# Analysis of Heat Recovery Techniques Applied to a Xylene Production Plant

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#### Abstract

The production of xylene (an important petrochemical in a variety of industries) has been steadily increasing over the past few years. Due to this, maximizing heat recovery in large scale xylene production facilities could have significant economic benefits. After analyzing the system using pinch analysis, the  $Q_{hmin}$ ,  $Q_{cmin}$  and  $T_{pinch}$  values of the pilot plant analyzed are 2855.987 KW, 2824.387 KW and 254.3° C when  $\Delta T_{min} = 10^{\circ}$  C. After integrating the network, the savings of doing so would prove to be greatly beneficial to both the company running the process as well as for the environment. By redirecting the energy appropriately, the yearly operational costs and carbon dioxide emissions can be reduced significantly.

The heat from the streams can also be utilized to run a Carnot engine and produce work that can be used to run other processes. Using carbon dioxide as the working fluid around supercritical conditions, an engine can be used to replace 1521.768 kW that would otherwise be supplied by a cooler to produce 225.746 Joules of work per cycle of the piston cylinder system. Carbon dioxide also proved to be the most appropriate supercritical working fluid for the network as compared to ethane, methane and water. Another process of heat recovery is steam raising, where an independent cold stream of water enters the process and absorbs as much heat as possible to become steam by maximizing the incoming flow rate through an iterative process carried out in Python. Using this process, we can calculate the theoretical value taken out of the system to be 27851 kW. Lastly, the developed networks from each of the different sections were analyzed by eigenvector centrality. Eigenvector centrality is a display of the connections between parts of the network and leads to conclusions of the dependence of the network on certain portions on a scale of 0 to 1. In each of the networks, there are a few important streams that have numerous connections and each of the heat exchanger areas calculated in order to analyze feasibility and vulnerabilities within the system.

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#### 1. INTRODUCTION

Xylene is a volatile hydrocarbon generated in many chemical plants as a product of the catalytic disproportionation of toluene. This reaction will yield ortho(o), para(p) and meta(m) isomers of xylene. In general, xylene has a wide variety of uses such as a solvent in printing, rubber and leather industries and can also be used in cleaning agents, paint thinners and varnishes. Most p-xylene is processed into into polyethylene terephthalate (PET), a common plastic used in many industries. One example of PET's usage is found in plastic water bottles and other plastic food containers. P-xylene is also used in the manufacture of purified terephthalic acid (PTA), a basic petrochemical used in the textile industry for the production of polyester[1]. Production of this chemical has been growing for the past 15 years at a steady pace[12]. In Asia specifically, polyester producers have gotten into the purified terephthalic acid business to increase cost competitiveness and as a result over 70% of global market of xylene is in Asia. In a recent news article from Houston Business Journal, ExxonMobil Chemical Co.'s Singapore affiliate will buy one of the world's largest aromatics plants from Jurong Aromatics Corporation Pte Ltd. [9]. This will allow Exxon to increase their production of paraxylene by 1.4 million additional tonnes per year. President of ExxonMobil Chemical claims, "Our growth in Singapore is driven by the expected increase in global demand for chemical products over the next decade of nearly 45%, or about 4% per year, which is a faster pace than energy demand and economic growth[9]. This data shows there will be a constant increase in the global production of xylene, specifically in Asia, and more plants will need to be built to satisfy the demand. This information gives context to the project as the plants that will be implemented are similar to the plant being analyzed, meaning the energy optimization techniques applied in this paper could be applied to actual systems in the near future.

### 2. Energy Analysis

The pilot plant for this process is a scaled down model for purification of benzene and xylenes. Through the process there are hot and cold streams, reboilers, and condensers that are used to produce the desired product on a large scale. While an arrangement of these streams and distillation columns work, it is not the optimal solution and has a lot of wasted energy and heat. By properly integrating the system, the wasted heat can be minimized so that the system can be optimized for the process development.

Proper heat exchange and column integration within the network begins with identifying and labeling the hot and cold streams available. At the surface of heat exchange networks, connections between hot and cold streams can be made so the energy of the hot streams can be used to heat the cold streams to their final temperatures. If there is any excess/deficit of heat such that a stream does not reach its target temperature, heaters/coolers can be applied to the system that require outside heat to power them.

For the entirety of process, it is highly preferred that a process be at steady state so that it can continually run. For that to be feasible, however, the mass and energy of running the production has to be balanced such that mass or energy in minus mass or energy out is equal to zero. For the mass balance at each section of the process can be balanced by equation 1 to show that there is no accumulation of any of the chemicals.

$$\frac{\partial m_i}{\partial t} = 0 \tag{1}$$

For the energy balance, the enthalpies of each of the sections of the stream need to be found such that it satisfies equation 2 that states that the difference between the beginning and ending enthalpies are equivalent to the enthalpy of a heat exchanger that transfers energy.

$$H_1 - H_2 = H_{exchanger} \tag{2}$$

When applied to each section of the network given, the mass and energy balances out at all parts allowing for this system to be optimized by pinch analysis.

Pinch analysis is the breakdown of understanding how to properly integrate a network based the temperature differences of hot and cold streams. The integration begins around the pinch temperature which is determined by the point where the hot and cold streams are exactly separated by  $T_{min}$  when compared graphically, meaning that there is no available heat for transfer at that exact point. The pinch temperature will decide how the network will be divided and provide a basis for establishing the connections between the streams [6].

The process that was integrated in this paper is shown in Appendix i.

The energy requirements of the pilot system at a  $T_{min}$  of 10° after integration are  $Q_h = 2856$  kW,  $Q_c = 2824$  kW, and  $T_{pinch} = 254.3^{\circ}$  (Appendix xiii). If  $T_{min}$  is set to 20°,  $Q_h = 2880.4$  kW,  $Q_c = 2848.8$  kW, and  $T_{pinch} = 259.3^{\circ}$  (Appendix xiv). For the full scale plant, each of these  $Q_s$  are multiplied by 10 to account for the difference in scale. The cost of the full scale plant can be calculated using Equations 3, 4, and 5.

$$CapitalCost = \frac{12.5 * 10^6 *^{\circ} C * \$}{.05T_{min}}$$
(3)

$$OperationCosts = \frac{\$.15Q_h t}{kW * hr} \tag{4}$$

$$TotalCost = \frac{12.5 * 10^6 * CC * \$}{.05T_{min}} + \frac{\$.15Q_h t}{kW * hr}$$
(5)

The  $Q_h$  versus  $T_{min}$  is shown in Figure 1 for  $T_{min}$  in the range of  $10^{\circ}$  to  $40^{\circ}$ .

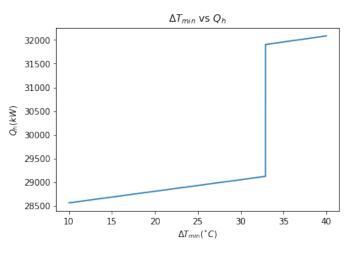


Figure 1:  $\Delta T_{min} vs T_{min}$ 

The spike in  $Q_h$  is due to a change in the pinch temperature. We can see that  $Q_h$  generally remains lowest below a  $T_{min}$  of 30°.

Capital cost versus  $T_{min}$  is shown in Figure 2 for  $T_{min}$  of 10-40°.

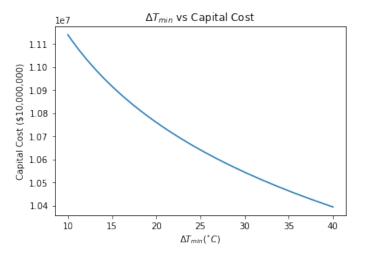


Figure 2:  $\Delta T_{min}$  vs Capitol Cost

This shows that capital cost declines with increasing  $T_{min}$ . Operation cost versus  $T_{min}$  for a period of 1 year is shown in Figure 3 over the same  $T_{min}$  range.

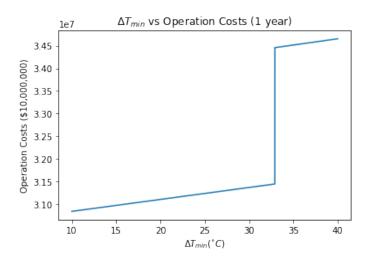


Figure 3:  $\Delta T_{min}$  vs Operational Cost

This graph follows a similar trend to  $Q_h$ , since operation cost is a variable of  $Q_h$  and time. The ideal  $T_{min}$  to minimize operating costs for the long term is 10°.

A 3D graph of Cost vs. Time vs.  $T_{min}$  is shown in Figure 4.

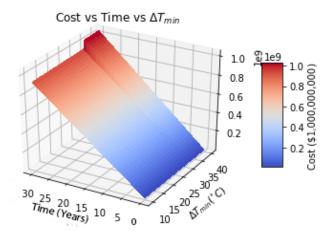


Figure 4: 3D Graph of Cost vs. Time vs. T<sub>min</sub>

This shows that while the initial cost is controlled by the capital cost, the final cost of the system will be mostly be controlled by the operating costs since these are a function of time. Because of this, depending on the number of years the plant operates, the ideal  $\Delta T_{min}$  will change over time.

Figure 5 shows the total cost for one year versus  $T_{min}$ .

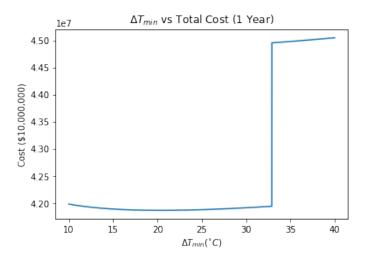


Figure 5: Costs After One Year

After 1 year of running the plant, we find that the lowest cost of the system would be \$41,870,000, at a  $T_{min}$  of 20.384°.

Due to observations above, a  $T_{min}$  of 10° will eventually become the most viable option at some time "t". This t was calculated in Appendix xv, along with the graphs above. From this, it can be seen that the optimal  $T_{min}$  will become 10° after 634 days (or 2 years and 34 days if running the system 300 days a year) and beyond. This means that all calculations in the following paper are most economically viable if the system runs for at least 634 days, since all following calculations assume 10°.

#### 3. Environmental Analysis

By utilizing the heat exchange network that was assembled in section 2, there are clear advantages to being more efficient with the energy available. Instead of underutilizing the available energy in the system, by integrating the pinch analysis there are not only cost savings involved which is beneficial to the company but the reduced impact on the environment is helpful on a global scale.

To be able to do the calculations of how much is saved by integrating, there were conversion values about the pricing and energy relations of coal. The information used to find the information was:

- 1. Coal's energy density is 6.67 kWh/kg.
- 2. Coal power plants are approximately 30% efficient.
- 3. The cost of coal is approximately 60.00/1000 kg coal.
- 4. 1 kg of coal produces approximately 1.83 kg carbon dioxide.
- 5. The plant runs 24 hours a day for 300 days a year.

The amount of heat that is required by the integrated network is the sum of the required heat to warm the cold streams as well as the heat necessary to run the reboilers of that system. With the integrated network, the heat needed is simply the  $Q_h$  value that is output after integration. Both of those values for heat apply to a full scale plant that is ten times larger than the pilot plant listed in the assignment details. The savings are listed in Table 1.

Unintegrated Plant Design		Integrated Plant Design	Savings
Total Heat Needed (kW)	42,678.00	28,559.87	14,118.13
kWh/year	307,281,600.00	205,631,078.40	101,650,521.60
Coal Needed (kg)	153,564,017.99	102,764,157.12	50,799,860.87
Cost of Coal	\$9,213,841.08	\$6,165,849.43	\$3,047991.65
Carbon Emissions (kg)	281,022,152.92	188,058,407.53	92,963,745.39

Table 1: Savings Made by Integration

#### 4. Steam Raising

In most factories, a significant portion of heat put into large scale processes is output as waste due to the inability of the plant to utilize that heat. Finding a way to use this waste heat would be of financial interest to any large scale manufacturing plant and pinch analysis, discussed in section 2, explains the methodology and techniques used to analyze the process system. While it is difficult to reuse low grade heat ( $< 100^{\circ}$ ), high grade heat ( $>100^{\circ}$ ) can be recycled in the form of steam. This is achieved by transferring heat between existing hot streams and streams of water or steam. In this situation the water stream is essentially a cooler since it removes heat from the system and therefore the water stream can replace coolers in the network. Due to the constraints of this system, this process can only be used below the pinch and in order to determine the constraints of the water stream, the Grand Composite Curve (GCC) of the system below the pinch can be analyzed in Figure 6.

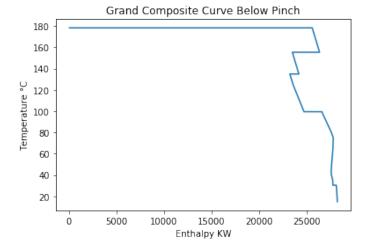


Figure 6: Grand Composite Curve Below Pinch

To generate the GCC graph, the interfacial temperatures from the heat cascade must be plotted with their corresponding enthalpies. By using the endpoints of a line segment and Equation 6, the points between any two endpoints can be plotted and a complete graph of line segments can be compiled using

$$\frac{T_2 - T_1}{H_2 - H_1} = \frac{T - T_1}{H - H_1} \tag{6}$$

where  $(H_1, T_1)$  and  $(H_2, T_2)$  are the end points to any of the GCC line segments and  $\frac{T_2-T_1}{H_2-H_1}$  is the slope of every point between the 2 endpoints. Using the slope, the values along the GCC between the endpoints can be calculated. This method is also used to calculate the points between each steam raising line. Values for H1, H2, T1, and T2 for each segment are from the steam raising code in Appendix vii.

The GCC is a graphical representation of the heat cascade analysis, with each temperature associated with a kW value and shows, graphically, the maximum heat that can be taken from the system. Steam lines are one way to find that maximum heat. These lines are graphed on the GCC using specific thermodynamic properties of water and steam[4]. By keeping your steam lines just within the GCC lines, the pinch condition is satisfied while attaining the maximum flow rate ie. the maximum heat transfer. For this system, water at the inlet is  $25^{\circ}$  ( $30^{\circ}$  shifted) and heated to  $120^{\circ}$  ( $125^{\circ}$  shifted). Heating the water to  $120^{\circ}$  will evaporate the water to steam and thus all the stages of heating water need to be considered. The calculations for this require the Equation 7, Equation 8, Equation 9 for the sensible, latent and superheating stages.

$$M_w = \frac{H_{start} - H_{wsat}}{C_{pw}(T_{sat} - T_{start})} \tag{7}$$

$$M_w = \frac{H_{Wsat} - H_{ssat}}{\Delta H_{vap}} \tag{8}$$

$$M_w = \frac{H_{ssat}}{C_{ps}(T_{final} - T_{start})} \tag{9}$$

These 3 equations give 4 unknowns;  $H_{start}$ ,  $H_{wsat}$ ,  $H_{ssat}$  and MW. With one degree of freedom, If  $H_{wsat}$  is guessed, the above 3 equations can be combined into:

$$H_{ssat} = \frac{C_{ps}H_{wsat}(Tfinal - Tsat)}{Hvap + Cps(Tfinal - Tsat)}$$
(10)

$$H_{start} = H_{wsat} \left(1 + C_{pw} \frac{T_{sat} - T_{start}}{\Delta H_{vap}}\right) - H_{wsat} \left(C_{pw} C_{ps} \frac{T_{sat} - T_{start}}{\Delta H_{vap}}\right) \left(\frac{T_{final} - T_{sat}}{\Delta H_{vap} - T_{sat}}\right)$$
(11)

$$Mw = \left(\frac{H_{wsat}}{\Delta H_{vap}}\right)\left(1 - C_{ps}\frac{T_{final} - T_{sat}}{\Delta H_{vap} + C_{ps}(T_{final} - T_{sat})}\right)$$
(12)

By guessing the  $H_{wsat}$  value just outside the GCC of the same temperature, a corresponding flow rate is produced. This analysis requires an iterative reduction of  $H_{wsat}$  until it is just touching the GCC. Once that is satisfied, look to make sure the "corner points" (GCC line segment endpoints) are all less than the corresponding GCC enthalpies at the same temperature. If any of these criteria are not met, Mw will iterate through at a smaller Hwsat changing the shape of the graph and the value of Mw. Finally, if  $H_{ssat}$  is less then or equal to 0, no solution can be found. This process can be verified using computational tools like Microsoft Excel or Python below. Using the GCC data and the initial conditions, the full scale plant can be calculated to have a maximum flow rate of 10.67 Kg/s. The is the maximum heat taken out of the system is equal to  $H_{start}$ , 27851 kW. All of this computation was done by a Python code in Appendix vii

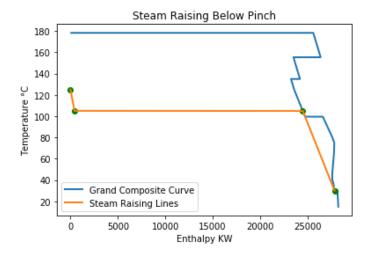


Figure 7: From right to left:  $(H_{start}, T_{start}), (H_{Wsat}, T_{sat}), (H_{ssat}, T_{sat}), (0, T_{Final})$ 

#### i. Integrating Steam Raising into the Heat Exchange Network

A new heat exchanger network was designed for the purpose of utilizing steam raising to get as much heat as possible out of the heat exchange network. This network will have multiple pinches due to the fact that no energy will be left in the system at the original pinch, and no energy will be available at two other points due to the steam raising process taking all available energy. These points are at shifted temperatures of  $105^{\circ}$ C and  $45^{\circ}$ C, in addition to the existing pinch at  $254.3^{\circ}$ C. These pinches were calculated through the python pinch analysis code in Appendix xvii. Due to the existence of three pinches, the network must be changed a great deal to adjust for steam raising and is pictured in Appendix iii. Realistically, the ideal  $Q_c$  and  $Q_h$  calculated from the code in Appendix xvii cannot be reached through the system. The actual  $Q_c$  the network can support in the full scale plant is is 660.39 kW, versus the calculated 441.77 kW. In the same vein, the  $Q_h$  that the network can actually support is 28,780 kW, versus the calculated 28,560 kW. Due to this, about 220 kW needs to be added to the system that will be removed by coolers later. However, steam raising uses 27,585 kW that would otherwise be unused, so this small change to  $Q_c$  and  $Q_h$  is well worth it because so much extra energy that would be wasted by the system is now being used. This steam could then be used to power a turbine if the plant wanted to use this energy to generate electrical energy.

#### 5. CARNOT CYCLE

#### i. Carnot Cycle Construction

Another method to utilize the waste heat is to convert to work using the Carnot Engine. The Carnot engine is a basic thermodynamic model of an engine that displays the change in pressure and volume between two specific isotherms. A piston cylinder system within the engine will expand and contract based on the limits that are created by the isotherms. The net result of the movement of the pistons produce work that can be used to move whatever is required by the system.

