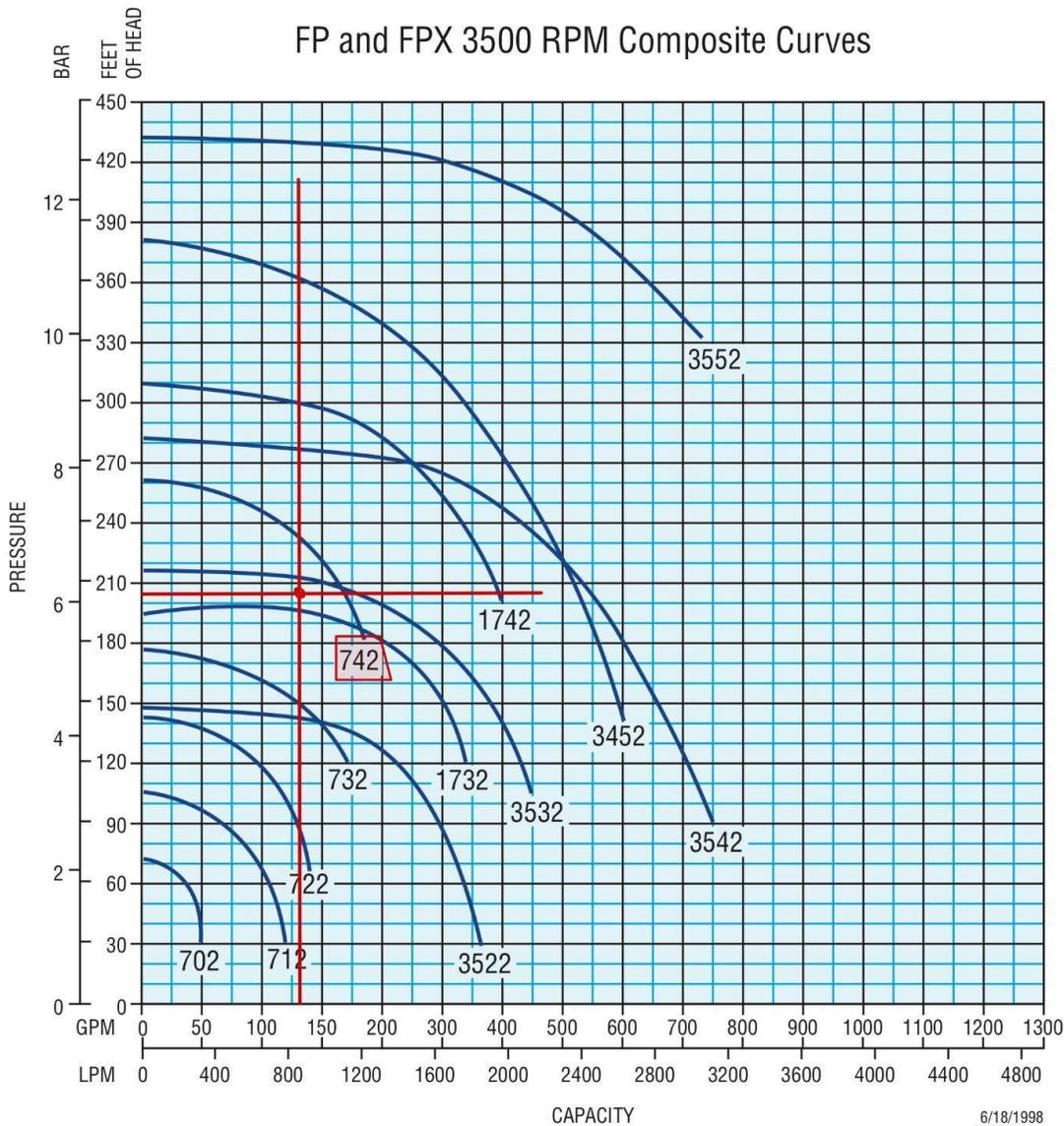


Performance curve based on tests using 70°F water and 0 psig inlet pressure. A tolerance of ± 5% applies to all figures. Actual performance may vary by application product. Please contact Fristam for different conditions.