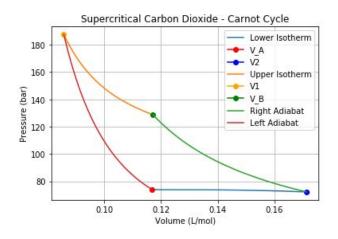


Figure 8: The Carnot Cycle of Supercritical Carbon Dioxide

To develop this system, the amount of work the engine produces depends on the fluid that is used to move the piston. For this engine, carbon dioxide near its critical conditions will be used. By staying near the super critical conditions, pressure becomes a weak function of volume and thus the isotherms become flatter. The flatter the isotherms, the greater the difference between them, which increases the potential work that can be extracted from the engine. The critical conditions dictate how some of the parameters of this analysis were established to allow for other parameters of the engine to be changed effecting the outcome of work.

In order to build the Carnot cycle, the volume range of any curve needs to be established. To stay around the critical conditions, the critical volume of the fluid can be calculated by Equation 13 [8], after being given critical pressure and temperature. By initially being given the critical pressure,  $P_c$ , and the critical temperature,  $T_c$ .

$$V_c = \frac{3RT_c}{8P_c} \tag{13}$$

Once the critical volume is established, the range of the volume can be determined by centering the range over the critical volume. The length of the range is determined by the compression ratio of the fluid. The compression ratio is the relation between the maximum and minimum volumes of the fluid represented by  $V_1$  and  $V_2$ , respectively. The compression ratio was set at 2 for the purposes of this project to allow for there to be a reasonable amount of movement of the fluid when the heat is added to the engine.

The next two parameters established were the isotherms that are used to create the heat difference that moves the piston. The lower isotherm was set as the critical temperature of carbon dioxide to ensure that the fluid can remain, at minimum, near the critical conditions. The upper isotherm was determined by selecting a unit that was attached to a hot stream and had a temperature that was reasonably higher than  $T_c$ . A cooler on stream 7 had an outgoing temperature of 353.13 K (80°C) which produced a sizeable amount of work. ix

Once the volume range and the temperatures were established, the curves of the isotherms can be created using Equation 14 [8]:

$$P_c = \frac{RT_c}{V_c - b} - \frac{a}{V_c^2} \tag{14}$$

Where  $V_c$  is the critical volume, T is the temp of the isotherm and constants a and b are constants that apply to the Van der Waals equation and can be calculated from Equation 15 [8] and Equation 16 [8]:

$$a = \frac{27R^2T_c^2}{64P_c}$$
(15)

$$b = \frac{RT_c}{8P_c} \tag{16}$$

After the isotherms are created, the adiabatic curves on the left and right sides of the Carnot cycle need to be established through Equation 17 [8]:

$$V_B - b = (V_2 - b) \frac{T_c}{T_h}^{\frac{C_v}{R}}$$
(17)

Where b is the Van der Waal's constant calculated prior,  $T_c$  is the the lower isotherm, R is the gas constant,  $V_b$  is the volume associated with the upper right corner of the Carnot cycle, and  $C_v$  is the heat capacity of the fluid at different temperatures. The range of volumes is then found by iterating  $T_h$  in Equation 17 from  $T_c$  to  $T_h$ . The range of volumes can then be used to calculate a range of pressures using Equation 14 and that will connect the two isotherms by the adiabat.

The left adiabat can be found in a similar way to the right adiabatic curve except that Va is used instead of  $V_b$ ,  $V_1$  is used instead of  $V_2$ , and the  $T_c/Th$  is inverted to  $T_h/T_c$  and  $T_c$  is varied instead of  $T_h$ .

 $C_v$  can be calculated by Equation 18 [8]:

$$C_{v} = \frac{R(A + BT + CT^{2} + DT^{-2})}{\gamma}$$
(18)

The A, B, C, D and gamma are constants that are specific to the fluid used in your system. The values to each of those constants can be found in Table 2 [10]:

Table 2: A,B, C, D and gamma constants for CO<sub>2</sub>

	$\rm CO_2$
А	5.457
В	$1.045^{*}10^{-3}$
С	0
D	$-1.157^*10^5$
$\gamma$	1.29

The  $C_v$  value that was used was an average of all the  $C_v$ 's found iterating temperature from  $T_c$  to  $T_h$ . The range of the  $C_v$  temperatures is not large and therefore taking an average is an accurate way to represent the  $C_v$ 's for this temperature range. After all four curves have been established, the Carnot cycle is complete and the work associated by expanding and contracting the piston in the engine can, numerically, be found. The work associated with one cycle of the Carnot engine is the area of the shape formed by connecting the curves. ix

#### ii. Numerical and Analytical Analysis

To run this engine however, there needs to be an amount of heat that is introduced to create isothermal expansion, and can be taken from the initial network design for our plant that is Figure i. The temperature of the cooler utilized needs to have a  $T_h$  value that is large enough to produce an optimal amount of work, but also cannot be too large as the work output becomes negative at some point.x With both of these considerations in mind, cooler 5 from our network fits this criteria for not being excessively large nor being to small to create very little work.

These amounts of work and heat that have been calculated from the network and plot, can also be done through equations, analytically. In Equation 19 [8] and Equation 20 [8], work and  $Q_H$  can be found based on some of the chosen parameters of our calculations.

$$Q_{H} = \int_{V_{1}}^{V_{B}} \frac{RT_{h}}{V - b} dv = RT_{h} ln \frac{V_{B} - b}{V_{1} - b}$$
(19)

$$W = Q_h \left(1 + \frac{T_c}{T_H}\right) \tag{20}$$

The implementation of using these equations allow for a good comparison of how much work that can be taken out of the system if the numerical analysis of the system and graph were correct.

Lastly, the efficiency of a Carnot engine is a simple calculation that compares the utilized isotherms with which the system runs. The equation for finding the efficiency is seen as Equation 21 [8]:

$$\eta = 1 - \frac{T_c}{T_h} \tag{21}$$

#### iii. Carnot Engine Specifications

To determine the rate at which the system has to complete a cycle, an accurate relationship between the work and heat needs to be found. The heat is being inputted to the system at the rate of J/sec and the work that is extracted occurs in J/cycle\*mol. The frequency of how fast the piston moves is then found through Equation 22.

$$Hz = \frac{\eta * Q_h}{W * mol} \tag{22}$$

The amount of moles is arbitrarily assigned to allow for an appropriate amount of cycles/sec to occur. In this regard, there cannot be too few moles assigned to the piston since that will cause for a preposterous amount of cycles needed to intake all of the heat. Oppositely, too many moles will call for too large of a system that will be unnecessarily expensive and large that the pistons may reach a point of underutilization of what could be a more efficient process.

The size of the engine can be calculated therefore based on the number of moles selected by the system and the maximum volume needed to run the system V2. The calculations for volume, pressure and work have been on a "per mole" bases thus far and therefore the volume of the engine needed is found through Equation 23.

$$V = mol * V_2 \tag{23}$$

The size of the engine is therefore based on the size of a one piston-cylinder system in an ideal setting. For the purposes of applying it to being able to handle the capacity of an entire plant however, there needs to be some consideration on how to better balance the capacity of absorbing heat and converting it to work.

To improve the reality of getting this engine to appropriately handle the impact of the incoming heat, dispersing the work amongst multiple cylinders better improves the engine and its ability to work. Instead of just working with one piston, the engine could be rearranged to have 6 cylinders in flat arrangement connected to a crankshaft that in turn does the work to run a process. By doing this, there is less of an impact on any one cylinder to have to produce all of the work and improve the longevity of the internal pieces to that engine. On top of this, the amount of supercritical fluid gets divided amongst the cylinders making it easier to maintain, and the volumes of each cylinder still surround the critical volumes to keep it in that state.

Table 3 displays the impact on one cylinder in both a one cylinder engine and 6 cylinder engine using 100 moles of  $CO_2$ , the work found numerically from our system and the  $Q_h$  that is being inputted into the Carnot engine from our heat exchange network.

Table 3: Comparisons of Numerical and Analytical values

	1 Cylinder Engine	6 Cylinder Engine
Frequency (Hz)	23.51	3.92
Size of Cylinder (L)	6.852	1.142

The Carnot cycle that applies to our network can finally be integrated into the system as seen in Appendix ii to use some of the heat that is available.

By adding this engine cycle to the system to the system to replace a cooler, not only is the engine producing work that can be used to run another process but there is a cost savings that is associated with no longer needing to run a cooler to reduce the temperature of the hot stream. In this case, assuming that coal is used to power the electricity needed, the work produced by the engine saves \$45,631.50 per year and no longer needing to run the cooler saves \$328,537.64 per year for a total savings of \$374,169.14 per year.

#### iv. Supercritical Working Fluid Comparison

The engine that was calculated for in the previous tables utilized supercritical  $CO_2$  for the working fluid within the piston cylinder system. The calculations therefore, were based around the characteristics of the  $CO_2$  such as the critical volume determining the range of the volumes the piston would move or the critical temperature acting as the lower isotherm of the PV diagram.

By varying the fluid within the engine, different parameters may be needed to better absorb the heat from the network and convert it to work, while still remaining around the supercritical conditions that benefit work production. Common supercritical fluids that can be used in this situation are methane, ethane and water. By comparing their properties to those of  $CO_2$  and how these fluids could possibly apply to our network, an optimal fluid can be found that suits the network better than  $CO_2$  would.

Each of the three other fluids have critical conditions that might lead to a better solution for this network. Methane has an extremely low critical temperature ( $-80^{\circ}$ C) and thus using an isotherm of room temperature would create the large difference between the two curves producing work. Ethane has a critical temperature that is very close to CO<sub>2</sub> (305.3K for Ethane, 304.1 for CO<sub>2</sub>) but has a critical pressure that is almost half of that of CO<sub>2</sub>. The resulting difference in critical volume based on critical temperature and pressure may be able to produce a more efficient Carnot engine. Lastly, water has a high critical temperature which can be applied to few portions of the available network, but exploring greater critical temperatures could also lead to a more efficient Carnot engine.

Table 4 [10] shows a comparison of the critical parameters of the four common supercritical fluids for quick comparison of differences.

	$CO_2$	Methane	Ethane	Water
$T_c$ (K)	304.1	190.6	305.3	647.1
$P_c$ (bar)	73.80	45.99	48.72	220.55
Vc (L/mol)	0.128	0.129	0.195	0.0915

 Table 4: Critical Parameters for Selected Fluids

 $T_c$  and  $P_c$  are from accepted literature and Vc is calculated via Equation 13.

The other individual parameter that needs to be established for each of the fluids is their heat capacity coefficients. The coefficients can be used to calculate a heat capacity that applies to finding a volume range. The coefficients for  $CO_2$  have been listed prior in Table 2, and the coefficients for the other supercritical fluids is listed in Table 5 [10].

	Methane	Ethane	Water
Α	1.702	1.131	3.470
В	9.081*10	19.225*10	1.450*10
Б	-3	-3	-3
С	-2.164*10 -6	-5.561*10 -6	0
D	0	0	0.121*10 5
$\gamma$	1.31	1.19	1.33

 Table 5: Coefficients for Selected Fluids

For the purposes of comparison, the critical parameters and the heat capacity constants are the only parameters that will change about the fluids. In order to have a logical argument for discussion on the best critical fluid for our scenario it is fair to keep consistency for outside conditions, beyond that of the fluid, to best see how the fluids compare. The constants that will remain the same between the fluids are the way each of the functions and results are calculated, the compression ratio, the critical volume being exactly between V1 and V2, and the number of moles that the engine will utilize to complete the Carnot cycle.

The first comparison of the fluids that can be looked at is how well each fluid performs under the same difference in temperature difference and same  $Q_h$  inlet. By comparing the critical parameters to each other, inferences can be made on which fluids may work best for the network given.

Each of the critical temperatures of the fluids will be used as  $T_c$  and  $T_h$  will be determined using the same temperature difference as calculated earlier when a CO<sub>2</sub> engine was integrated into the network which is 49.05 K. The reason that the temperature difference is remaining same and not the temperatures themselves is that by using different temperatures other than the critical temperatures for each fluid, the fluid is not going to be around supercritical conditions and therefore the information gathered from that approximation would not make conclusions about the fluid as a supercritical fluid. The same  $Q_h$  is being applied to each of the fluids to accurately compare the frequency of cycles needed to produce the calculated work.

The results of this comparison is listed in Table 6.  $T_h$  for each fluid was 49.05K higher than  $T_c$ ,  $Q_h$  is 1,521,768 Watts, the number of moles in each system is 40 moles of each fluid. CO<sub>2</sub> results, although previously listed, were added to Table 4 for comparative reasons.

	Carbon Dioxide	Methane	Ethane	Water
$T_c$ (K)	304.1	190.6	305.3	647.1
$T_h$ (K)	353.1	239.65	354.35	696.15
Efficiency	13.9%	20.5%	13.8%	7.05%
$Q_h~{ m (J/s)}$	1,521,768	1,521,768	1,521,768	1,521,768
Work (J/cycle*mol)	224.749	194.590	97.464	347.872
$Q_c ~({ m J/s})$	1,310,405	1,210,302	1,311,121	1,414,546
Hz $(1/s)$	23.51	40.02	54.03	7.71
Engine Size (L)	6.852	6.891	10.42	4.88

Table 6:	Calculated	Values	for	Selected	Fluids
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Methane as compared to carbon dioxide at these conditions proves to simply not match up in quality of output in most categories of comparison. Despite the methane based engine being more efficient, the work output with the same temperature difference as carbon dioxide is considerably smaller due to the fact that lower overall temps causes smaller calculated area outputs. This reduction in work, causes a higher required frequency which creates more wear on the engine over time.

Ethane, despite having similar isotherms to carbon dioxide, also produces results that are not as preferable as an engine based on carbon dioxide. The issue mainly stems from the critical volume of ethane being significantly greater than that of carbon dioxide's. The larger the critical volume, the greater the size of the engine, however the isotherms stretch the Carnot graph and ultimately produce less work. This causes required frequency to increase which is less desirable than the original design.

Water, at its high temperatures, produces results that rival the results of carbon dioxide in numerous ways. Most noticeably, the work that is produced by this cycle is greater than carbon dioxide's because the upper isotherm extends to such high temperatures producing a greater area of the Carnot plot. The increased amount of work, decreases the required frequency and the lower critical volume produces a smaller engine size overall. The results of the supercritical water engine make it possible that if it can be successfully integrated into the heat exchange network, it could be more profitable in the long run than the given carbon dioxide engine.

#### v. Supercritical Working Fluid Integrations

After reviewing the comparative results based on the already integrated supercritical carbon dioxide engine, the engines based on the other supercritical fluids can also be attempted to be integrated into the network. If they can be appropriately integrated to the network, the outputs need to be considered to see if it is profitable to use that type of engine over the given carbon dioxide.

Any attempts to integrate an engine type into the network will first be based on if it is even possible to work it into the system based on the critical temperatures, and then placed on the diagram to find the optimal location for it.

The constants that are kept in this comparison include the calculations, the compression ratio, the critical volume of the fluid being exactly between V1 and V2, and the number of moles of the system which will be set to 40 moles. The results of this comparison is listed in Table 7.  $CO_2$  results, although previously listed, were added to Table 4 for comparative reasons. (App.ix through xii)

	Carbon Dioxide	Methane	Ethane	Water
$T_c$ (K)	304.1	190.6	305.3	647.1
$T_h$ (K)	353.1	298.15	353.15	683.15
Effeciency	13.9%	36.1%	13.5%	5.28%
$Q_h ~({ m J/s})$	1,521,768	81,000	1,521,768	976,668
Work (J/cycle*mol)	224.749	-175.060	103.317	274.777
$Q_c~({ m J/s})$	1,310,405	51,781.3	$1,\!315,\!576$	925,128.8
Hz (1/s)	23.51	-4.17	49.89	4.69
Engine Size (L)	6.852	6.891	10.42	4.88

 Table 7: Integrated Calculated Values for Selected Fluids

For methane, the trouble begins with integrating it into our network by the fact that the critical temperature of methane is comparatively low (190.6 K,  $-82.55^{\circ}$ C) and the lowest possible temperature on the network is 20 ° C, located

on Stream 2 in Figure i. For consistency between engines, the lower isotherm will be the critical temperature for each of the fluids and the upper isotherm will be the temperature of the stream in the network. The result of having such a dramatic difference in temperature becomes problematic when trying to run a Carnot engine.

Disregarding the energy required to maintain a lower isotherm that is so low in temperature, the calculation method of finding work is limited by the temperature difference. In this instance, the temperature difference is large enough that the resulting work is negative (App.v). Needless to say, a Carnot engine that uses methane as a working fluid is not appropriate, considering the temperatures of the network.

For ethane, due to its similar critical temperature to carbon dioxide, can reasonably be integrated into the system at the same place as the integrated carbon dioxide Carnot engine. Similar to the results found when the fluids were compared at similar conditions, the results of using ethane at this section of the network gives inferior results to that of the carbon dioxide results (App.vi). The greater required size of the engine, higher required frequency, and lower work output prove that carbon dioxide working fluid is more appropriate than the ethane working fluid for this network.

While methane and ethane did not prove to be properly suited for this network, which was consistent with the comparison of the fluids, water showed promising results when attempted to be integrated into the system.

If the original network is redesigned and the Carnot engine with water as the working fluid is integrated at stream two, the calculations can be done to remove heat up until the temperature of the exiting fluid is 410°C. The results from that integration produce the results shown in Table 7 which prove to be better than the carbon dioxide based engine. The work output is increased, the size of the engine decreases, and the frequency decreases. Water is also abundantly accessible to apply to this system so from a cost standpoint of installing one of these engines, the benefits prove to beat the benefits of the carbon dioxide based engine.

When integrating the engine utilizing water as its working fluid, the possible energy production is higher than that of any other fluids tested (App.iv). However, this cannot be integrated into the existing heat exchange network, since the water engine would only function above the pinch, and there is no energy available for this engine to use above the pinch.

Although none of the other explored fluids could be better applied than the given carbon dioxide based engine, the comparison of them proved to show interesting insights about when a supercritical fluid is appropriate for a system. In terms of cost reduction, integrating engines should optimally be done to replace current machinery to create productivity out of waste heat. It is also important to understand that the critical temperature will determine where the engine can be possibly integrated, lower critical temperatures apply to colder systems and higher critical temperatures apply to hotter systems. Lastly, the size of the engine, and the costs associated with it, are determined by the critical volume of the fluid where lower critical volumes reduce size and therefore there is less fluid needed to make the engine work and less capital costs for material and installation.

### 6. EIGENVECTOR CENTRALITY

One method used to look at the interconnectedness of heat exchanger networks is eigenvector centrality. Eigenvector centrality is a numerical measure from 0 to 1 of how important a node (or in our case, stream) is to the network as a whole. Eigenvector centrality is more specific than other types of centrality like degree centrality since eigenvector centrality considers a node more useful if it is connected to other well connected nodes. Additionally, the edges (which in our case are heat exchanges) can be weighted, meaning that centrality can be calcualted based on how much heat each stream is transferring.