P-21



FP/FPX Performance Curves Models: 3500 RPM (Composite)



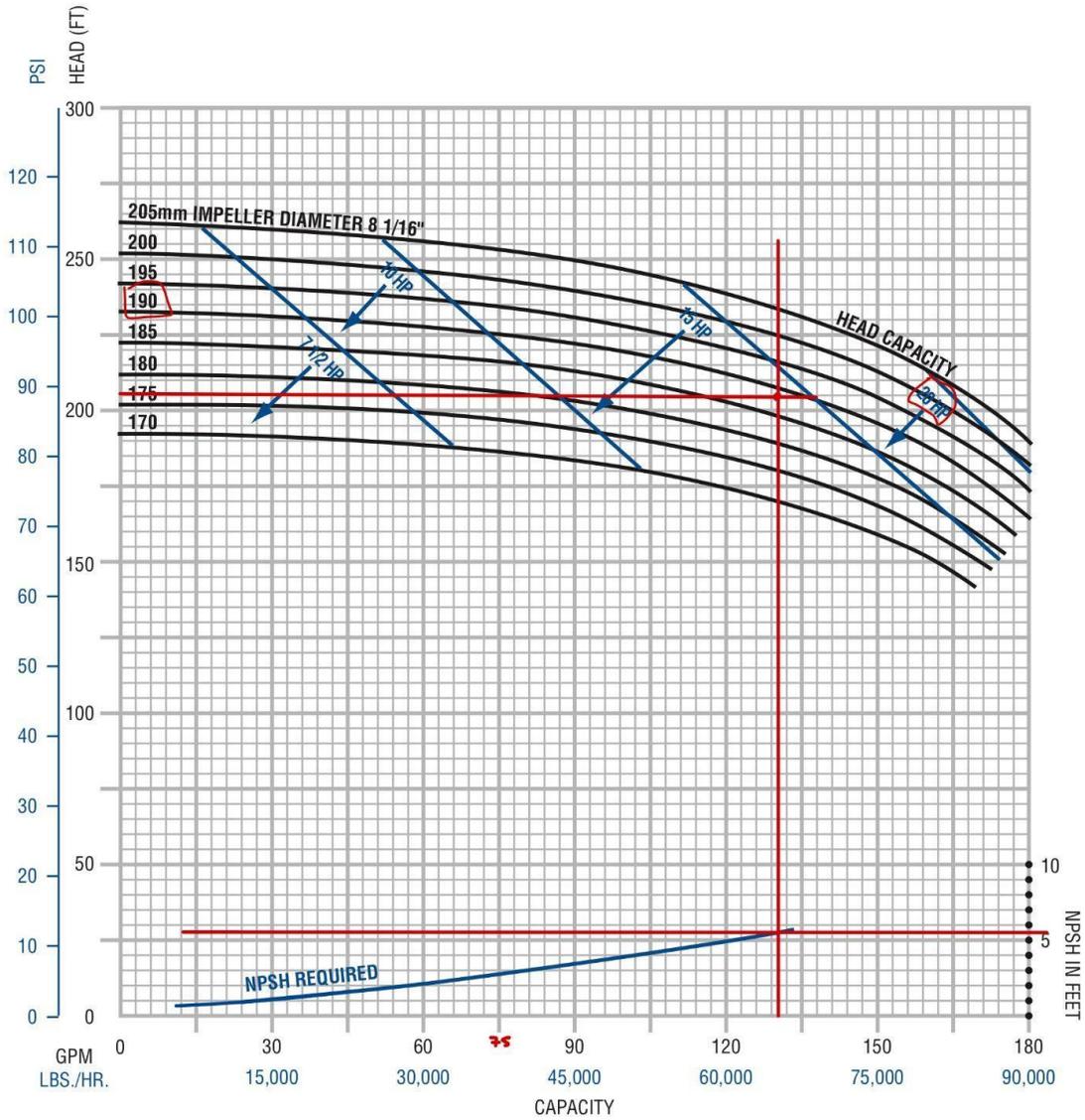
Performance curve based on tests using 70°F water and 0 psig inlet pressure. A tolerance of ± 5% applies to all figures. Actual performance may vary by application product. Please contact Fristam for different conditions.