## i. Original Network

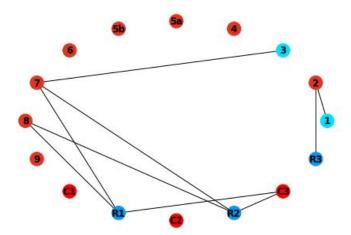


Figure 9: The original network designed for the plant was the network above. C1-3 represent condensers, and R1-3 represent reboilers.

The eigenvector centrality values are as follows:

#### Table 8: Original Network

Stream	Centrality
1	$9.05^{*}10^{-6}$
2	$1.28^{*}10^{-5}$
3	0.180
4	$2.03^{*}10^{-16}$
5a	$2.03*10^{-16}$
5b	$2.03*10^{-16}$
6	$2.03^{*}10^{-16}$
7	0.454
8	0.383
9	$2.03^{*}10^{-16}$

Centrality
$2.03*10^{-16}$
$2.03*10^{-16}$
0.383
0.484
0.484
$9.05*10^{-6}$

From these values, reboilers 1 and 2 are the most connected, followed by stream 8 and condenser 3, and then stream 3. Streams 1 and 2, and reboiler 3 are connected in their own less important network, so they have lower centralities, with stream 2 being the most important of the three. All other streams are unconnected, and therefore very unimportant in the network, so they are given extremely low centrality values. These values are incredibly small, but still non-zero since they are still part of the network as a whole, even though they have no connections. From this, reboilers 1 and 2 are most important for our system as a whole when it comes to their general connectedness, meaning that if they fail in some way, this hurts the rest of the network the most.

The weighted eigenvector centrality based on the amount of heat transfer in each connection is as follows:

 Table 9: Original Network Weighted

Stream	Centrality
1	0.707
2	0.707
3	$8.61^{*}10^{-6}$
4	$7.61^{*}10^{-19}$
5a	$7.61^{*}10^{-19}$
5b	$7.61^{*}10^{-19}$
6	$7.61^{*}10^{-19}$
7	$4.84^{*}10^{-5}$
8	$2.55^{*}10^{-6}$
9	$7.61^{*}10^{-19}$

Stream	Centrality
Condenser 1	$7.61^{*}10^{-19}$
Condenser 2	$7.61^{*}10^{-19}$
Condenser 3	$1.05^{*}10^{-4}$
Reboiler 1	$2.71^{*}10^{-5}$
Reboiler 2	$1.07^{*}10^{-4}$
Reboiler 3	$1.20^{*}10^{-4}$

From these, we see that streams 1 and 2 are the most important to our overall network, since they transfer so much heat (986.8 kW in the pilot plant, 9868 kW in the full scale) between one another. Reboiler 3 is given a high centrality value since it's interconnected with these two streams. Reboilers 3 and 2, and condenser 3, followed by streams 7, 3, then 8 all have middling centrality values since they are transferring a fair amount of heat, and are interconnected with each other. Finally, all other streams are not connected, giving very low centrality values. From this, we see that if there are problems with streams 1 and 2, this becomes quickly problematic for the network because of how much heat they are transferring. However, these failing would really only affect each other, since they are only connected to each other and reboiler 3. The code used to calculate these values is in Appendix xvi.

Note that everything within this section also applies to the alternate network with the Carnot engine integrates since the Carnot engine will just be replacing an existing cooler.

### ii. Steam Raising Network

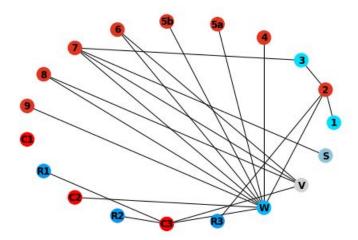


Figure 10: The redesigned network for steam raising is pictured above. C1-3 are condensers, R1-3 are reboilers, W is the water stream before it is vaporized, S is the steam after being vaporized, and V is the water as it is being vaporized.

The eigenvector centrality values for this network are below.

Stream	Centrality
1	0.0670
2	0.243
3	0.153
4	0.164
5a	0.164
5b	0.164
6	0.248
7	0.314
8	0.248
9	0.16

### Table 10: Steam Raised Network

Stream	Centrality
Condenser 1	$2.91^{*}10^{-19}$
Condenser 2	0.164
Condenser 3	0.292
Reboiler 1	0.0804
Reboiler 2	0.0804
Reboiler 3	0.0670
Water	0.596
Steam	0.0864
Vaporization	0.303

From this, we see that water is the most connected stream by far. This is largely due to its high CP value. The vaporization stream also has a high number of connections, due to its high CP value and very high energy requirements (2400 kW in the pilot plant, and 24000 kW in the full scale). Then, condenser 3 is connected to both of these important streams (and reboiler 2), so it is next most important stream. The rest of the streams follow this sort of pattern, with the only notable stream being condenser 1, which has no connections within the network, and as such has a super low centrality value. This shows us that if the water stream fails, a huge number of streams would be affected by this.

The weighted eigenvector centrality based on the amount of heat transfer in each connection is shown in the table below.

 Table 11: Steam Raised Network Weighted

Stream	Centrality	Ctrooper	Controlid
1	0.0257	Stream	Centralit
2	0.0254	Condenser 1	
3	0.00126	Condenser 2	
4	$4.95^{*}10^{-7}$	Condenser 3	0.000
5a	$4.06*10^{-5}$	Reboiler 1	0.0313
5b	$3.67^{*}10^{-6}$	Reboiler 2	0.0944
6	0.00713	Reboiler 3	4.35*10-
7	0.0607	Water	0.00311
8	0.00508	Steam	0.721
		Vaporization	0.00125
9	$1.02^{*}10^{-5}$	(apolization	0.0012

From this table, it can be seen that the vaporization stream is most important, with condenser 3 relatively close behind it, and stream 7 behind that. This is due to the vast amounts of heat (for vaporization: 2400 kW in the pilot plant, and 24000 kW in the full scale, and for condenser 3: 2552.7 kW in the pilot plant, and 25527 kW in the full scale)

that condenser 3 and the vaporization stream are exchanging. Stream 7 is considered important mostly because of the streams it exchanges heat with. Stream 7 exchanges heat with the vaporization stream, and two streams which connect to stream 2, which has our next biggest heat exchange behind condenser 3 and the vaporization stream. What all of this means is that stream 7, the vaporization stream, and condenser 3 are all important to this network, due to how much heat they are exchanging, and their connectivity, so if any of these fail in some way, the network will be heavily affected.

#### iii. Heat Exchanger Energy/Area Analysis

Two ways to measure each heat exchanger's significance in the overall network are the amount of energy transferred, and the area of each heat exchanger. It is important to keep each of these in mind, because if important heat exchangers fail for any reason, this could cause the whole system to stop functioning properly since the processes will not be at the desired temperatures. This section analyzes which heat exchanger should be monitored the most closely due to this fact.

#### iii.1 Original Network

In the original network (Appendix i), the heat exchanger energies and areas needed are in Table 12. Numbers in Table 12 are for the full scale plant.

Heat Exchanger	Power (kW)	Area (m2)
1	4652.252	1624.3
2	5215.8	1819.3
3	431	20.2
Reboiler 1 and Stream 7	665.04	-
Reboiler 2 and Stream 7	746.54	-
Reboiler 1 and Stream 8	24.0	-
Reboiler 2 and Stream 8	104.753	-
Reboiler 3 and Stream 2	1.6726	-
Reboiler 1 and Condenser 3	261	-
Reboiler 2 and Condenser 3	2013.7	-

Table 12: Powers and Areas for Original Flowsheet

Areas were calculated using Equations 24 and 25. Note that areas of heat exchange cannot be easily calculated for connections to reboilers or condensers since they do not change temperature. LMTD of the reboiler connections is shown below in a Equation 26 [7] [2]. This equation could be modified for condenser connections, and condenser-reboiler connections to get a heat transfer area. Additionally, note that  $T^{sat}$  is needed to calculate this area, and since a number of the streams used for this will be at vapor liquid equilibrium in mixtures of multiple substances, these would need to be categorized before calculating these areas. In addition, the spatial requirements of the facility would need to be taken into account since all of the heat transfer occurring at the reboilers and condensers needs to happen in relatively the same location, complicating things further, thus why calculations for these areas were forgone in this analysis.

$$Q = UA * LMTD \tag{24}$$

$$LMTD = \frac{\Delta T_A - \Delta T_B}{\ln(\Delta T_A / \Delta T_B)}$$
(25)

$$LMTD = \frac{(T^{sat} - T_{2o}) - (T^{sat} - T_{2i})}{\ln \frac{T^{sat} - T_{2o}}{T^{sat} - T_{2i}}}$$
(26)

Through this method, we see that the most heat power is transferred through exchangers 1 and 2. This means that these failing would likely have the largest effect on other streams. This is also supported by the weighted edge eigenvector centrality values, since streams 1 and 2, the streams exchanging heat in exchangers 1 and 2, have the highest weighted centrality values. The connection between reboiler 2 and condenser 3 also transfers a great deal of heat, so the same is true if this connection fails. The areas for heat exchangers 1 and 2 will be very large, so this means that they will be harder to maintain since they will take up more overall space in the plant, and there will be a greater area for them to possibly fail. Because these two exchangers also transfer the most heat, precautionary measures should be taken to make these exchangers less likely to fail, or easier to repair, since they are most likely to have issues, and contribute the most to the overall network.

#### iii.2 Steam Raising Network

In the network where steam raising is integrated into the process (Appendix iii), the heat exchanger energies and areas needed are in Table 13. Numbers in Table 13 are for the full scale plant. Areas for connections to condensers, reboilers, and the vaporization stream are not calculated for the same reasons as above.

Heat Exchanger	Power (kW)	Area $(m^2)$
1	4652.252	1624.3
2	109.78	38.64720065
3	2.763	0.9521834871
4	17.582	3.860317573
5	19.012	4.174289484
6	8.47	1.868626706
7	13.439	3.128161073
8	430.474	54.9356993
9	425.1344	22.47118525
10	547.14	48.41905523
11	226	24.83970954
12	345.09	25.55337162
13	12.0	2.453482018
14	70.62	8.274748874
15	38.182	6.484044467
16	3642.3	1274.172275
17	1463.74	514.84686

Table 13:	Powers	and Ar	reas for	Steam	Raised	Flowsheet
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Heat Exchanger	Power (kW)
Area $(m^2)$	
Water Stream and Condenser 2 (Connection 1)	485.793
Water Stream and Condenser 2 (Connection 2)	1185.4
Water Stream and Condenser 3	28.83
Vap. Stream and Stream 6	228.91
Vap. Stream and Stream 7	1960.251
Vap. Stream and Stream 8	163.955
Vap. Stream and Condenser 3	21683.17

Within this network, There are several heat exchangers that are very important to the overall network. These are exchangers 1, 16, and 17, the second connection between water and condenser 2, V (the vaporization stream) connected with stream 7, and V connected with condenser 3, since these all transfer more than 1 MW of power. The connection between V and condenser 3 is especially important since it is transferring 21.683 MW, so if this fails, the impact on the system would be disastrous. This observation is supported by the fact that condenser 3 has the second highest weighted centrality value, meaning that if something goes wrong here, the entire system becomes affected, so extra precaution needs to be taken to ensure that this exchange does not fail. Due to the interconnectedness of this network (Section ii , Figure 10), any of these exchangers encountering problems could be devastating for the system as a whole. The exchangers with the largest heat transfer areas are exchangers 1, 16, and 17. Coincidentally, these exchangers are also some of the most important to the system, so it would be prudent to design the layout of these heat exchangers in such a way where they are not likely to get damaged, or can be fixed easily if they fail.

### 7. CONCLUSION

Upon full integration of the system from the given diagram, we were able to recover the maximum amount of heat given the network. After analyzing the system using pinch analysis, the  $Q_{hmin}$ ,  $Q_{cmin}$  and  $T_{pinch}$  values of the pilot plant analyzed are 2855.987 KW, 2824.387 KW and 254.3°C when  $T_{min} = 10^{\circ}$ C.

An analysis of finding the lowest cost for operating the plant over time was conducted to find the appropriate measures for developing this plant. After 1 year of running the plant, the lowest cost to develop the system is \$41,870,000 if the  $T_{min}$  is set at 20.384°C. If the system were to be run for a longer period of time, however (at least 634 days), the best  $T_{min}$  for the system would become 10°C, since this would produce the lowest possible overall cost.

There are great incentives to implement this heat exchange network from both a business perspective and from an environmental perspective. Based on given information regarding energy facts about coal, the integrated system saves over \$3,000,000 per year and reduces over 94,000,000 kilograms of carbon dioxide emissions to the atmosphere per year.

When comparing other common supercritical fluids (methane, ethane and water) to carbon dioxide as working fluids, the results are mainly dependent on the critical conditions of the fluid. Methane and ethane showed to be less effective at producing work than carbon dioxide, but water had promising results before the fluids were attempted to be integrated. After integration, methane could not be appropriately integrated and ethane did not work as well as carbon dioxide in the network. Water could be integrated into the system and produced more work than carbon dioxide, but the arrangement of the network for that to be successful was not feasible overall and thus supercritical carbon dioxide was the best working fluid for our Carnot engine.

Using eigenvector centrality, the relationships between streams can be analyzed, and the most interconnected streams can be identified. This type of analysis can be used to find the most important parts of a system. Additionally, heat exchanger areas and energies were calculated to find the most important exchangers and the amount of area they take up, since exchangers with larger areas are often more vulnerable to leaks or other problems.

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## 9. Appendix

## i. Original Network Flowsheet

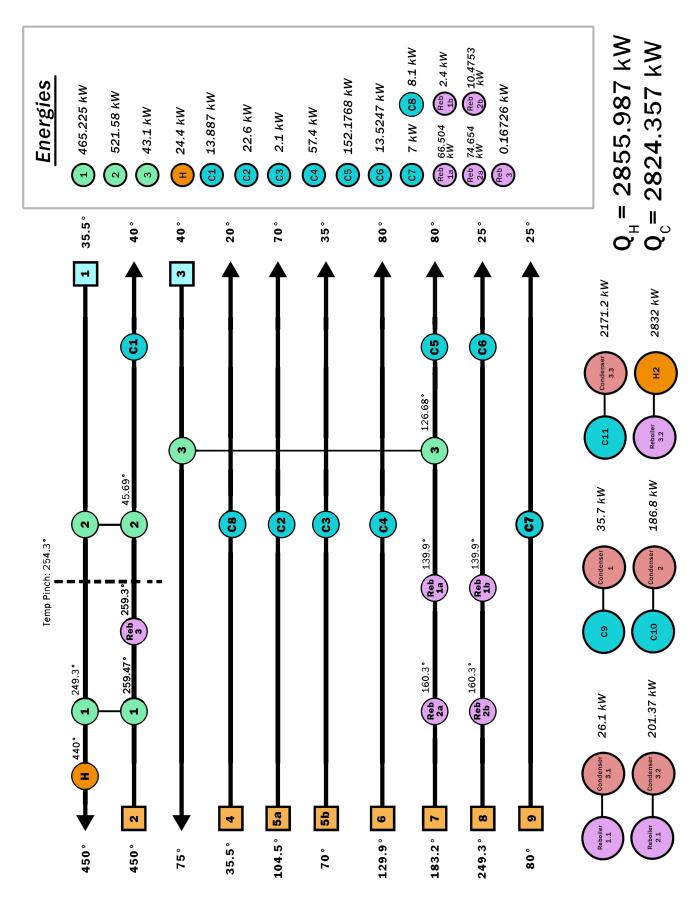


Figure 11: Design Process Flowsheet

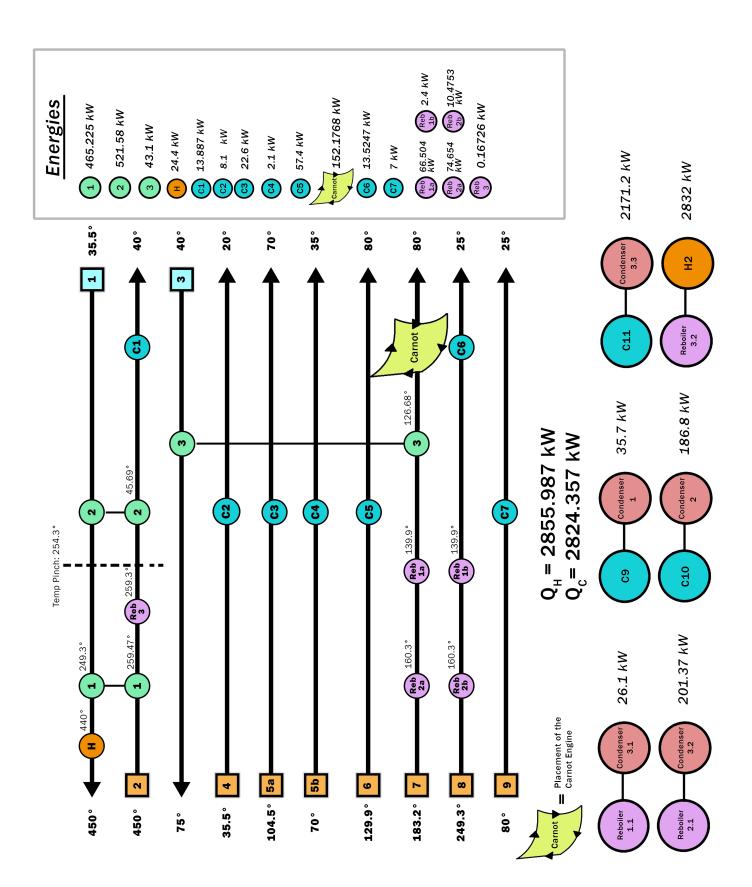
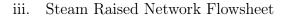