P-21



FP/FPX Performance Curves Model: 742 (3500 RPM, Inlet 2.5", Outlet 2")

FPR model 742 covers the range of both the FP/FPX 732 and 742

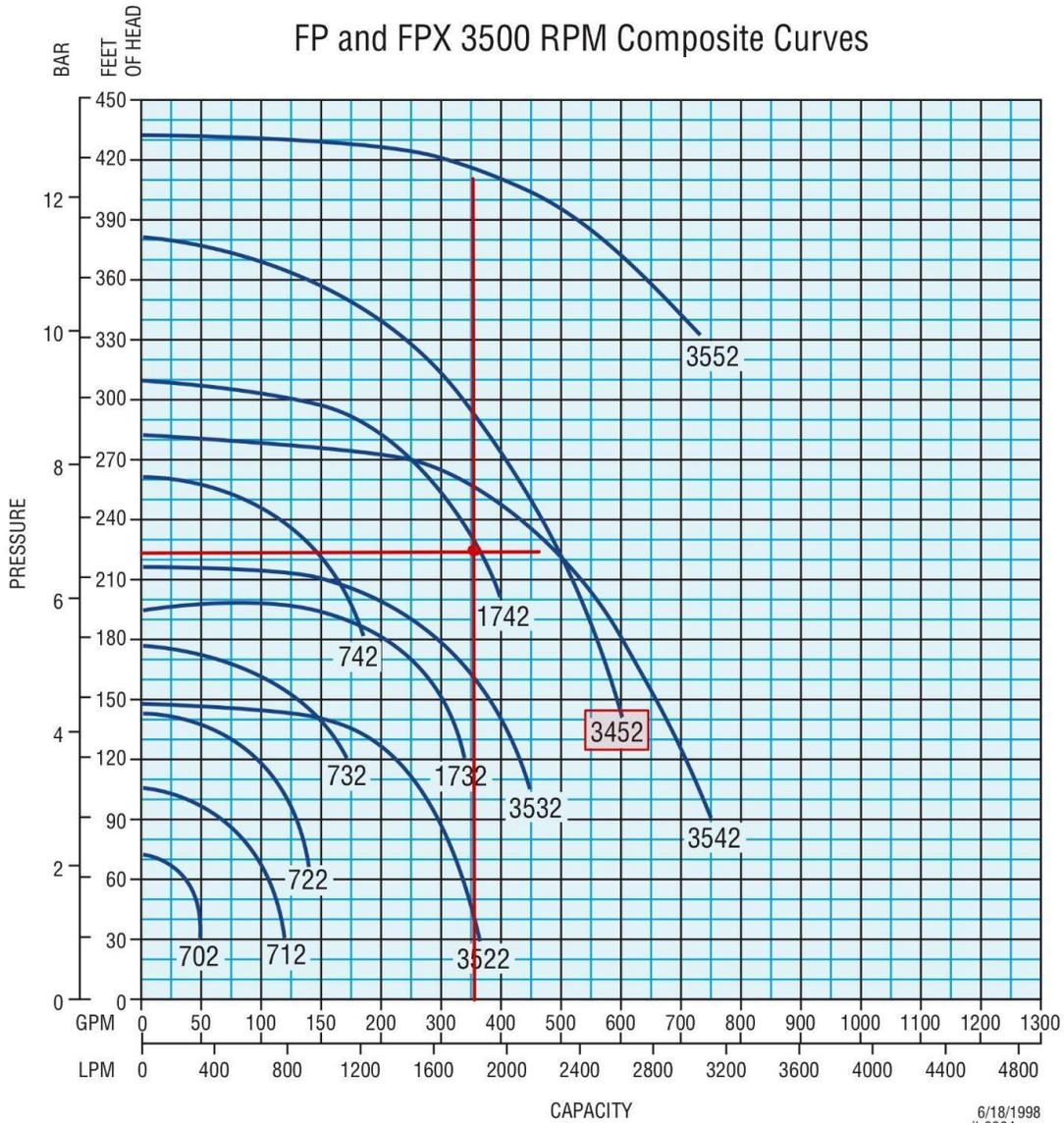


Performance curve based on tests using 70°F water and 0 psig inlet pressure. A tolerance of ± 5% applies to all figures. Actual performance may vary by application product. Please contact Fristam for different conditions.

P-22



FP/FPX Performance Curves Models: 3500 RPM (Composite)

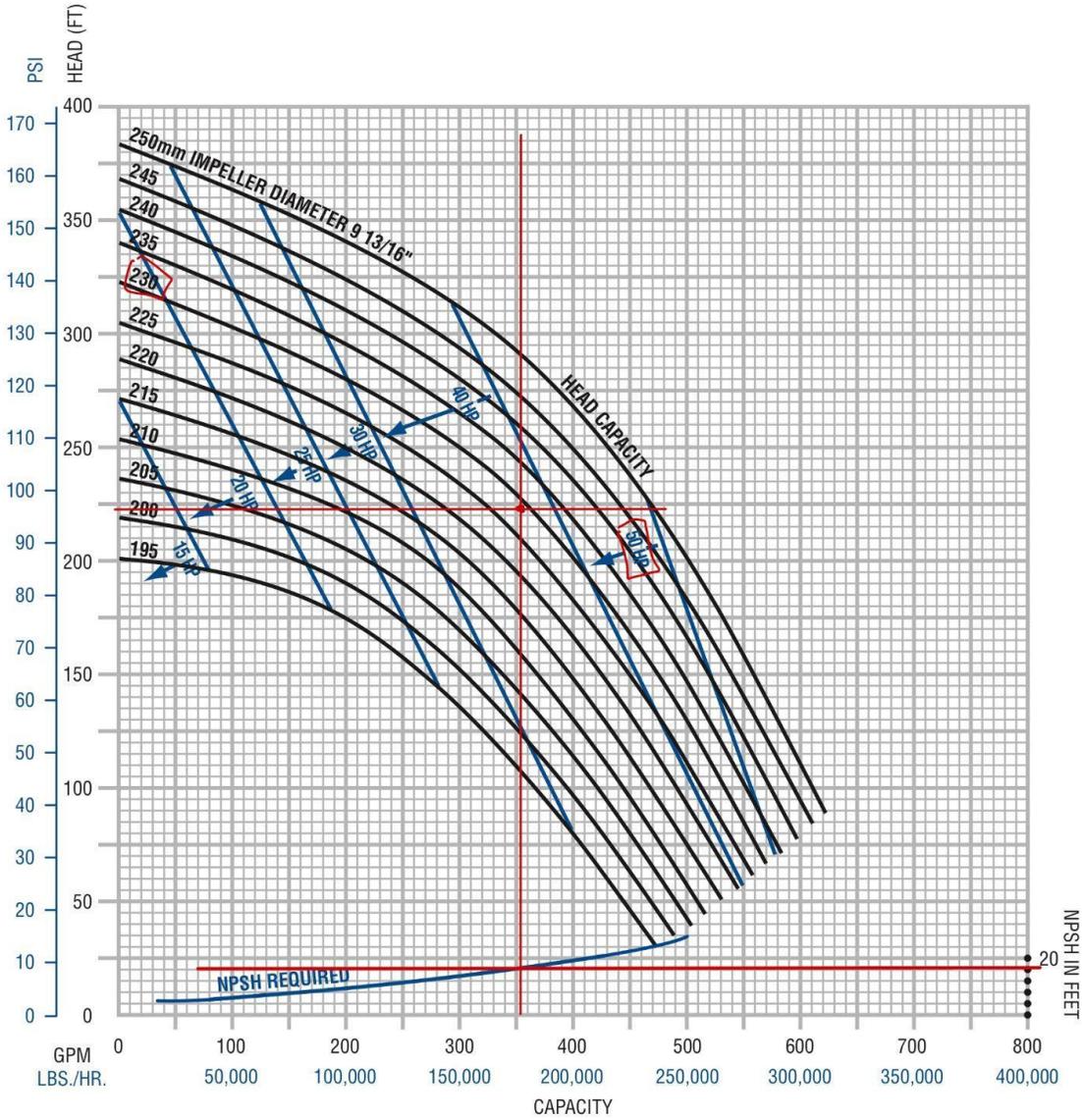


Performance curve based on tests using 70°F water and 0 psig inlet pressure. A tolerance of ± 5% applies to all figures. Actual performance may vary by application product. Please contact Fristam for different conditions.