Figure 12: Carnot Integrated Process Flowsheet



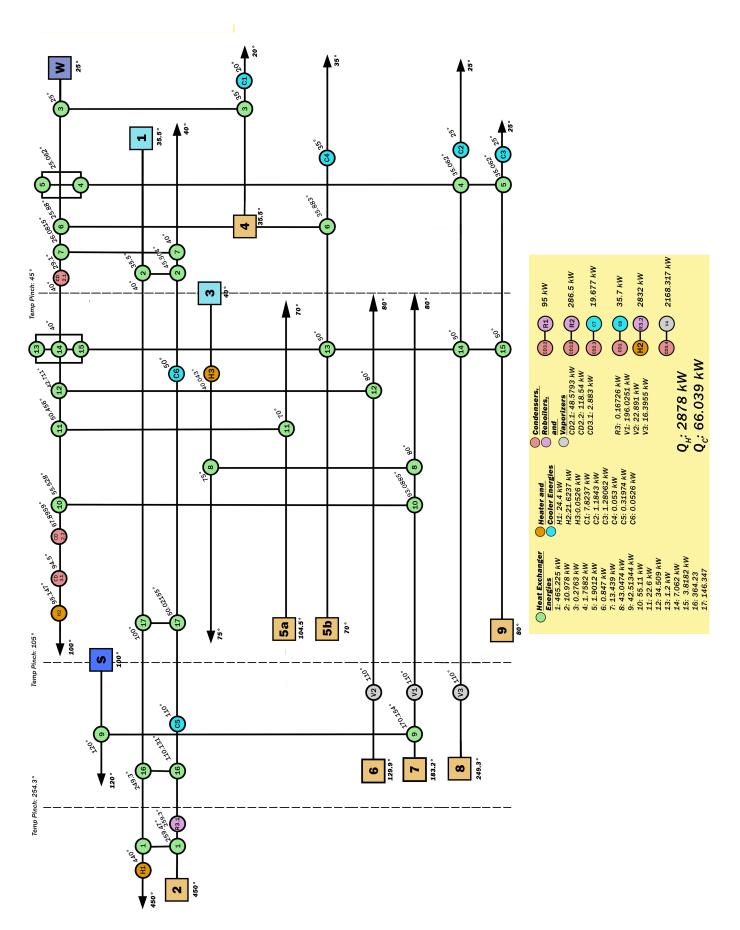
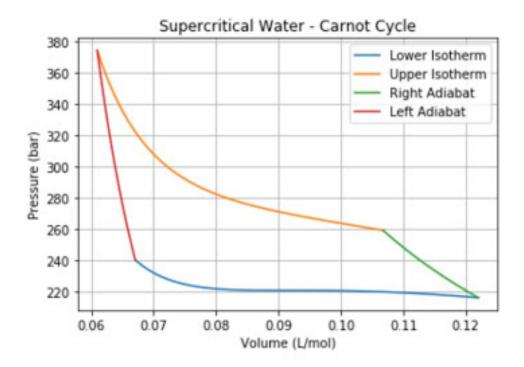


Figure 13: Steam Raised Process Flowsheet

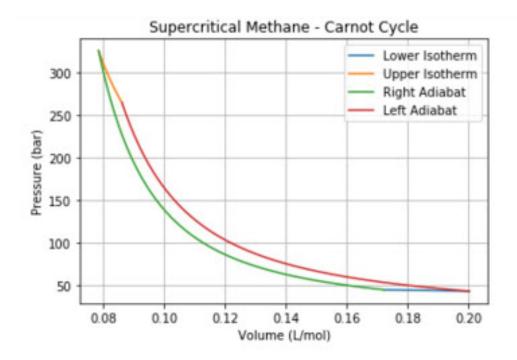
## iv. Supercritical Water Carnot Cycle



The efficiency of this system is 5.28 %. The theoretical input energy, Qh, is 5206.802 Joules/sec. The theoretical work removed from the engine is 4932.038 Joules/sec The theoretical work of this system is 274.7643 Joules/cycle\*mol The work from the system is 274.7768 Joules/cycle. The power available from the network is 1521768 Joules/sec The power lost by the engine is 1441463.9 Joules/sec The number of moles that the engine contains is 40 moles. The RPS of the Carnot Engine is 7.306 Cycles/second. The size of the Carnot Engine is 4.879 L

Figure 14: Steam Raised Process Flowsheet

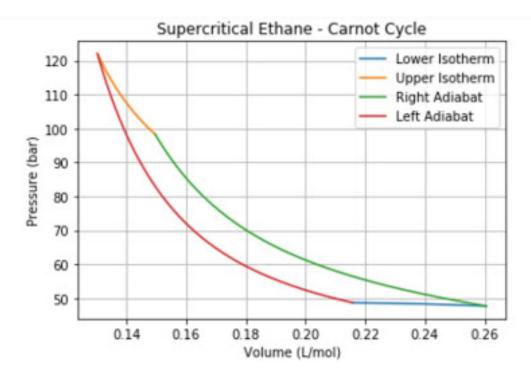
## v. Supercritical Methane Carnot Cycle



The efficiency of this system is 36.1 %. The theoretical input energy, Qh, is -485.3017 Joules/sec. The theoretical work of this system is -175.0602 Joules/cycle\*mol The theoretical work removed from the engine is -310.2415 Joules/sec The work from the system is -175.0604 Joules/cycle\*mol. The power available from the network is 81000 Joules/sec The power lost by the engine is 51781.318 Joules/sec The number of moles that the engine contains is 40 moles. The RPS of the Carnot Engine is -4.173 Cycles/second. The size of the Carnot Engine is 6.891 L

Figure 15: Steam Raised Process Flowsheet

## vi. Supercritical Ethane Carnot Cycle



The efficiency of this system is 13.5 %. The theoretical input energy, Qh, is 762.5147 Joules/sec. The theoretical work of this system is 103.3168 Joules/cycle\*mol The theoretical work removed from the engine is 659.1979 Joules/sec The work from the system is 103.3172 Joules/cycle. The power available from the network is 1521768 Joules/sec The power lost by the engine is 1315576.3 Joules/sec The number of moles that the engine contains is 40 moles. The RPS of the Carnot Engine is 49.89 Cycles/second. The size of the Carnot Engine is 10.42 L

Figure 16: Steam Raised Process Flowsheet

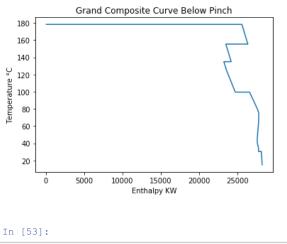
vii. Steam Raising Code

These thermodynamic values were taken from Appendix viii

```
In [51]:
```

```
import numpy as np
import matplotlib.pyplot as plt
### I multipy by 10 for all of my enthalpy values so that I can
#test the full scale plant
Qc = 2824.38725*10 \ #Qc \ of \ the \ real \ plant
Qh = 2855.9872*10 # Qh of the real plant
#[[30.5, 35.7], [99.5, 186.8], [178.2, 2552.7]]
#[[134.9, -95], [155.3, -286.5], [254.3, -2832]]
temps = [455.0, 445.0, 254.3, 254.3,
         244.3, 178.2, 178.2, 155.3, 155.3, 134.9, 134.9, 124.9,
         99.5, 99.5, 80.0, 75.0, 65.0, 45.0, 40.5, 35.0, 30.5, 30.5, 30.0, 20.0, 15.0]
Q = [0, -24.39565742, 0.4083983525000012, -2832, 0.02141575000000067,
     7.921495692060003, 2552.7, 77.36907013433992, -286.5, 68.92266509784002, -95,
     33.785620146, 115.03311043624004, 186.8, 101.0867340483, 19.762532542, -3.292422953,
     -18.486295181999996, 1.3820121535499998, 15.106737546449999, 1.3723750660499998, 35.7,
     0.41377644105, 7.6755288209999994, 2.6129032260000002]
\#\texttt{temps} and \textit{Q} are lists corrisponding to the "corner points" of the GCC
Q = [i * 10 for i in Q] # turnes the Q's into the real plants Q
print(0)
newq =[]
Sum = Qh
for i in range(len(Q)):
    Sum = Sum + O[i]
    newq.append(Sum) #creates a list enthaklpuied corresponding from the high temp to low
plt.plot(newq[5::], temps[5::]) # this plots the Grand Composite Curve
plt.title("Grand Composite Curve Below Pinch")
plt.ylabel("Temperature °C")
plt.xlabel("Enthalpy KW")
plt.show()
[0, -243.95657419999998, 4.083983525000012, -28320, 0.21415750000000067, 79.21495692060003,
```

[0, -243.95657419999998, 4.083983525000012, -28320, 0.21415750000000067, 79.21495692060003, 25527.0, 773.6907013433993, -2865.0, 689.2266509784002, -950, 337.85620145999997, 1150.3311043624003, 1868.0, 1010.867340483, 197.62532542, -32.92422953, -184.86295181999995, 13.820121535499998, 151.0673754645, 13.723750660499999, 357.0, 4.1377644105, 76.75528820999999, 26.129032260000002]

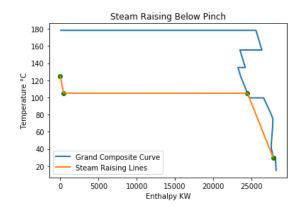


Hwsat = 2450\*10 #guess from graph Hvap =2256 #Kj/Kg Cpw = 4.19 #Kj/Kg\*C Tsat = 105 #C assumed Cps = 1.996 #Kj/Kg\*C Tstart = 30 #C Tfinal = 125 # Final temp of steam

```
count = 0
#creating the graph physically
Main_temps = [] #254.3-->30
C = \overline{254.3} #this starts the list below the pinch so we can look at the
#pertinent values of the eqaution
while C>=30:
   Main_temps.append(C)
   C = C-.1 #gves temperature values for the
graphenthalpy = [] #the raw data
for i in range(len(temps)-1):
    slope = (temps[i+1]-temps[i]) / (newq[i+1]-newq[i]) #this calculates the slope.
    if slope == 0:
       slope =.000000001
    for j in range(len(Main_temps)):
        if (Main_temps[j] < temps[i] and Main_temps[j]</pre>
            > temps[i+1]):
            H = (1/slope)*(Main temps[j]-temps[i])
            +newq[i]
            graphenthalpy.append(H)
Main_temps.pop() #removes the last element from the list
#making the optomal steam lines based on equations
graphenthalpysteam = []
graphtempssteam = []
holder = True
while holder == True: # thsi is ideration,
   count = 0
   Hssat = Cps*Hwsat*(Tfinal-Tsat)/(Hvap +Cps*
                                     (Tfinal - Tsat))
   Hstart = Hwsat*(1+Cpw*((Tsat-Tstart)/Hvap))-Hwsat*
    ((Cpw*Cps*(Tsat-Tstart)/Hvap)
    *((Tfinal-Tsat)/(Hvap+Cps*(Tfinal-Tsat))))
    Mw = (Hwsat/Hvap)*(1-Cps*(Tfinal-Tsat)/(
       Hvap + Cps*(Tfinal-Tsat)))
    crit_S_enthalpies = [0,Hssat,Hwsat,Hstart]
    # important x values for slope
    crit_S_temps = [Tfinal,Tsat,Tsat,Tstart]
    # important y values for slope
    graphenthalpysteam = []
    #the graphing enthalpies for steam
    graphtempssteam = []
    #the graphing temps for steam
    for i in range(len(crit_S_temps)-1):
        slope = (crit_S_temps[i+1]-crit_S_temps[i]) /
        (crit_S_enthalpies[i+1]-crit_S_enthalpies[i])
        if slope == 0:
            slope = .000000001
            #Deals with when you get an undefined slope aka a horizonal line.
        for j in range(len(Main_temps)):
            if Main_temps[j] < crit_S_temps[i] and</pre>
            Main temps[j] > crit S temps[i+1]:
                H = (1/slope) * (Main temps[j]-
                        crit_S_temps[i])+crit_S_enthalpies[i]
                graphenthalpysteam.append(H)
                #appends the enthalpy at a specific temoperature
                graphtempssteam.append(Main temps[j])
                #appends the temperature used to caculate the enthalpy
    if Hwsat > 2449.797*10: #this makes sure that the
                            #value of Hwsat is always
                            #barely touvhing th GCC
        count = count + 1
    #this let me check for any other values where the GCC may cross.
    if graphenthalpysteam[graphtempssteam.index(30.50000000010353)]
    > 2813.85*10:
       count = count + 1
```



the mass flow rate is 10.670188856754605



#### In [4]:

```
# Value Finder for graph
#for i in range(len(Main_temps)):
    # if Main_temps[i] <= 35 and Main_temps[i] >= 25:
    # print(graphenthalpy[i])
```

#### In [37]:

```
for i in range(len(graphtempssteam)):
    if graphtempssteam[i] <= 29 and graphtempssteam[i]>= 31 :
        print(graphenthalpysteam[i])
```

# viii. Table of Steam Raising Variables

Variable	Definition	Units	Value
$M_w$	Mass Flow Rate	m kg/S	Unknown
$C_{pw}$	Heat Capacity of Water In	kJ/kg*°C	4.19
$C_{ps}$	Heat Capacity of Steam In	kJ/kg*°C	1.996
$H_{start}$	Enthalpy of the Inlet Water	kW	Unknown
$T_{start}$	Temperature of the Inlet Water	$^{\circ}\mathrm{C}$	$20^{\circ}\mathrm{C}$
$H_{wsat}$	Enthalpy of Saturated Water In	kW	Manually Changed
$T_{sat}$	Water Vaporization Temperature	$^{\circ}\mathrm{C}$	$100^{\circ}(105^{\circ}\text{shifted})$
$H_{ssat}$	Enthalpy of Saturated Steam In	kW	unknown
$\Delta H_{vap}$	Vaporization Enthalpy In	kJ/Kg	2265
$T_{final}$	Final Temperature of Steam In	$^{\circ}\mathrm{C}$	$120^{\circ}\mathrm{C}$

 Table 14: Variables Used Within Steam Raising Equations. All values come from Introduction to Chemical Engineering [10]

ix. Supercritical CO2 Carnot Cycle Code

## Carnot Cycle - Super Critical CO2

November 19, 2018

In [21]: import numpy as np import matplotlib.pyplot as plt In [184]: R = .08314 #L-bar/mol\*K Tc = 304.1 #K, lower isotherm Pc = 73.8 *#bar* Th = 353.15 #80 degrees Celsius, upper isotherm  $r = 8.314 \ #J/mol *K$ n = 1 - (Tc/Th) #Efficiency of the Carnot engine equation a = 27/64\*(R\*\*2)\*(Tc\*\*2)/Pc #Parameter calculations that apply to the Van der Waal b = 1/8 \* R \* Tc/PcVc = 3/8\*R\*Tc/Pc #Critical Volume CompRatio = 2 #V2/V1 V1 = .085647V2 = V1\*CompRatio Tspace = np.linspace(Tc, Th, 1000) #array of temperatures that will be used to est list(Tspace) #converting the array to a list A = 5.457 #Heat Capacity coefficients B = 1.045 \* 10 \* \* - 3**C** = 0 D = -1.157\*10\*\*5 $y = 1.29 \ \#Cp - Cv$ testCv = (R\*(A + B\*Tspace + C\*(Tspace\*\*2) + D\*(Tspace\*\*-2)))/y #Calculating Cv Cv = np.mean(testCv)Var = ((V2-b)\*((Tc/Tspace)\*\*(Cv/R))) + b #Volume range of the right adiabat Par = ((R\*Tspace)/(Var-b))-(a/(Var\*\*2)) #Pressure list based on parameters, temp 1-Val = ((V1-b)\*((Th/Tspace)\*\*(Cv/R))) + b #Volume range of the left adiabatPal = ((R\*Tspace)/(Val-b))-(a/(Val\*\*2)) #Pressure list based on parameters, temp let a state of the state

```
hVspace = np.linspace(V1, Var[-1], 100) #Volume range for upper isotherm
Ph = ((R*Th)/(hVspace-b))-(a/(hVspace**2)) #Pressure list for the upper isotherm
cVspace = np.linspace(Val[0], V2, 100) #Volume range for lower isotherm
Pc = ((R*Tc)/(cVspace-b))-(a/(cVspace**2)) #Pressure list for lower isotherm
```

#Plotting all curves, adding specific points

```
plt.plot(cVspace, Pc, label = 'Lower Isotherm')
plt.plot(cVspace[0], Pc[0], marker = 'o', color = 'red', label = "V_A")
plt.plot(cVspace[-1], Pc[-1], marker = 'o', color = 'blue', label = "V2")
plt.plot(hVspace, Ph, label = 'Upper Isotherm')
plt.plot(hVspace[0], Ph[0], marker = 'o', color = 'orange', label = "V1")
plt.plot(hVspace[-1], Ph[-1], marker = 'o', color = 'green', label = "V_B")
plt.plot(Var, Par, label= 'Right Adiabat')
plt.plot(Val, Pal, label = 'Left Adiabat')
plt.grid(True)
plt.xlabel('Volume (L/mol)')
plt.ylabel('Pressure (bar)')
plt.title("Supercritical Carbon Dioxide - Carnot Cycle")
plt.legend(loc = 'best')
plt.show()
#Finding the work associated with the plot of the graph
War = -np.trapz(Par, Var)
Wth = np.trapz(Ph, hVspace)
Wal = -np.trapz(Pal, Val)
Wtc = np.trapz(Pc, cVspace)
#Using equations given to solve for and report findings for this supercritical flu
print('The efficiency of this system is {:.3}'.format(n*100), '%.')
```

```
Qh = r*Th*np.log((Var[-1]-b)/(V1-b)) #Qh for one cycle
print('The theoretical input energy, Qh, is {:.7}'.format(Qh), "Joules/sec.")
```

```
TheoWORK = Qh*(1-(Tc/Th))
print('The theoretical work of this system is {:.7}'.format(TheoWORK), "Joules/cycl
```

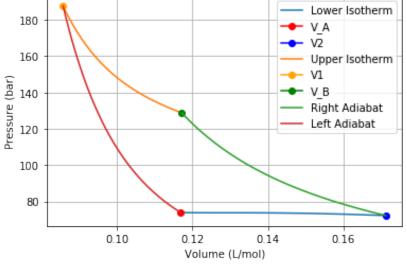
```
TheoQc = Qh*(1-n)
print('The theoretical work removed from the engine is {:.7}'.format(TheoQc), "Jou"
```

```
WORK = ((War+Wth)-(Wal+Wtc))*100
print('The work from the system is {:.7}'.format(WORK), "Joules/cycle.")
```

Qhnetwork = 1521768 #From cooler 5, W #Full scale size, 10x greater than the number print('The power available from the network is',(Qhnetwork), 'Joules/sec')

```
Qcnetwork = Qhnetwork*(1-n)
print('The power lost by the engine is {:.8}'.format(Qcnetwork), 'Joules/sec')
Moles = 40
print('The number of moles that the engine contains is',(Moles), 'moles.')
Hz = (n*Qhnetwork)/(WORK*Moles)
print('The RPS of the Carnot Engine is {:.4}'.format(Hz), "Cycles/second.")
V_Engine = V2*Moles
print('The size of the Carnot Engine is {:.4}'.format(V_Engine), "L")
Work_Cost_Savings = WORK*Hz*Moles*300*24*(1/1000)*(1/6.67)*(60/1000)*(1/.3)
print('The amount of money saved by utilizing this engine is ${:.6}'.format(Work_Co
Cooler_Cost_Savings = (Qhnetwork/1000)*24*300*(1/6.67)*(60/1000)*(1/.3)
print('The amount of money saved by no longer needing to run the cooler is \{:.7\}'
            Supercritical Carbon Dioxide - Carnot Cycle
                                                 Lower Isotherm
180
                                                - V A

    V2
```



The efficiency of this system is 13.9 %. The theoretical input energy, Qh, is 1618.123 Joules/sec. The theoretical work of this system is 224.7457 Joules/cycle\*mol The theoretical work removed from the engine is 1393.377 Joules/sec The work from the system is 224.7488 Joules/cycle.

cle - Super Critical CO2.pdf

The power available from the network is 1521768 Joules/sec The power lost by the engine is 1310405.3 Joules/sec The number of moles that the engine contains is 40 moles. The RPS of the Carnot Engine is 23.51 Cycles/second. The size of the Carnot Engine is 6.852 L The amount of money saved by utilizing this engine is \$45631.5 The amount of money saved by no longer needing to run the cooler is \$328537.6 x. Supercritical Methane Carnot Cycle Code

# Carnot Cycle - Super Critical Methane

```
November 19, 2018
```

In [34]: import numpy as np import matplotlib.pyplot as plt In [44]: R = .08314 #L-bar/mol\*K Tc = 190.6 #K, lower isotherms Pc = 45.99 #bar, critical pressure Th = 298.15 #20 degrees celsius, best attempt to integrate Methane to the network **r** = 8.314 #J/mol\*K n = 1 - (Tc/Th) #efficiency of the Carnot Engine a = 27/64\*(R\*\*2)\*(Tc\*\*2)/Pc #Parameter calculations that apply to the Van der Waal b = 1/8 \* R \* Tc/PcVc = 3/8\*R\*Tc/Pc #Critical Volume CompRatio = 2 #V2/V1 V1 = .086141V2 = V1\*CompRatio Tspace = np.linspace(Tc, Th, 1000) #array of temperatures that will be used to esta list(Tspace) #converting the array to a list A = 1.702 #Heat Capacity coefficient B = 9.081 \* 10 \* \* -3C = -2.164 \* 10 \* \* -6**D** = 0 y = 1.31 testCv = (R\*(A + B\*Tspace + C\*(Tspace\*\*2) + D\*(Tspace\*\*-2)))/y #Calculating Cv Cv = np.mean(testCv) Var = ((V2-b)\*((Tc/Tspace)\*\*(Cv/R))) + b #Volume range of the right adiabat Par = ((R\*Tspace)/(Var-b))-(a/(Var\*\*2)) #Pressure list based on parameters, temp la Val = ((V1-b)\*((Th/Tspace)\*\*(Cv/R))) + b #Volume range of the left adiabatPal = ((R\*Tspace)/(Val-b))-(a/(Val\*\*2)) #Pressure list based on parameters, temp la

```
hVspace = np.linspace(V1, Var[-1], 100) #Volume range for upper isotherm

Ph = ((R*Th)/(hVspace-b))-(a/(hVspace**2)) #Pressure list for the upper isotherm

cVspace = np.linspace(Val[0], V2, 100) #Volume range for lower isotherm

Pc = ((R*Tc)/(cVspace-b))-(a/(cVspace**2)) #Pressure list for lower isotherm
```

*#Plotting all curves* 

```
plt.plot(cVspace, Pc, label = 'Lower Isotherm')
plt.plot(hVspace, Ph, label = 'Upper Isotherm')
plt.plot(Var, Par, label = 'Right Adiabat')
plt.plot(Val, Pal, label = 'Left Adiabat')
plt.grid(True)
plt.xlabel('Volume (L/mol)')
plt.ylabel('Pressure (bar)')
plt.title("Supercritical Methane - Carnot Cycle")
plt.legend(loc = 'best')
plt.show()
```

#Finding the work associated with the plot of the graph

War = -np.trapz(Par, Var)
Wth = np.trapz(Ph, hVspace)
Wal = -np.trapz(Pal, Val)
Wtc = np.trapz(Pc, cVspace)

#Using equations given to solve for and report findings for this supercritical flux

print('The efficiency of this system is {:.3}'.format(n\*100), '%.')

Qh = r\*Th\*np.log((Var[-1]-b)/(V1-b)) #Qh for one cycle print('The theoretical input energy, Qh, is {:.7}'.format(Qh), "Joules/sec.")

TheoWORK = Qh\*(1-(Tc/Th)) print('The theoretical work of this system is {:.7}'.format(TheoWORK), "Joules/cycl

TheoQc = Qh\*(1-n) print('The theoretical work removed from the engine is {:.7}'.format(TheoQc), "Joul

WORK = ((War+Wth)-(Wal+Wtc))\*100
print('The work from the system is {:.7}'.format(WORK), "Joules/cycle\*mol.")

Qhnetwork = 81000
print('The power available from the network is',(Qhnetwork), 'Joules/sec')

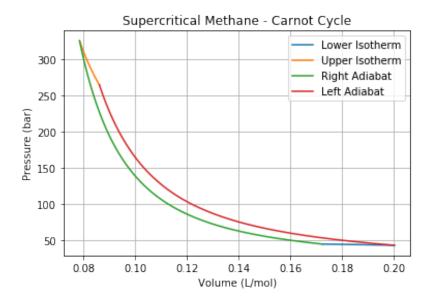
Qcnetwork = Qhnetwork\*(1-n)
print('The power lost by the engine is {:.8}'.format(Qcnetwork), 'Joules/sec')

Moles = 40 print('The number of moles that the engine contains is',(Moles), 'moles.')

Hz = (n\*Qhnetwork)/(WORK\*Moles)
print('The RPS of the Carnot Engine is {:.4}'.format(Hz), "Cycles/second.")

#### V\_Engine = V2\*Moles

print('The size of the Carnot Engine is {:.4}'.format(V\_Engine), "L")



The efficiency of this system is 36.1 %. The theoretical input energy, Qh, is -485.3017 Joules/sec. The theoretical work of this system is -175.0602 Joules/cycle\*mol The theoretical work removed from the engine is -310.2415 Joules/sec The work from the system is -175.0604 Joules/cycle\*mol. The power available from the network is 81000 Joules/sec The power lost by the engine is 51781.318 Joules/sec The number of moles that the engine contains is 40 moles. The RPS of the Carnot Engine is -4.173 Cycles/second. The size of the Carnot Engine is 6.891 L

le - Super Critical Methane.pdf

xi. Supercritical Ethane Carnot Cycle Code

# Carnot Cycle - Super Critical Ethane

```
November 19, 2018
```

```
In [6]: import numpy as np
        import matplotlib.pyplot as plt
In [23]: R = .08314 #L-bar/mol*K
         Tc = 305.3 #K, critical temperature
         Pc = 48.72 #bar
         Th = 353.15 #80 degrees Celsius, upper isotherm
        n = 1 - (Tc/Th) #Efficiency of the Carnot engine equation
         a = 27/64*(R**2)*(Tc**2)/Pc #Parameter calculations that apply to the Van der Waal
        b = 1/8 * R * T c/P c
         Vc = 3/8*R*Tc/Pc #Critical Volume
         CompRatio = 2 # V2/V1
         V1 = .130248
         V2 = V1*CompRatio
         Tspace = np.linspace(Tc, Th, 1000) #array of temperatures that will be used to esta
         list(Tspace) #converting the array to a list
         A = 1.131 #Heat Capacity coefficients
        B = 19.225*10**-3
        C = -5.561 \times 10 \times 10
        D = 0
        y = 1.19
         testCv = (R*(A + B*Tspace + C*(Tspace**2) + D*(Tspace**-2)))/y
         Cv = np.mean(testCv) #Calculating Cv
         Var = ((V2-b)*((Tc/Tspace)**(Cv/R))) + b #Volume range of the right adiabat
         Par = ((R*Tspace)/(Var-b))-(a/(Var**2)) #Pressure list based on parameters, temp l
         Val = ((V1-b)*((Th/Tspace)**(Cv/R))) + b #Volume range of the left adiabat
         Pal = ((R*Tspace)/(Val-b))-(a/(Val**2)) #Pressure list based on parameters, temp la
```

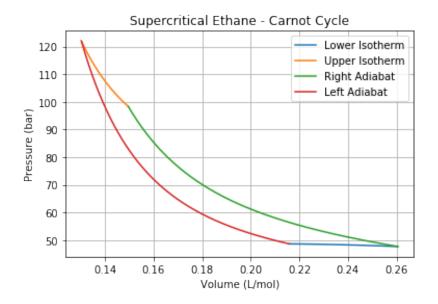
```
hVspace = np.linspace(V1, Var[-1], 100) #Volume range for upper isotherm
Ph = ((R*Th)/(hVspace-b))-(a/(hVspace**2)) #Pressure list for the upper isotherm
cVspace = np.linspace(Val[0], V2, 100) #Volume range for lower isotherm
Pc = ((R*Tc)/(cVspace-b))-(a/(cVspace**2)) #Pressure list for lower isotherm
#Plotting all curves
plt.plot(cVspace, Pc, label = 'Lower Isotherm')
plt.plot(hVspace, Ph, label = 'Upper Isotherm')
plt.plot(Var, Par, label = 'Right Adiabat')
plt.plot(Val, Pal, label = 'Left Adiabat')
plt.grid(True)
plt.xlabel('Volume (L/mol)')
plt.ylabel('Pressure (bar)')
plt.title("Supercritical Ethane - Carnot Cycle")
plt.legend(loc = 'best')
plt.show()
#Finding the work associated with the plot of the graph
War = -np.trapz(Par, Var)
Wth = np.trapz(Ph, hVspace)
Wal = -np.trapz(Pal, Val)
Wtc = np.trapz(Pc, cVspace)
#Using equations given to solve for and report findings for this supercritical flux
print('The efficiency of this system is {:.3}'.format(n*100), '%.')
Qh = r*Th*np.log((Var[-1]-b)/(V1-b)) #Qh for one cycle
print('The theoretical input energy, Qh, is {:.7}'.format(Qh), "Joules/sec.")
TheoWORK = Qh * (1 - (Tc/Th))
print('The theoretical work of this system is {:.7}'.format(TheoWORK), "Joules/cycl
TheoQc = Qh * (1-n)
print('The theoretical work removed from the engine is {:.7}'.format(TheoQc), "Joul
WORK = ((War+Wth)-(Wal+Wtc))*100
print('The work from the system is {:.7}'.format(WORK), "Joules/cycle.")
Qhnetwork = 1521768 #From cooler 5, W #Full scale size, 10x greater than the number
print('The power available from the network is',(Qhnetwork), 'Joules/sec')
Qcnetwork = Qhnetwork*(1-n)
print('The power lost by the engine is {:.8}'.format(Qcnetwork), 'Joules/sec')
Moles = 40
```

le - Super Critical Ethane .pdf

print('The number of moles that the engine contains is',(Moles), 'moles.')

Hz = (n\*Qhnetwork)/(WORK\*Moles)
print('The RPS of the Carnot Engine is {:.4}'.format(Hz), "Cycles/second.")

V\_Engine = V2\*Moles
print('The size of the Carnot Engine is {:.4}'.format(V\_Engine), "L")



The efficiency of this system is 13.5 %. The theoretical input energy, Qh, is 762.5147 Joules/sec. The theoretical work of this system is 103.3168 Joules/cycle\*mol The theoretical work removed from the engine is 659.1979 Joules/sec The work from the system is 103.3172 Joules/cycle. The power available from the network is 1521768 Joules/sec The power lost by the engine is 1315576.3 Joules/sec The number of moles that the engine contains is 40 moles. The RPS of the Carnot Engine is 49.89 Cycles/second. The size of the Carnot Engine is 10.42 L

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xii. Supercritical Water Carnot Cycle Code

# Carnot Cycle - Super Critical H2O

November 19, 2018

In [1]: import numpy as np import matplotlib.pyplot as plt In [14]: R = .08314 #L-bar/mol\*K Tc = 647.1 #K, critical temperature Pc = 220.55 #bar, critical pressure Th = 683.15 #410 degrees Celsius r = 8.314 #J/mol\*K n = 1 - (Tc/Th) #Efficiency of the Carnot engine equation  $a = \frac{27}{64*(R**2)*(Tc**2)}/Pc$  #Parameter calculations that apply to the Van der Waal's b = 1/8 \* R \* Tc/PcVc = 3/8\*R\*Tc/Pc #Critical Volume CompRatio = 2 #V2/V1 V1 = .060984 V2 = V1\*CompRatio Tspace = np.linspace(Tc, Th, 1000) #array of temperatures that will be used to establish list(Tspace) #converting the array to a list A = 3.470 #Heat Capacity coefficients B = 1.450 \* 10 \* \* - 3**C** = 0 D = 0.121\*10\*\*5y = 1.33testCv = (R\*(A + B\*Tspace + C\*(Tspace\*\*2) + D\*(Tspace\*\*-2)))/y #Calculating Cv Cv = np.mean(testCv)Var = ((V2-b)\*((Tc/Tspace)\*\*(Cv/R))) + b #Volume range of the right adiabat Par = ((R\*Tspace)/(Var-b))-(a/(Var\*\*2)) #Pressure list based on parameters, temp li Val = ((V1-b)\*((Th/Tspace)\*\*(Cv/R))) + b #Volume range of the left adiabatPal = ((R\*Tspace)/(Val-b))-(a/(Val\*\*2)) #Pressure list based on parameters, temp li

```
hVspace = np.linspace(V1, Var[-1], 100) #Need to keep this array at a length of 100
Ph = ((R*Th)/(hVspace-b))-(a/(hVspace**2)) #Pressure list for the upper isotherm
cVspace = np.linspace(Val[0], V2, 100) #Volume range for lower isotherm
Pc = ((R*Tc)/(cVspace-b))-(a/(cVspace**2)) #Pressure list for lower isotherm
```

```
#Plotting all curves
```

```
plt.plot(cVspace, Pc, label = 'Lower Isotherm')
plt.plot(hVspace, Ph, label = 'Upper Isotherm')
plt.plot(Var, Par, label = 'Right Adiabat')
plt.plot(Val, Pal, label = 'Left Adiabat')
plt.grid(True)
plt.xlabel('Volume (L/mol)')
plt.ylabel('Pressure (bar)')
plt.title("Supercritical Water - Carnot Cycle")
plt.legend(loc = 'best')
plt.show()
```

#Finding the work associated with the plot of the graph

```
War = -np.trapz(Par, Var)
Wth = np.trapz(Ph, hVspace)
Wal = -np.trapz(Pal, Val)
Wtc = np.trapz(Pc, cVspace)
```

#Using equations given to solve for and report findings for this supercritical flui

print('The efficiency of this system is {:.3}'.format(n\*100), '%.')

```
Qh = r*Th*np.log((Var[-1]-b)/(V1-b)) #Qh for one cycle
print('The theoretical input energy, Qh, is {:.7}'.format(Qh), "Joules/sec.")
```

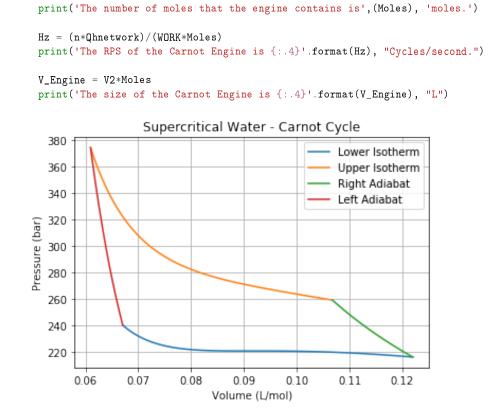
```
TheoQc = Qh*(1-n)
print('The theoretical work removed from the engine is {:.7}'.format(TheoQc), "Joule
```

TheoWORK = Qh\*(1-(Tc/Th))
print('The theoretical work of this system is {:.7}'.format(TheoWORK), "Joules/cycle")

WORK = ((War+Wth)-(Wal+Wtc))\*100
print('The work from the system is {:.7}'.format(WORK), "Joules/cycle.")

Qhnetwork = 976668 #From cooler 5, W #Full scale size, 10x greater than the numbers print('The power available from the network is', (Qhnetwork), 'Joules/sec')

Qcnetwork = Qhnetwork\*(1-n)
print('The power lost by the engine is {:.8}'.format(Qcnetwork), 'Joules/sec')



The efficiency of this system is 5.28 %. The theoretical input energy, Qh, is 5206.802 Joules/sec. The theoretical work removed from the engine is 4932.038 Joules/sec The theoretical work of this system is 274.7643 Joules/cycle\*mol The work from the system is 274.7768 Joules/cycle. The power available from the network is 976668 Joules/sec The power lost by the engine is 925128.98 Joules/sec The number of moles that the engine contains is 40 moles. The RPS of the Carnot Engine is 4.879 L

Moles = 40

3

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xiii. Pinch Calculations at Tmin of 10 degrees C Code

```
In [518]:
```

```
#COLUMN INTEGRATION
CP = [2.439565742, 2.441707317, 1.231428571, 0.5225806452, 0.6550724638, 0.06, 1.150300601, 3.25872
093, 0.1176995096, 0.1272727273, 0,0, 0, 0, 0, 0] #input CP values (0 for columns)
Ts = [35.5, 450, 40, 35.5, 104.5, 70, 129.9, 183.2, 249.3, 80, 35.5, 129.9, 104.5, 150.3, 183.2, 24
9.3] #input temperatures at inlets
Tt = [450, 40, 75, 20, 70, 35, 80, 80, 25, 25, 35.5, 129.9, 104.5, 150.3, 183.2, 249.3] #input
temperatures at outlets
Qcol = [0,0,0,0,0,0,0,0,0,0,0, 35.7, -95, 186.8, -286.5, 2552.7, -2832] #input 0 if not a column, -Qre
b for reboiler, or Ocond for condenser
Tmin = 10 #input Tmin
o = list(range(len(CP))) #list of length of the number of streams
Tss = list(range(len(Ts))) #list that will become shifted inlet temperatures
Tts = list(range(len(Tt))) #list that will become shifted outlet temperatures
coldnum = [] #list used to identify cold streams
hotnum = [] #list used to identify hot streams
disnumC = [] #list used to identify condensers
disnumR = [] #list used to identify reboilers
columntempsC = [] #used to identify where the condenders fit into the heat cascade
columntempsR = [] #used to identify where the reboilers fit into the heat cascade
for i in o: #function creating modified temps and identifying hot vs cold streams
   if Ts[i] > Tt[i]:
        Tss[i] = Ts[i] - (Tmin*.5)
        Tts[i] = Tt[i] - (Tmin*.5)
        hotnum.append(i)
    if Ts[i] < Tt[i]:</pre>
        Tss[i] = Ts[i] + (Tmin*.5)
        Tts[i] = Tt[i] + (Tmin*.5)
        coldnum.append(i)
    if Ts[i] == Tt[i]: #identifies columns/shifts temps
        if Qcol[i] > 0:
            Tss[i] = Ts[i] - (Tmin*.5)
            Tts[i] = Tt[i] - (Tmin*.5)
            disnumC.append(i)
            columntempsC.append([Tts[i], Qcol[i]])
        if Qcol[i] < 0:</pre>
            Tss[i] = Ts[i] + (Tmin*.5)
            Tts[i] = Tt[i] + (Tmin*.5)
            disnumR.append(i)
            columntempsR.append([Tts[i], Qcol[i]])
```