P-22

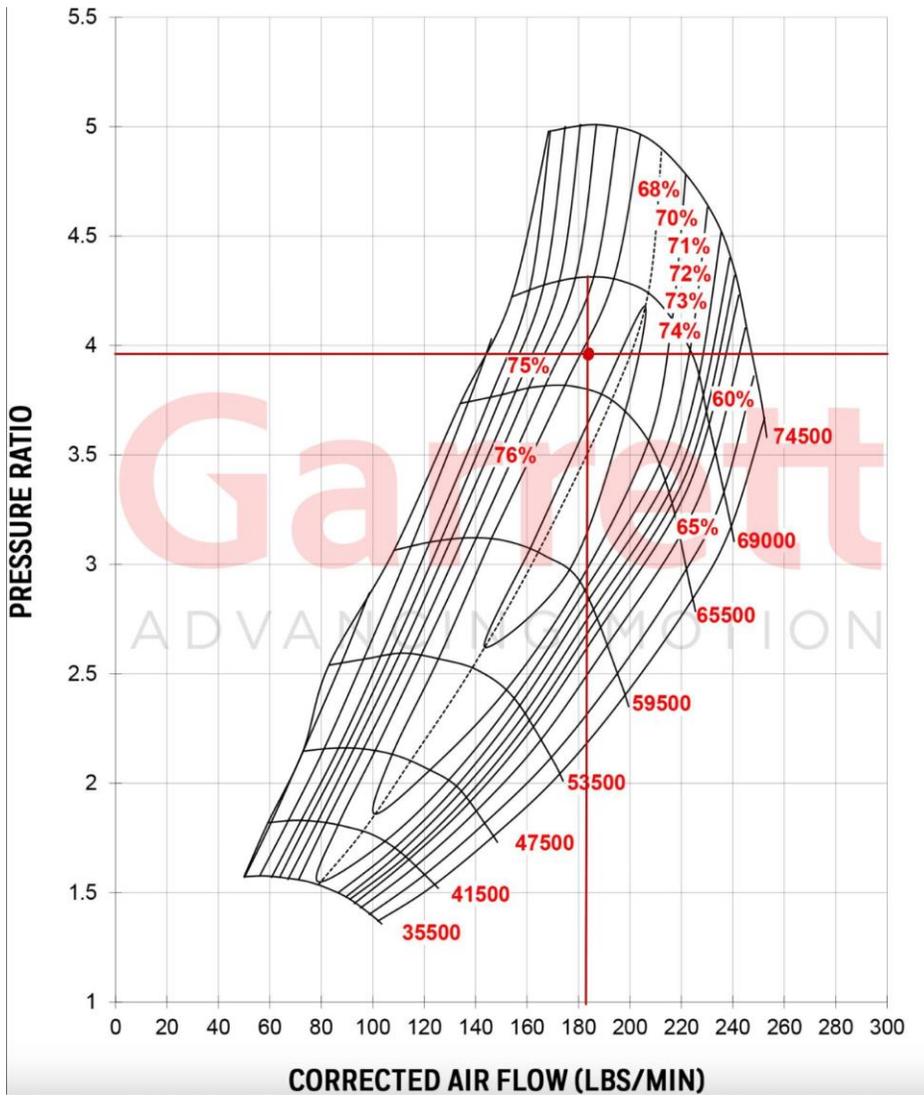


FP/FPX/FPR Performance Curves Model: 3452 (3500 RPM, Inlet 3", Outlet 2")



Performance curve based on tests using 70°F water and 0 psig inlet pressure. A tolerance of ± 5% applies to all figures. Actual performance may vary by application product. Please contact Fristam for different conditions.

Appendix F: Compressor Curve



Appendix G: Heat Exchanger Correction Factor Curves

Correction factor graphs used in heat exchanger design. All are sourced from Seider, W. D., et al. (2017).