# In [519]:

```
Tall = [] #list of all shifted temperatures
for i in o:
    Tall.append(Tss[i])
    Tall.append(Tts[i])
Tstar = list(set(Tall)) #list of all temperatures, without repeats, in descending order
Tstar.sort(reverse=True)
print(Tstar) #HEAT CASCADE TEMPS
print()
CPtot = [] #will be list of net CPs for each temp interval
lenT = list(range(len(Tstar) - 1)) #list for iterating through temperature intervals
p=0
lentempc = list(range(len(coldnum))) #iterates over cold streams
lentemph = list(range(len(hotnum))) #iterates over hot streams
#function to calculate net CPs
for i in lenT: #iterate through temp intervals
```

```
p=0
                     for j in o: #iterate through streams
                                           for k in lentempc:
                                                                \label{eq:if_j} \ensuremath{\texttt{if}}\ \ensuremath{\texttt{j}}\ \ensuremath{\texttt{=}}\ \ensuremath{\texttt{cold}}\ \ensuremath{\texttt{increments}}\ \ensuremath{\texttt{to}}\ \ensuremath{\texttt{see}}\ \ensuremath{\texttt{increments}}\ \ensuremath{\texttt{to}}\ \ensuremath{\texttt{see}}\ \ensuremath{\texttt{increments}}\ \ensuremath{\texttt{to}}\ \ensuremath{\texttt{see}}\ \ensuremath{\texttt{increments}}\ \ensuremath{\texttt{to}}\ \ensuremath{\texttt{see}}\ \ensuremath{\texttt{increments}}\ \ensuremath{\texttt{increments}}\ \ensuremath{\texttt{increments}}\ \ensuremath{\texttt{to}}\ \ensuremath{\texttt{see}}\ \ensuremath{\texttt{increments}}\ \ensuremath{\ensuremath{}}\ \ensuremath{\ensuremath{increments}}\ \ensuremath{\ensuremath{increments}}\ \ensuremath{\ensuremath{increments}}\ \ensuremath{\ensuremath{increments}}\ \ensuremath{\ensuremath{increments}}\ \ensuremath{\ensuremath{increments}}\ \en
                                                                                                                                                                            #if it's in the selected temp range
                                                                                     x = Tss[j]
                                                                                     while Tts[j] >= x:
                                                                                                           if -.005 +x <Tstar[i] -.1 < x +.005:</pre>
                                                                                                                              p = p-CP[j]
                                                                                                           x = x + .1
                                           for k in lentemph: #same for hot streams, but decreasing temp
                                                                if j == hotnum[k]:
                                                                                     x = Tss[j]
                                                                                     while Tts[j] <= x:</pre>
                                                                                                          if -.005 + x<Tstar[i] -.1 <x+.005:</pre>
                                                                                                                              p = p+CP[j]
                                                                                                            x = x - .1
                     CPtot.append(p)
print(CPtot) #NET CP VALUES
[455.0, 445.0, 254.3, 244.3, 178.2, 155.3, 134.9, 124.9, 99.5, 80.0, 75.0, 65.0, 45.0, 40.5, 35.0,
```

30.5, 30.0, 20.0, 15.0]

[-2.439565742, 0.002141575000000067, 0.002141575000000067, 0.11984108460000001, 3.3785620146, 3. 3785620146, 3.3785620146, 4.5288626156000005, 5.1839350794, 3.9525065084, -0.3292422953, -0.9243147590999998, 0.3071138119, 2.7466795539, 0.30497223689999997, 0.8275528821, 0.7675528821, 0. 5225806452] ◀

In [520]:

```
H = [] #list of delta H values for intervals
Hval = list(range((len(Tstar) - 1))) #list to iterate through temperature intervals
for i in Hval:
    H.append((Tstar[i]-Tstar[i+1])*(CPtot[i])) #calculates delta H
print(H) #delta Hs before column integration
print()
count = 0
for i in range(len(Tstar)): #adds in column values
    for j in range(len(columntempsR)):
        if Tstar[i] == columntempsR[j][0]:
            H.insert(count + i, columntempsR[j][1])
            count = count+1
    for j in range(len(columntempsC)):
        if Tstar[i] == columntempsC[j][0]:
            H.insert(count + i, columntempsC[j][1])
            count = count+1
print(H) #delta Hs after column integration
[-24.39565742,\ 0.4083983525000012,\ 0.02141575000000067,\ 7.921495692060003,\ 77.36907013433992,\ 68.
92266509784002, 33.785620146, 115.03311043624004, 101.0867340483, 19.762532542, -3.292422953, -18.
486295181999996, 1.3820121535499998, 15.106737546449999, 1.3723750660499998, 0.41377644105,
7.6755288209999994, 2.612903226000002]
[-24.39565742, 0.4083983525000012, -2832, 0.02141575000000067, 7.921495692060003, 2552.7,
77.36907013433992, -286.5, 68.92266509784002, -95, 33.785620146, 115.03311043624004, 186.8,
101.0867340483, 19.762532542, -3.292422953, -18.486295181999996, 1.3820121535499998,
15.106737546449999, 1.3723750660499998, 35.7, 0.41377644105, 7.6755288209999994,
2.612903226000002]
In [521]:
Hlen = list(range(len(H))) #list of delta H values for intervals
Hsum = []
```

n = 0
for i in Hlen:
 n = n+H[i]
 Hsum.append(n)
Qh = -min(Hsum) #Qh is -largest negative number when adding through H

print(Qh) #Qh
Hnewsum = list(range(len(Hsum))) #\*\*\*HEAT CASCADE Hs\*\*\*

for i in Hlen: Hnewsum[i] = Hsum[i] + Qh print() print(Hnewsum) #Heat Cascade after Qh

2855.9872590675

[2831.5916016475, 2832.0, 0.0, 0.0214157499999601, 7.942911442059994, 2560.64291144206, 2638.0119815763996, 2351.5119815763996, 2420.43464667424, 2325.43464667424, 2359.22026682024, 2474.25337725648, 2661.05337725648, 2762.1401113047796, 2781.90264384678, 2778.61022089378, 2760.12392571178, 2761.50593786533, 2776.61267541178, 2777.9850504778296, 2813.68505047783, 2814.0988269188797, 2821.77435573988, 2824.38725896588]

In [522]:

```
Qc = sum(H)+Qh #Qc is ending value of cacade after adding Qc
print(Qc)
pinch = 0
count = 0
recheckR = len(columntempsR)*[0]
recheckC = len(columntempsC)*[0]
O = Qh
for i in Hlen: #finds pinch by checking for zero value in cascade
    Q = Q + H[i]
    if -.01 < Q < .01:
       pinch = Tstar[i+1-count]
    for j in range(len(columntempsR)):
        if Tstar[i+1-count] == columntempsR[j][0]:
            if recheckR[j] == 0:
                count = count + 1
                recheckR[j] = 1
            else:
                recheckR[j] = 0
    for j in range(len(columntempsC)):
        if Tstar[i+1-count] == columntempsC[j][0]:
            if recheckC[j] == 0:
                count = count + 1
                recheckC[j] = 1
            else:
                recheckC[j] = 0
print(pinch) #pinch temperature
```

2824.38725896588 254.3

# In [523]:

#COLUMN INTEGRATION (Tmin of 20) CP = [2.439565742, 2.441707317, 1.231428571, 0.5225806452, 0.6550724638, 0.06, 1.150300601, 3.25872 093, 0.1176995096, 0.1272727273, 0,0, 0, 0, 0, 0] #input CP values (0 for columns) Ts = [35.5, 450, 40, 35.5, 104.5, 70, 129.9, 183.2, 249.3, 80, 35.5, 129.9, 104.5, 150.3, 183.2, 24 9.3] #input temperatures at inlets Tt = [450, 40, 75, 20, 70, 35, 80, 80, 25, 25, 35.5, 129.9, 104.5, 150.3, 183.2, 249.3] #input temperatures at outlets Qcol = [0,0,0,0,0,0,0,0,0, 35.7, -95, 186.8, -286.5, 2552.7, -2832] #input 0 if not a column, -Qre b for reboiler, or Qcond for condenser Tmin = 20 #input Tmin o = list(range(len(CP))) #list of length of the number of streams Tss = list(range(len(Ts))) #list that will become shifted inlet temperatures Tts = list(range(len(Tt))) #list that will become shifted outlet temperatures xiv. Pinch Calculations at Tmin of 20 degrees C Code

print(Qh) #Qh
Hnewsum = list(range(len(Hsum))) #\*\*\*HEAT CASCADE Hs\*\*\*

for i in Hlen: Hnewsum[i] = Hsum[i] + Qh print() print(Hnewsum) #Heat Cascade after Qh

2855.9872590675

[2831.5916016475, 2832.0, 0.0, 0.0214157499999601, 7.942911442059994, 2560.64291144206, 2638.0119815763996, 2351.5119815763996, 2420.43464667424, 2325.43464667424, 2359.22026682024, 2474.25337725648, 2661.05337725648, 2762.1401113047796, 2781.90264384678, 2778.61022089378, 2760.12392571178, 2761.50593786533, 2776.61267541178, 2777.9850504778296, 2813.68505047783, 2814.0988269188797, 2821.77435573988, 2824.38725896588]

In [522]:

```
Qc = sum(H)+Qh #Qc is ending value of cacade after adding Qc
print(Qc)
pinch = 0
count = 0
recheckR = len(columntempsR)*[0]
recheckC = len(columntempsC)*[0]
O = Qh
for i in Hlen: #finds pinch by checking for zero value in cascade
    Q = Q + H[i]
    if -.01 < Q < .01:
       pinch = Tstar[i+1-count]
    for j in range(len(columntempsR)):
        if Tstar[i+1-count] == columntempsR[j][0]:
            if recheckR[j] == 0:
                count = count + 1
                recheckR[j] = 1
            else:
                recheckR[j] = 0
    for j in range(len(columntempsC)):
        if Tstar[i+1-count] == columntempsC[j][0]:
            if recheckC[j] == 0:
                count = count + 1
                recheckC[j] = 1
            else:
                recheckC[j] = 0
print(pinch) #pinch temperature
```

2824.38725896588 254.3

# In [523]:

#COLUMN INTEGRATION (Tmin of 20) CP = [2.439565742, 2.441707317, 1.231428571, 0.5225806452, 0.6550724638, 0.06, 1.150300601, 3.25872 093, 0.1176995096, 0.1272727273, 0,0, 0, 0, 0, 0] #input CP values (0 for columns) Ts = [35.5, 450, 40, 35.5, 104.5, 70, 129.9, 183.2, 249.3, 80, 35.5, 129.9, 104.5, 150.3, 183.2, 24 9.3] #input temperatures at inlets Tt = [450, 40, 75, 20, 70, 35, 80, 80, 25, 25, 35.5, 129.9, 104.5, 150.3, 183.2, 249.3] #input temperatures at outlets Qcol = [0,0,0,0,0,0,0,0,0, 35.7, -95, 186.8, -286.5, 2552.7, -2832] #input 0 if not a column, -Qre b for reboiler, or Qcond for condenser Tmin = 20 #input Tmin o = list(range(len(CP))) #list of length of the number of streams Tss = list(range(len(Ts))) #list that will become shifted inlet temperatures Tts = list(range(len(Tt))) #list that will become shifted outlet temperatures

```
coldnum = [] #list used to identify cold streams
hotnum = [] #list used to identify hot streams
disnumC = [] #list used to identify condensers
disnumR = [] #list used to identify reboilers
columntempsC = [] #used to identify where the condenders fit into the heat cascade
columntempsR = [] #used to identify where the reboilers fit into the heat cascade
for i in o: #function creating modified temps and identifying hot vs cold streams
    if Ts[i] > Tt[i]:
        Tss[i] = Ts[i] - (Tmin*.5)
        Tts[i] = Tt[i]-(Tmin*.5)
        hotnum.append(i)
    if Ts[i] < Tt[i]:</pre>
        Tss[i] = Ts[i] + (Tmin*.5)
        Tts[i] = Tt[i] + (Tmin*.5)
        coldnum.append(i)
    if Ts[i] == Tt[i]: #identifies columns/shifts temps
        if Qcol[i] > 0:
            Tss[i] = Ts[i] - (Tmin*.5)
            Tts[i] = Tt[i] - (Tmin*.5)
            disnumC.append(i)
            columntempsC.append([Tts[i], Qcol[i]])
        if Qcol[i] < 0:</pre>
            Tss[i] = Ts[i] + (Tmin*.5)
            Tts[i] = Tt[i] + (Tmin*.5)
            disnumR.append(i)
            columntempsR.append([Tts[i], Qcol[i]])
```

```
In [524]:
```

```
Tall = [] #list of all shifted temperatures
for i in o:
    Tall.append(Tss[i])
    Tall.append(Tts[i])
Tstar = list(set(Tall)) #list of all temperatures, without repeats, in descending order
Tstar.sort(reverse=True)
print(Tstar) #HEAT CASCADE TEMPS
print()
CPtot = [] #will be list of net CPs for each temp interval
lenT = list(range(len(Tstar) - 1)) #list for iterating through temperature intervals
p=0
lentempc = list(range(len(coldnum))) #iterates over cold streams
lentemph = list(range(len(hotnum))) #iterates over hot streams
#function to calculate net CPs
for i in lenT: #iterate through temp intervals
    p=0
    for j in o: #iterate through streams
        for k in lentempc:
            if j == coldnum[k]: #if cold, increase temp in integer increments to see
                                 #if it's in the selected temp range
                x = Tss[j]
                while Tts[j] >= x:
                    if -.005 +x <Tstar[i] -.1 < x +.005:
                        p = p-CP[j]
                    x = x + .1
        for k in lentemph: #same for hot streams, but decreasing temp
            if j == hotnum[k]:
                x = Tss[j]
                while Tts[j] <= x:</pre>
                    if -.005 + x<Tstar[i] -.1 <x+.005:</pre>
                        p = p+CP[j]
                    x = x - .1
    CPtot.append(p)
print(CPtot) #NET CP VALUES
```

[460.0, 440.0, 259.3, 239.3, 173.2, 160.3, 139.9, 119.9, 94.5, 85.0, 70.0, 60.0, 50.0, 45.5, 30.0, 25.5, 25.0, 15.0, 10.0]

 $[-2.439565742,\ 0.002141575000000067,\ 0.002141575000000067,\ 0.11984108460000001,\ 3.3785620146,\ 3.$ 

```
3785620146, 3.3785620146, 4.5288626156000005, 5.1839350794, 3.9525065084, -0.3292422953, -
0.9243147590999998, 0.3071138119, 2.7466795539, 0.30497223689999997, 0.8275528821, 0.7675528821, 0.
5225806452]
```

In [525]:

```
H = [] #list of delta H values for intervals
Hval = list(range((len(Tstar) - 1))) #list to iterate through temperature intervals
for i in Hval:
   H.append((Tstar[i]-Tstar[i+1])*(CPtot[i])) #calculates delta H
print(H) #delta Hs before column integration
print()
count = 0
for i in range(len(Tstar)): #adds in column values
    for j in range(len(columntempsR)):
        if Tstar[i] == columntempsR[j][0]:
            H.insert(count + i, columntempsR[j][1])
            count = count+1
    for j in range(len(columntempsC)):
        if Tstar[i] == columntempsC[j][0]:
            H.insert(count + i, columntempsC[j][1])
            count = count+1
print(H) #delta Hs after column integration
```

[-48.79131484, 0.38698260250000116, 0.0428315000000013, 7.921495692060003, 43.58344998833992, 68.92266509784002, 67.571240292, 115.03311043624004, 49.247383254300004, 59.287597626, -3.292422953, -9.243147590999998, 1.3820121535499998, 42.57353308545, 1.3723750660499998, 0.41377644105, 7.6755288209999994, 2.6129032260000002]

[-48.79131484, 0.38698260250000116, -2832, 0.0428315000000013, 7.921495692060003, 2552.7, 43.58344998833992, -286.5, 68.92266509784002, -95, 67.571240292, 115.03311043624004, 186.8, 49.247383254300004, 59.287597626, -3.292422953, -9.243147590999998, 1.3820121535499998, 42.57353308545, 1.3723750660499998, 35.7, 0.41377644105, 7.6755288209999994, 2.6129032260000002]

#### In [526]:

Hlen = list(range(len(H))) #list of delta H values for intervals
Hsum = []
n = 0
for i in Hlen:
 n = n+H[i]
 Hsum.append(n)
Qh = -min(Hsum) #Qh is -largest negative number when adding through H
print(Qh) #Qh
Hnewsum = list(range(len(Hsum))) #\*\*\*HEAT CASCADE Hs\*\*\*
for i in Hlen:
 Hnewsum[i] = Hsum[i] + Qh
print()
print(Hnewsum) #Heat Cascade after Oh

2880.4043322375

[2831.6130173975002, 2832.0, 0.0, 0.0428314999999202, 7.9643271920599545, 2560.66432719206, 2604.2477771803997, 2317.7477771803997, 2386.6704422782395, 2291.6704422782395, 2359.24168257024, 2474.2747930064797, 2661.07479300648, 2710.32217626078, 2769.6097738867797, 2766.31735093378, 2757.0742033427796, 2758.4562154963296, 2801.0297485817796, 2802.4021236478297, 2838.10212364783, 2838.51590008888, 2846.19142890988, 2848.8043321358796]

#### In [527]:

Qc = sum(H)+Qh #Qc is ending value of cacade after adding Qc print(Qc)

pinch = 0
count = 0
recheckR = len(columntempsR)\*[0]

```
O = Oh
for i in Hlen: #finds pinch by checking for zero value in cascade
    Q = Q + H[i]
    if -.01 < Q < .01:
        pinch = Tstar[i+1-count]
    for j in range(len(columntempsR)):
        if Tstar[i+1-count] == columntempsR[j][0]:
            if recheckR[j] == 0:
                count = count + 1
                recheckR[j] = 1
            else:
                recheckR[j] = 0
    for j in range(len(columntempsC)):
        if Tstar[i+1-count] == columntempsC[j][0]:
            if recheckC[j] == 0:
                count = count + 1
                recheckC[j] = 1
            else:
                recheckC[j] = 0
print(pinch) #pinch temperature
```

Tee[i] = Te[i] + (Tmin \* 5)

2848.8043321358796 259.3

recheckC = len(columntempsC)\*[0]

In [485]:

```
def HXColInt(T): #uses program from before, but have Tmin as an input, and spits out
                #Qh, Qc, and Tpinch for each value put in
    CP = [24.39565742, 24.41707317, 12.31428571, 5.225806452, 6.550724638, 0.6, 11.50300601,
          32.5872093, 1.176995096, 1.272727273, 0, 0, 0, 0, 0, 0, 0] #input CP values (0 for columns)
    Ts = [35.5, 450, 40, 35.5, 104.5, 70, 129.9, 183.2, 249.3, 80, 35.5, 129.9, 104.5, 150.3,
          183.2, 249.3] #input temperatures at inlets
    Tt = [450, 40, 75, 20, 70, 35, 80, 80, 25, 25, 35.5, 129.9, 104.5, 150.3, 183.2, 249.3]
            #input temperatures at outlets
    Qcol = [0,0,0,0,0,0,0,0,0, 357, -950, 1868, -2865, 25527, -28320]
            #input 0 if not a column, -Qreb for reboiler, or Qcond for condenser
    Tmin = T #input Tmin
    o = list(range(len(CP))) #list of length of the number of streams
    Tss = list(range(len(Ts))) #list that will become shifted inlet temperatures
    Tts = list(range(len(Tt))) #list that will become shifted outlet temperatures
    coldnum = [] #list used to identify cold streams
    hotnum = [] #list used to identify hot streams
    disnumC = [] #list used to identify condensers
    disnumR = [] #list used to identify reboilers
    columntempsC = [] #used to identify where the condenders fit into the heat cascade
    columntempsR = [] #used to identify where the reboilers fit into the heat cascade
    for i in o: #function creating modified temps and identifying hot vs cold streams
        if Ts[i] > Tt[i]:
            Tss[i] = Ts[i] - (Tmin*.5)
            Tts[i] = Tt[i] - (Tmin*.5)
            hotnum.append(i)
        if Ts[i] < Tt[i]:</pre>
            Tss[i] = Ts[i] + (Tmin*.5)
            Tts[i] = Tt[i] + (Tmin*.5)
            coldnum.append(i)
        if Ts[i] == Tt[i]: #identifies columns/shifts temps
            if Qcol[i] > 0:
                Tss[i] = Ts[i]-(Tmin*.5)
                Tts[i] = Tt[i] - (Tmin*.5)
                disnumC.append(i)
                columntempsC.append([Tts[i], Qcol[i]])
            if Qcol[i] < 0:</pre>
```

xv. Cost Analysis Code

```
O = Oh
for i in Hlen: #finds pinch by checking for zero value in cascade
    Q = Q + H[i]
    if -.01 < Q < .01:
        pinch = Tstar[i+1-count]
    for j in range(len(columntempsR)):
        if Tstar[i+1-count] == columntempsR[j][0]:
            if recheckR[j] == 0:
                count = count + 1
                recheckR[j] = 1
            else:
                recheckR[j] = 0
    for j in range(len(columntempsC)):
        if Tstar[i+1-count] == columntempsC[j][0]:
            if recheckC[j] == 0:
                count = count + 1
                recheckC[j] = 1
            else:
                recheckC[j] = 0
print(pinch) #pinch temperature
```

Tee[i] = Te[i] + (Tmin \* 5)

2848.8043321358796 259.3

recheckC = len(columntempsC)\*[0]

In [485]:

```
def HXColInt(T): #uses program from before, but have Tmin as an input, and spits out
                #Qh, Qc, and Tpinch for each value put in
    CP = [24.39565742, 24.41707317, 12.31428571, 5.225806452, 6.550724638, 0.6, 11.50300601,
          32.5872093, 1.176995096, 1.272727273, 0, 0, 0, 0, 0, 0, 0] #input CP values (0 for columns)
    Ts = [35.5, 450, 40, 35.5, 104.5, 70, 129.9, 183.2, 249.3, 80, 35.5, 129.9, 104.5, 150.3,
          183.2, 249.3] #input temperatures at inlets
    Tt = [450, 40, 75, 20, 70, 35, 80, 80, 25, 25, 35.5, 129.9, 104.5, 150.3, 183.2, 249.3]
            #input temperatures at outlets
    Qcol = [0,0,0,0,0,0,0,0,0, 357, -950, 1868, -2865, 25527, -28320]
            #input 0 if not a column, -Qreb for reboiler, or Qcond for condenser
    Tmin = T #input Tmin
    o = list(range(len(CP))) #list of length of the number of streams
    Tss = list(range(len(Ts))) #list that will become shifted inlet temperatures
    Tts = list(range(len(Tt))) #list that will become shifted outlet temperatures
    coldnum = [] #list used to identify cold streams
    hotnum = [] #list used to identify hot streams
    disnumC = [] #list used to identify condensers
    disnumR = [] #list used to identify reboilers
    columntempsC = [] #used to identify where the condenders fit into the heat cascade
    columntempsR = [] #used to identify where the reboilers fit into the heat cascade
    for i in o: #function creating modified temps and identifying hot vs cold streams
        if Ts[i] > Tt[i]:
            Tss[i] = Ts[i] - (Tmin*.5)
            Tts[i] = Tt[i] - (Tmin*.5)
            hotnum.append(i)
        if Ts[i] < Tt[i]:</pre>
            Tss[i] = Ts[i] + (Tmin*.5)
            Tts[i] = Tt[i] + (Tmin*.5)
            coldnum.append(i)
        if Ts[i] == Tt[i]: #identifies columns/shifts temps
            if Qcol[i] > 0:
                Tss[i] = Ts[i]-(Tmin*.5)
                Tts[i] = Tt[i] - (Tmin*.5)
                disnumC.append(i)
                columntempsC.append([Tts[i], Qcol[i]])
            if Qcol[i] < 0:</pre>
```

```
199[T] - T9[T] + (THTH, "))
            Tts[i] = Tt[i]+(Tmin*.5)
            disnumR.append(i)
            columntempsR.append([Tts[i], Qcol[i]])
Tall = [] #list of all shifted temperatures
for i in o:
   Tall.append(Tss[i])
   Tall.append(Tts[i])
Tstar = list(set(Tall)) #list of all temperatures, without repeats, in descending order
Tstar.sort(reverse=True) #***HEAT CASCADE TEMPS**
CPtot = [] #will be list of net CPs for each temp interval
lenT = list(range(len(Tstar) - 1)) #list for iterating through temperature intervals
p=0
lentempc = list(range(len(coldnum))) #iterates over cold streams
lentemph = list(range(len(hotnum))) #iterates over hot streams
#function to calculate net CPs
for i in lenT: #iterate through temp intervals
   p=0
    for j in o: #iterate through streams
        for k in lentempc:
            if j == coldnum[k]: #if cold, checks if terget temp is in range
                if Tss[j] <Tstar[i] -.01 < Tts[j]:</pre>
                    p = p-CP[j]
        for k in lentemph: #same for hot streams w/ target temp
            if j == hotnum[k]:
                if Tts[j] <Tstar[i] -.01 < Tss[j]:</pre>
                    p = p+CP[j]
    CPtot.append(p)
H = [] #list of delta H values for intervals
Hval = list(range((len(Tstar) - 1))) #list to iterate through temperature intervals
for i in Hval:
   H.append((Tstar[i]-Tstar[i+1])*(CPtot[i])) #calculates delta H
count = 0
for i in range(len(Tstar)): #adds in column values
   for j in range(len(columntempsR)):
        if Tstar[i] == columntempsR[j][0]:
            H.insert(count + i, columntempsR[j][1])
            count = count+1
    for j in range(len(columntempsC)):
        if Tstar[i] == columntempsC[j][0]:
            H.insert(count + i, columntempsC[j][1])
            count = count+1
Hlen = list(range(len(H))) #list of delta H values for intervals
Hsum = []
n = 0
for i in Hlen:
   n = n+H[i]
   Hsum.append(n)
Qh = -min(Hsum) #Qh is -largest negative number when adding through H
QH.append(Qh) #Adds Qh to list
Hnewsum = list(range(len(Hsum))) #***HEAT CASCADE Hs***
for i in Hlen:
   Hnewsum[i] = Hsum[i] + Qh
Qc = sum(H)+Qh #Qc is ending value of cacade after adding Qc
QC.append(Qc) #Adds Qc to list
pinch = 0
count = 0
recheckR = len(columntempsR)*[0]
recheckC = len(columntempsC)*[0]
O = Oh
for i in Hlen: #finds pinch by checking for zero value in cascade
   Q = Q + H[i]
    if -.01 < Q < .01:
        pinch = Tstar[i+1-count]
   for i in range (lon (columntemper)).
```

```
LOL J III Lange (Len (COLUMNICEMPSK)):
        if Tstar[i+1-count] == columntempsR[j][0]:
            if recheckR[j] == 0:
                count = count + 1
                recheckR[j] = 1
            else:
                recheckR[j] = 0
    for j in range(len(columntempsC)):
        if Tstar[i+1-count] == columntempsC[j][0]:
            if recheckC[j] == 0:
                count = count + 1
                recheckC[j] = 1
            else:
                recheckC[j] = 0
Tpinch.append(pinch) #adds Tpinch to list
return
```

In [489]:

# In [491]:

```
hrs = 300*24 #setting hrs equal to hours in a year
print(hrs)
```

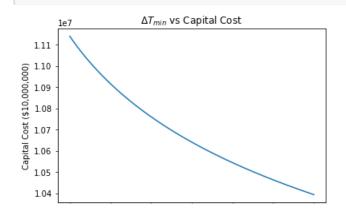
7200

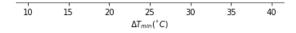
# In [492]:

```
cost = [] #calculating all three costs in terms of Tmin
Ccost = []
Tcost = []
for i in list(range(30001)):
    cost.append(QH[i]*hrs*.15)
    Ccost.append((12.5*10**6)/(Tmins[i]**.05))
    Tcost.append(cost[i]+Ccost[i])
```

In [493]:

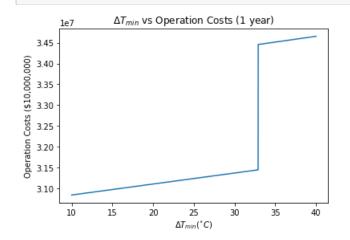
```
import matplotlib.pyplot as plt #Graphing Tmin vs Capital cost
plt.plot(Tmins, Ccost)
plt.title('$\Delta T_{min}$ vs Capital Cost')
plt.xlabel('$\Delta T_{min} (^{\circ}C)$')
plt.ylabel('Capital Cost ($10,000,000)')
plt.show()
```





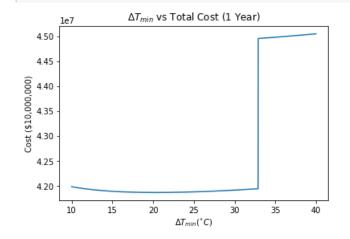
In [494]:

```
import matplotlib.pyplot as plt #graphing Tmin vs operation costs
plt.plot(Tmins, cost)
plt.title('$\Delta T_{min}$ vs Operation Costs (1 year)')
plt.xlabel('$\Delta T_{min} (^{\circ}C)$')
plt.ylabel('Operation Costs ($10,000,000)')
plt.show()
```



In [495]:

```
import matplotlib.pyplot as plt #graphing Tmin vs total cost for 1 year
plt.plot(Tmins, Tcost)
plt.title('$\Delta T_{min}$ vs Total Cost (1 Year)')
plt.xlabel('$\Delta T_{min} (^{\circ}C)$')
plt.ylabel('Cost ($10,000,000)')
plt.show()
```



In [357]:

minimum = min(Tcost) #calculating minimum cost for 1 year, and the Tmin needed to achieve this
for i in list(range(30001)):
 if minimum == Tcost[i]:
 print(Tcost[i])
 print(Tmins[i])
41869410.86540445
20.384
In [471]:
hours = list(range(360\*5)) #calculation of the number of days until the best Tmin value is 10
degrees

```
for i in hours:
```

```
hours[i] = i * 24
```

```
i in range(len(nours)):
    num = (QH[0]*.15*hours[i]) + ((12.5*10**6)/(Tmins[0]**.05))
    num2 = (QH[1]*.15*hours[i]) + ((12.5*10**6)/(Tmins[1]**.05))
    if num<num2:
        days = i
        break</pre>
```

# print(i)

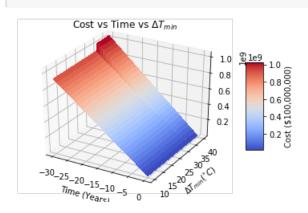
634

#### In [496]:

```
hours = [] #calculating cost in terms of Tmin and time
for i in range(31):
    hours.append(i*7200)
cost = list(range(31))
Tcost = list(range(31))
for i in cost:
    cost[i] = list(range(len(hours)))
Tcost[i] = list(range(len(hours)))
Ccost = []
for i in list(range(31)):
    for j in range(31):
        cost[i][j] = (QH[i]*hours[j]*.15)
    Ccost.append((12.5*10**6)/(Tmins[i]**.05))
    for j in range(31):
        Tcost[i][j] = (cost[i][j]+Ccost[i])
```

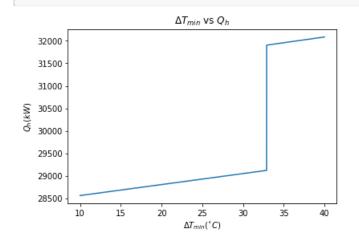
In [475]:

```
import numpy as np #using the relations between cost, Tmin, and time, makes a 3D plot to show
these relationships
from mpl_toolkits.mplot3d import Axes3D
from matplotlib import cm
from matplotlib.ticker import LinearLocator, FormatStrFormatter
xthree1 = np.array(Tmins)
ythree1 = np.array(hours)
Qthree = np.array(QH)
xthree1, ythree1 = np.meshgrid(xthree1, ythree1)
zthree1 = ((12.5*10**6) / (xthree1)) + (Qthree*ythree1*.15)
fig1 = plt.figure() #here we create our 3d coordinate system
ax1 = fig1.gca(projection='3d')
three1 = ax1.plot surface(-ythree1/7200, xthree1, zthree1, cmap='coolwarm', linewidth=0, antialiase
d = False) #creates our 3d plot as a surface plot.
figl.colorbar(three1, shrink=0.5, aspect=5, label = 'Cost ($100,000,000)') #creates a bar to displa
y what z values each color cooresponds to
plt.xlabel('Time (Years)')
plt.ylabel('$\Delta T {min} (^{\circ}C)$')
plt.title('Cost vs Time vs $\Delta T_{min}$')
plt.show()
```



### In [453]:

```
plt.xlabel('$\Delta T_{min} (^{\circ}C)$')
plt.ylabel('$Q_h (kW)$')
plt.show()
```

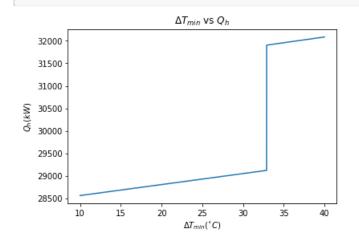


#### In [360]:

```
import networkx as nx #don't use!
G = nx.Graph()
G.add node('1', node color= '#f20d0d')
G.add node('2', node color= '#f2690d')
G.add node('3', node color= '#f2ba0d')
G.add node('4', node color= '#d9f20d')
G.add_node('5a', node_color= '#5af20d')
G.add_node('5b', node_color= '#0df23f')
G.add_node('6', node_color= '#0df279')
G.add_node('7', node_color= '#0df2b3')
G.add_node('8', node_color= '#0df2ec')
G.add node('9', node color= '#0d79f2')
G.add_node('C1', node_color= '#0d28f2')
G.add_node('R1', node_color= '#2c0df2')
G.add_node('C2', node_color= '#710df2')
G.add_node('R2', node_color= '#d90df2')
G.add node('C3', node color= '#f20d98')
G.add_node('R3', node_color= '#f20d52')
G.add edge('1', '2', weight=465.2252+521.58)
G.add_edge('2', 'R3', weight=.16726)
G.add_edge('3', '7', weight=43.1)
G.add_edge('7', 'R1', weight=74.654)
G.add_edge('7', 'R2', weight=66.504)
G.add_edge('8', 'R1', weight=10.4753)
G.add_edge('8', 'R2', weight=2.4)
G.add_edge('R1', 'C3', weight=26.1)
G.add edge('R2', 'C3', weight=201.37)
color_map = []
for node in G:
    if node == '1':
        color_map.append('#f20d0d')
    if node == '2':
        color_map.append('#f2690d')
    if node == '3':
        color_map.append('#f2ba0d')
    if node == '4':
        color map.append('#ecee0a')
    if node == '5a':
        color map.append('#5af20d')
    if node == '5b':
        color_map.append('#0df23f')
    if node == '6':
        color_map.append('#0df279')
    if node == '7':
        color_map.append('#0df2b3')
    if node == '8':
        color_map.append('#0df2ec')
    if node == '9':
        color map.append('#0d79f2')
    if node == 'C1':
```

xvi. Eigenvector Centrality for Original Network Code

```
plt.xlabel('$\Delta T_{min} (^{\circ}C)$')
plt.ylabel('$Q_h (kW)$')
plt.show()
```



#### In [360]:

```
import networkx as nx #don't use!
G = nx.Graph()
G.add node('1', node color= '#f20d0d')
G.add node('2', node color= '#f2690d')
G.add node('3', node color= '#f2ba0d')
G.add node('4', node color= '#d9f20d')
G.add_node('5a', node_color= '#5af20d')
G.add_node('5b', node_color= '#0df23f')
G.add_node('6', node_color= '#0df279')
G.add_node('7', node_color= '#0df2b3')
G.add_node('8', node_color= '#0df2ec')
G.add node('9', node color= '#0d79f2')
G.add_node('C1', node_color= '#0d28f2')
G.add_node('R1', node_color= '#2c0df2')
G.add_node('C2', node_color= '#710df2')
G.add_node('R2', node_color= '#d90df2')
G.add node('C3', node color= '#f20d98')
G.add_node('R3', node_color= '#f20d52')
G.add edge('1', '2', weight=465.2252+521.58)
G.add_edge('2', 'R3', weight=.16726)
G.add_edge('3', '7', weight=43.1)
G.add_edge('7', 'R1', weight=74.654)
G.add_edge('7', 'R2', weight=66.504)
G.add_edge('8', 'R1', weight=10.4753)
G.add_edge('8', 'R2', weight=2.4)
G.add_edge('R1', 'C3', weight=26.1)
G.add edge('R2', 'C3', weight=201.37)
color_map = []
for node in G:
    if node == '1':
        color_map.append('#f20d0d')
    if node == '2':
        color_map.append('#f2690d')
    if node == '3':
        color_map.append('#f2ba0d')
    if node == '4':
        color map.append('#ecee0a')
    if node == '5a':
        color map.append('#5af20d')
    if node == '5b':
        color_map.append('#0df23f')
    if node == '6':
        color_map.append('#0df279')
    if node == '7':
        color_map.append('#0df2b3')
    if node == '8':
        color_map.append('#0df2ec')
    if node == '9':
        color map.append('#0d79f2')
    if node == 'C1':
```

```
color_map.append('#5e6fee')
if node == 'R1':
```

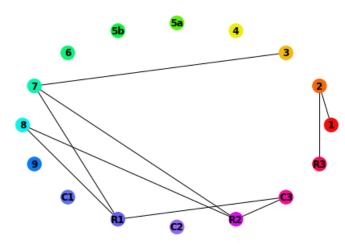
```
color_map.append('#635eee')
if node == 'C2':
```

- color\_map.append('#906aee')
  if node == 'R2':
- color\_map.append('#d90df2')
  if node == 'C3':
- color\_map.append('#f20d98')
  if node == 'R3':
  - color\_map.append('#f20d52')

# import matplotlib.pyplot as plt

nx.draw\_circular(G,node\_color = color\_map,with\_labels = True, font\_weight='bold')
plt.show()

EC = nx.eigenvector\_centrality(G)
print(EC)