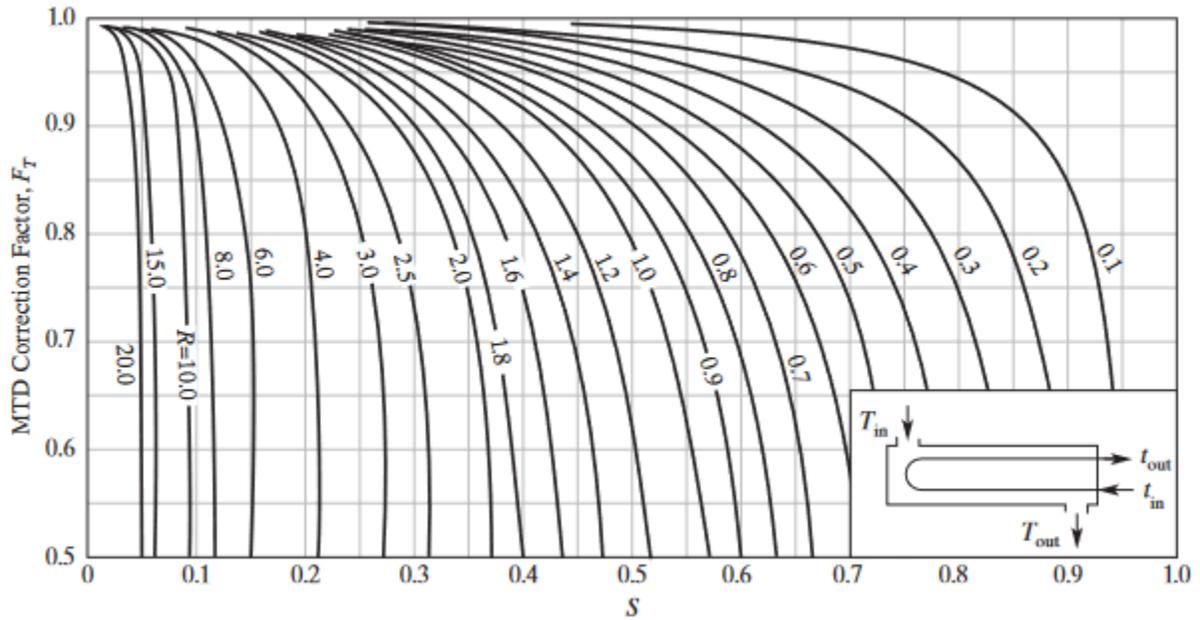


Figure B.1. “Temperature-driving-force correction factor for 1-2 shell-and-tube heat exchanger”.

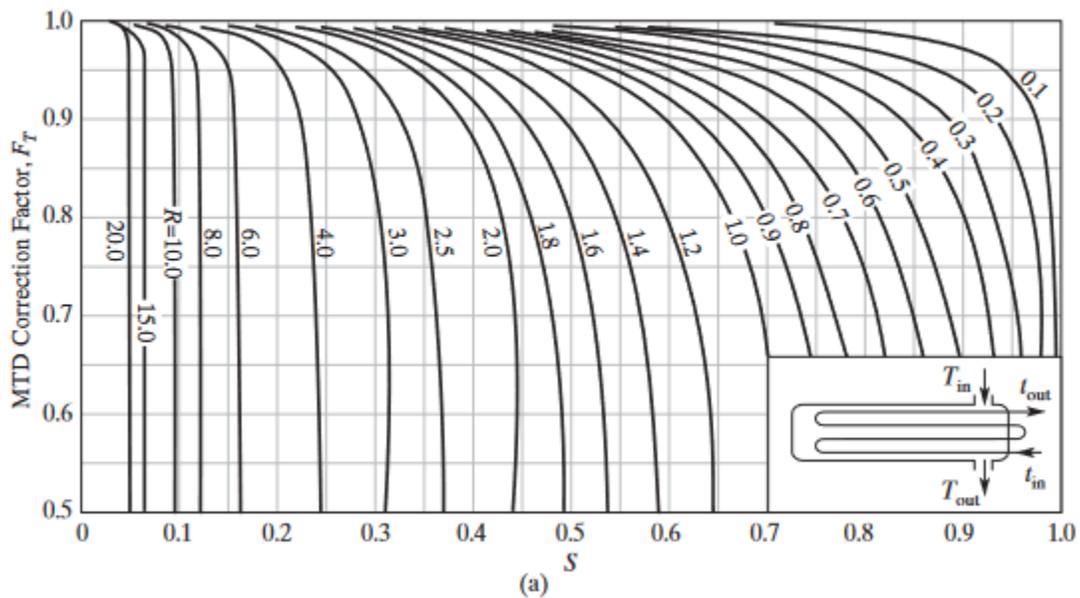


Figure B.2. “Temperature-driving-force correction factor for 2-4 shell-and-tube heat exchanger”.

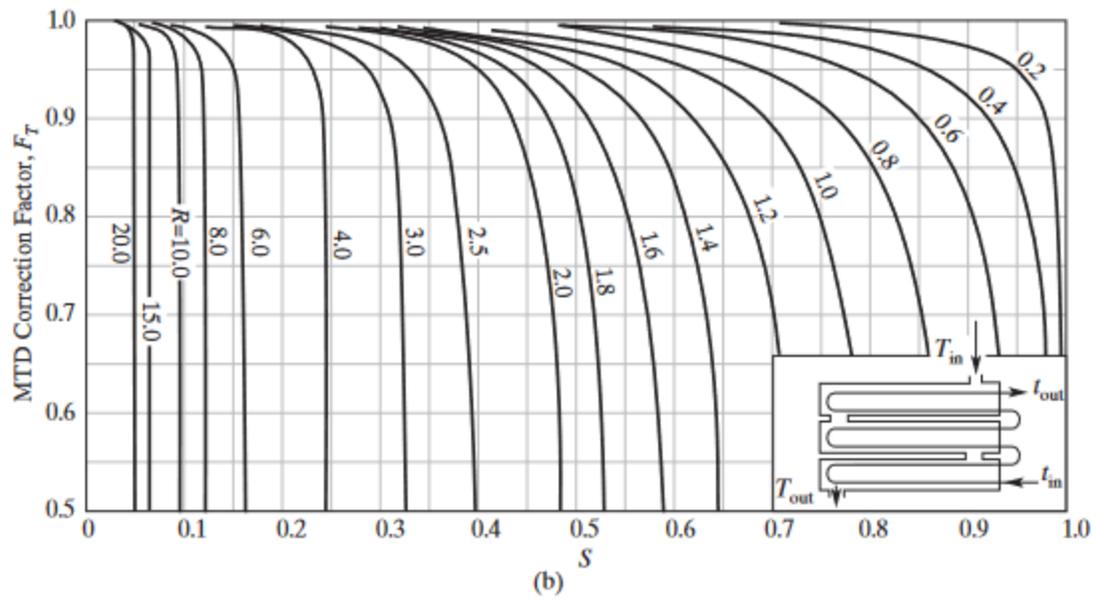


Figure B.3. “Temperature-driving-force correction factor for 3-6 shell-and-tube heat exchanger”.

Appendix H: Addendum to Section 9

- The plant capacity was found to be 443,557,259 gal per year. This value was found by summing all four product streams and multiplying that value by 8040 operating hours per year.
 - The operating hours were obtained by subtracting the 30 days of maintenance per year, and converting the remaining 335 days to hours since the plant runs continuously.
- The availability/purity of ingredients was found to be \$2.74 per gallon of product. This contributed, alongside utilities and byproduct credits, to a total variable cost of \$1.72 per gallon of product.
- This plant is an addition to an existing facility.
- Located in California. County unknown. Estimated as a West Coast area plant in the Economics spreadsheet with Macros.
- Availability of Utilities
 - It should be noted that all utilities were hand calculated from values in Aspen and not taken from the Heat Integration results. This is due to the fact that there are non-real heat exchangers in the simulation to emulate reactor environments (because of black box reactors) and this led to non-real utility results. As such, all utility values should be treated as a rough estimate given limited information.
 - Steam
 - LP Steam: Available at a price of \$27.78 per klb. LP Steam usage was calculated from utility flow in Aspen of low temperature or pressure columns. Specifically; LPG Sep, C3 Sep, and iC4 Sep Lyt. Column names are listed verbatim to how they are labeled in the Aspen Simulation. This totalled to 2.95E06 klb/year, which translates to 0.01 units required per gallon of product.
 - HP Steam: Available at a price of \$30.03 per klb. Inversely to LP Steam, HP Steam usage was calculated from utility flow of high temperature or pressure columns. Specifically; Hvy Sep, C4 Sep Lyt, iC5 Sep, and Jet Splitter. This totalled to 2.26E06 klb/year, which also translates to 0.01 units required per gallon of product.
 - Electricity
 - Available at a price of \$0.42 per kWh, the sum of load of the heat exchangers, pumps, and cooler equalled 3.56E08 kWh/year. This translates to 0.80 units required per gallon of product. The pumps used the most power out of any piece of equipment, at a sum of 5.04E06 kWh for all 22 pumps.
 - Cooling Water
 - Restated price of cooling water from \$10 per year per GPM to terms of \$/gal via time conversion factors, resulting in a volume basis price of effectively \$0/gal. Amount of cooling water needed was summed across all heat exchangers from the heat exchanger design, totalling to 3.21E08 ft³/year, translating to 0.72 units of cooling water required per gallon of product. Due to the extremely cheap price, cooling water did not contribute significantly to the cost.
- This plant is continuous.
- Recycle stream considerations:
- Purity of Product(s): detailed in the Refinery Table in **Appendix D**
- Assumptions made for all equipment/utilities:
 - assumed that cooling water is onsite

- assumed that all pumps are included in new equipment
- assumed a cartridge filter for all filters
- assumed a packed bed absorption unit for Chlorine absorbers, with molecular sieves as the absorber and carbon steel & API horizontal tanks of sizes equal to the volumes determined in **Section 7.5.2**