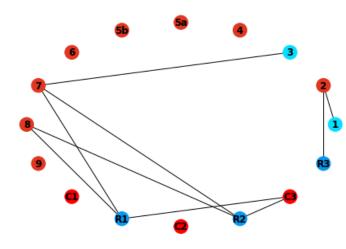


{'1': 9.046110461023596e-06, '2': 1.27931321007047e-05, '3': 0.18000813939677104, '4': 2.030074636709603e-16, '5a': 2.030074636709603e-16, '5b': 2.030074636709603e-16, '6': 2.030074636709603e-16, '7': 0.45440134941833504, '8': 0.38309229533177, '9': 2.030074636709603e-16 , 'C1': 2.030074636709603e-16, 'R1': 0.483527181027733, 'C2': 2.030074636709603e-16, 'R2': 0.483527181027733, 'C3': 0.38309229533177, 'R3': 9.046110461023596e-06}

```
In [498]:
```

<pre>import networkx as nx #creates graph G = nx.Graph()</pre>
G.add_node('1') G.add_node('2')
G.add_node('3') G.add_node('4') G.add_node('5a')
G.add_node('5b') G.add_node('6') G.add_node('7')
G.add_node('8') G.add_node('9') G.add_node('C1')
G.add_node('R1') G.add_node('C2')
G.add_node('R2') G.add_node('C3') G.add_node('R3')
<pre>G.add_edge('1', '2', weight=465.2252+521.58) #creates edges and edge weights G.add_edge('2', 'R3', weight=.16726) G.add_edge('3', '7', weight=43.1) G.add_edge('7', 'R1', weight=74.654)</pre>
G.add_edge('7', 'R2', weight=66.504) G.add_edge('8', 'R1', weight=10.4753) G.add_edge('8', 'R2', weight=2.4) G.add edge('R1', 'C3', weight=26.1)

```
G.add_edge('R2', 'C3', weight=201.37)
color map = [] #colors the nodes
for node in G:
   if node == '1':
        color_map.append('#05dfff')
    if node == '2':
        color map.append('#e13622')
    if node == '3':
       color_map.append('#05dfff')
    if node == '4':
       color_map.append('#e13622')
    if node == '5a':
       color_map.append('#e13622')
    if node == '5b':
       color map.append('#e13622')
    if node == '6':
        color_map.append('#e13622')
    if node == '7':
        color map.append('#e13622')
    if node == '8':
       color map.append('#e13622')
    if node == '9':
       color map.append('#e13622')
    if node == 'C1':
       color_map.append('#fd0000')
    if node == 'R1':
       color_map.append('#0998f0')
    if node == 'C2':
        color map.append('#fd0000')
    if node == 'R2':
       color_map.append('#0998f0')
    if node == 'C3':
       color_map.append('#fd0000')
    if node == 'R3':
        color map.append('#0998f0')
nx.draw circular(G,node color = color map,with labels = True, font weight='bold') #draws our graph
plt.show()
EC = nx.eigenvector_centrality(G) #prints unweighted centralities
print(EC)
print()
ECW = nx.eigenvector centrality(G, max iter=100, tol=1e-04, weight = 'weight') #prints weighted cen
tralities
print(ECW)
```



{'1': 9.046110461023596e-06, '2': 1.27931321007047e-05, '3': 0.18000813939677104, '4': 2.030074636709603e-16, '5a': 2.030074636709603e-16, '5b': 2.030074636709603e-16, '6': 2.030074636709603e-16, '7': 0.45440134941833504, '8': 0.38309229533177, '9': 2.030074636709603e-16 , 'C1': 2.030074636709603e-16, 'R1': 0.483527181027733, 'C2': 2.030074636709603e-16, 'R2': 0.483527181027733, 'C3': 0.38309229533177, 'R3': 9.046110461023596e-06}

{'1': 0.7071659513667207, '2': 0.707047578120793, '3': 8.609888467230922e-06, '4': 7.610624739699129e-19. '5a': 7.610624739699129e-19. '5b': 7.610624739699129e-19. '6':

```
7.610624739699129e-19, '7': 4.4838164426463e-05, '8': 2.554859928484192e-06, '9':
7.610624739699129e-19, 'C1': 7.610624739699129e-19, 'R1': 2.7112364662527182e-05, 'C2':
7.610624739699129e-19, 'R2': 0.00010650607344006016, 'C3': 0.00010471126102060963, 'R3': 0.00011986
213391011565}
```

#### In [362]:

4

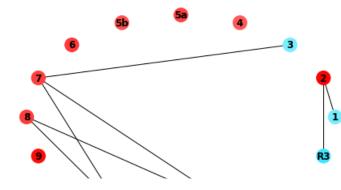
print(['%s %0.4f'%(node,EC[node]) for node in EC]) #Prints centrality and weighted centrality to 4
decimal places
print()
print(['%s %0.4f'%(node,ECW[node]) for node in ECW])

['1 0.0000', '2 0.0000', '3 0.1800', '4 0.0000', '5a 0.0000', '5b 0.0000', '6 0.0000', '7 0.4544',
'8 0.3831', '9 0.0000', 'C1 0.0000', 'R1 0.4835', 'C2 0.0000', 'R2 0.4835', 'C3 0.3831', 'R3 0.000
0']
['1 0.7072', '2 0.7070', '3 0.0000', '4 0.0000', '5a 0.0000', '5b 0.0000', '6 0.0000', '7 0.0000',
'8 0.0000', '9 0.0000', 'C1 0.0000', 'R1 0.0000', 'C2 0.0000', 'R2 0.0001', 'C3 0.0001', 'R3 0.000
1']

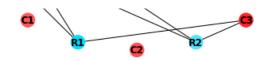
#### In [257]:

```
color map = [] #not used!
for node in G:
   if node == '1':
       color map.append('#75edff')
   if node == '2':
       color_map.append('#ff0000')
   if node == '3':
       color_map.append('#79eeff')
   if node == '4':
       color_map.append('#ff5858')
   if node == '5a':
       color map.append('#ff4040')
   if node == '5b':
       color_map.append('#ff4e4e')
   if node == '6':
       color_map.append('#ff3939')
   if node == '7':
       color map.append('#ff3e3e')
   if node == '8':
       color_map.append('#ff3c3c')
   if node == '9':
       color_map.append('#ff0a0a')
   if node == 'C1':
       color map.append('#ff5555')
   if node == 'R1':
       color map.append('#00dfff')
   if node == 'C2':
       color_map.append('#ff4d4d')
   if node == 'R2':
       color_map.append('#4fe6ff')
   if node == 'C3':
       color map.append('#ff2121')
   if node == 'R3':
       color map.append('#3ee5ff')
nx.draw circular(G,node color = color map,with labels = True, font weight='bold')
```

```
plt.show()
```



xvii. Pinch Calculations for Steam Raising Code



# In [499]:

```
#STEAM RAISING NETWORK
#Very similar to earlier code, but not with 2 more streams and a
#"reboiler" which is our vaporization stream
CP = [2.439565742, 2.441707317, 1.231428571, 0.5225806452, 0.6550724638, 0.06, 1.150300601,
      3.25872093, 0.1176995096, 0.1272727273, 0, 0, 0, 0, 0, 0, 4.184*1.064965, 1.996*1.064965,
      ((4.184+1.996)/2)*1.064965] #input CP values (0 for columns)
Ts = [35.5, 450, 40, 35.5, 104.5, 70, 129.9, 183.2, 249.3, 80, 35.5, 129.9, 104.5, 150.3,
      183.2, 249.3, 25, 100, 100] #input temperatures at inlets
Tt = [450, 40, 75, 20, 70, 35, 80, 80, 25, 25, 35.5, 129.9, 104.5, 150.3, 183.2, 249.3,
      100, 120, 100] #input temperatures at outlets
Qcol = [0,0,0,0,0,0,0,0,0,0,0, 35.7, -95, 186.8, -286.5, 2552.7, -2832, 0, 0, -2257*1.064965]
                    #input 0 if not a column, -Qreb for reboiler, or Qcond for condenser
Tmin = 10 #input Tmin
o = list(range(len(CP))) #list of length of the number of streams
Tss = list(range(len(Ts))) #list that will become shifted inlet temperatures
Tts = list(range(len(Tt))) #list that will become shifted outlet temperatures
coldnum = [] #list used to identify cold streams
hotnum = [] #list used to identify hot streams
disnumC = [] #list used to identify condensers
disnumR = [] #list used to identify reboilers
columntempsC = [] #used to identify where the condenders fit into the heat cascade
columntempsR = [] #used to identify where the reboilers fit into the heat cascade
for i in o: #function creating modified temps and identifying hot vs cold streams
    if Ts[i] > Tt[i]:
        Tss[i] = Ts[i] - (Tmin*.5)
        Tts[i] = Tt[i] - (Tmin*.5)
        hotnum.append(i)
    if Ts[i] < Tt[i]:</pre>
        Tss[i] = Ts[i] + (Tmin*.5)
        Tts[i] = Tt[i] + (Tmin*.5)
        coldnum.append(i)
    if Ts[i] == Tt[i]: #identifies columns/shifts temps
        if Ocol[i] > 0:
            Tss[i] = Ts[i] - (Tmin*.5)
            Tts[i] = Tt[i] - (Tmin*.5)
            disnumC.append(i)
            columntempsC.append([Tts[i], Qcol[i]])
        if Qcol[i] < 0:</pre>
            Tss[i] = Ts[i] + (Tmin*.5)
            Tts[i] = Tt[i] + (Tmin*.5)
            disnumR.append(i)
            columntempsR.append([Tts[i], Qcol[i]])
```

```
In [500]:
```

```
Tall = [] #list of all shifted temperatures
for i in o:
    Tall.append(Tss[i])
    Tall.append(Tts[i])

Tstar = list(set(Tall)) #list of all temperatures, without repeats, in descending order
Tstar.sort(reverse=True) #***HEAT CASCADE TEMPS***
print(Tstar)
print()

CPtot = [] #will be list of net CPs for each temp interval
lenT = list(range(len(Tstar) - 1)) #list for iterating through temperature intervals
p=0
```

```
lentempc = list(range(len(coldnum))) #iterates over cold streams
lentemph = list(range(len(hotnum))) #iterates over hot streams
#function to calculate net CPs
for i in lenT: #iterate through temp intervals
    p=0
    for j in o: #iterate through streams
        for k in lentempc:
            if j == coldnum[k]: #if cold, increase temp in integer increments to see
                                #if it's in the selected temp range
                x = Tss[i]
                while Tts[j] >= x:
                    if -.005 +x <Tstar[i] -.1 < x +.005: #WILL FAIL IF TEMPS ARE NOT INTEGERS
                        p = p-CP[j]
                    x = x + .1
        for k in lentemph: #same for hot streams, but decreasing temp
            if j == hotnum[k]:
                x = Tss[j]
                while Tts[j] <= x:</pre>
                    if -.005 + x<Tstar[i] -.1 <x+.005:</pre>
                        p = p+CP[j]
                    x = x - .1
    CPtot.append(p)
print(CPtot)
[455.0, 445.0, 254.3, 244.3, 178.2, 155.3, 134.9, 125.0, 124.9, 105.0, 99.5, 80.0, 75.0, 65.0, 45.
0, 40.5, 35.0, 30.5, 30.0, 20.0, 15.0]
[-2.439565742, 0.002141575000000067, 0.002141575000000067, 0.11984108460000001, 3.3785620146, 3.
3785620146, 3.3785620146, 2.4031924756000005, 2.4031924756000005, 0.0730490556000003,
0.7281215194000001, -0.5033070516000002, -4.7850558553, -5.3801283191, -4.1486997481, -
1.7091340061000002, -4.1508413231, -3.6282606779, 0.7675528821, 0.5225806452]
In [501]:
H = [] #list of delta H values for intervals
Hval = list(range((len(Tstar) - 1))) #list to iterate through temperature intervals
for i in Hval:
    H.append((Tstar[i]-Tstar[i+1])*(CPtot[i])) #calculates delta H
print(H) #before column integration
count = 0
for i in range(len(Tstar)): #adds in column values
    for j in range(len(columntempsR)):
        if Tstar[i] == columntempsR[j][0]:
            H.insert(count + i, columntempsR[j][1])
            count = count+1
    for j in range(len(columntempsC)):
        if Tstar[i] == columntempsC[j][0]:
            H.insert(count + i, columntempsC[j][1])
            count = count+1
print()
print(H) #after column integration
[-24.39565742, 0.4083983525000012, 0.02141575000000067, 7.921495692060003, 77.36907013433992, 68.
92266509784002, 33.44776394454002, 0.24031924755998638, 47.82353026444002, 0.40176980580000166,
14.198369628300004, -2.516535258000001, -47.850558553000006, -107.60256638199999, -18.66914886645,
-9.40023703355, -18.678785953949998, -1.81413033895, 7.6755288209999994, 2.6129032260000002]
```

[-24.39565742, 0.4083983525000012, -2832, 0.02141575000000067, 7.921495692060003, 2552.7, 77.36907013433992, -286.5, 68.92266509784002, -95, 33.44776394454002, 0.24031924755998638, 47.82353026444002, -2403.626005, 0.40176980580000166, 186.8, 14.198369628300004, -2.516535258000001, -47.850558553000006, -107.60256638199999, -18.66914886645, -9.40023703355, -18. 678785953949998, 35.7, -1.81413033895, 7.6755288209999994, 2.6129032260000002]

In [502]:

Hlen = list(range(len(H))) #list of delta H values for intervals
Hsum = []
n = 0
form i in Uler:

```
For i in Hien:
    n = n+H[i]
    Hsum.append(n)
Qh = -min(Hsum) #Qh is -largest negative number when adding through H
print(Qh)
Hnewsum = list(range(len(Hsum))) #***HEAT CASCADE Hs***
for i in Hlen:
    Hnewsum[i] = Hsum[i] + Oh
```

```
Hnewsum[i] = Hsum[i] + Qh
print()
print(Hnewsum)
```

2855.9872590675

```
[2831.5916016475, 2832.0, 0.0, 0.0214157499999601, 7.942911442059994, 2560.64291144206,
2638.0119815763996, 2351.5119815763996, 2420.43464667424, 2325.43464667424, 2358.88241061878,
2359.12272986634, 2406.9462601307796, 3.3202551307795147, 3.7220249365796008, 190.52202493657978,
204.72039456487983, 202.20385930687962, 154.35330075387947, 46.75073437187939, 28.081585505429302,
18.68134847187912, 0.0025625179291637323, 35.70256251792898, 33.8884321789792, 41.56396099997937,
44.17686422597944]
```

In [503]:

```
Qc = sum(H)+Qh #Qc is ending value of cacade after adding Qc
print(Qc)
pinch = 0
count = 0
recheckR = len(columntempsR)*[0]
recheckC = len(columntempsC)*[0]
O = Oh
for i in Hlen: #finds pinch by checking for zero value in cascade
    Q = Q + H[i]
    if -.01 < Q < .01:
       pinch = Tstar[i+1-count]
        print(pinch)
    for j in range(len(columntempsR)):
        if Tstar[i+1-count] == columntempsR[j][0]:
            if recheckR[j] == 0:
                count = count + 1
                recheckR[j] = 1
            else:
                recheckR[j] = 0
    for j in range(len(columntempsC)):
        if Tstar[i+1-count] == columntempsC[j][0]:
            if recheckC[j] == 0:
                count = count + 1
                recheckC[j] = 1
            else:
                recheckC[j] = 0
```

#note that two pinches are printed. In the readout of the code above this, heat cascade values are
displayed,
#and the point at which the cascade is at ~3.32 kW is also a pinch, even if it is not reflected ex
actly through
#the code.

44.17686422597944 254.3 45.0

In [507]:

import networkx as nx #same graph procedure as above but for the steam raising network
G = nx.Graph()
G.add\_node('1', node\_color= '#f20d0d')
G.add\_node('2', node\_color= '#f2690d')
G.add\_node('3', node\_color= '#f2ba0d')
G.add\_node('4', node\_color= '#d9f20d')
G.add\_node('4', node\_color= '#d9f20d')

xviii. Eigenvector Centrality for Steam Raising Network Code

```
For i in Hien:
    n = n+H[i]
    Hsum.append(n)
Qh = -min(Hsum) #Qh is -largest negative number when adding through H
print(Qh)
Hnewsum = list(range(len(Hsum))) #***HEAT CASCADE Hs***
for i in Hlen:
    Hnewsum[i] = Hsum[i] + Oh
```

```
Hnewsum[i] = Hsum[i] + Qh
print()
print(Hnewsum)
```

2855.9872590675

```
[2831.5916016475, 2832.0, 0.0, 0.0214157499999601, 7.942911442059994, 2560.64291144206,
2638.0119815763996, 2351.5119815763996, 2420.43464667424, 2325.43464667424, 2358.88241061878,
2359.12272986634, 2406.9462601307796, 3.3202551307795147, 3.7220249365796008, 190.52202493657978,
204.72039456487983, 202.20385930687962, 154.35330075387947, 46.75073437187939, 28.081585505429302,
18.68134847187912, 0.0025625179291637323, 35.70256251792898, 33.8884321789792, 41.56396099997937,
44.17686422597944]
```

In [503]:

```
Qc = sum(H)+Qh #Qc is ending value of cacade after adding Qc
print(Qc)
pinch = 0
count = 0
recheckR = len(columntempsR)*[0]
recheckC = len(columntempsC)*[0]
O = Oh
for i in Hlen: #finds pinch by checking for zero value in cascade
    Q = Q + H[i]
    if -.01 < Q < .01:
       pinch = Tstar[i+1-count]
        print(pinch)
    for j in range(len(columntempsR)):
        if Tstar[i+1-count] == columntempsR[j][0]:
            if recheckR[j] == 0:
                count = count + 1
                recheckR[j] = 1
            else:
                recheckR[j] = 0
    for j in range(len(columntempsC)):
        if Tstar[i+1-count] == columntempsC[j][0]:
            if recheckC[j] == 0:
                count = count + 1
                recheckC[j] = 1
            else:
                recheckC[j] = 0
```

#note that two pinches are printed. In the readout of the code above this, heat cascade values are
displayed,
#and the point at which the cascade is at ~3.32 kW is also a pinch, even if it is not reflected ex
actly through
#the code.

44.17686422597944 254.3 45.0

In [507]:

import networkx as nx #same graph procedure as above but for the steam raising network
G = nx.Graph()
G.add\_node('1', node\_color= '#f20d0d')
G.add\_node('2', node\_color= '#f2690d')
G.add\_node('3', node\_color= '#f2ba0d')
G.add\_node('4', node\_color= '#d9f20d')
G.add\_node('4', node\_color= '#d9f20d')

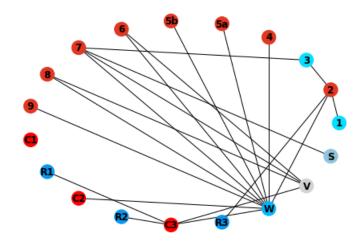
```
G.add node('ba', node color= '#bat20d')
G.add_node('5b', node_color= '#0df23f')
G.add node('6', node color= '#0df279')
G.add node('7', node color= '#0df2b3')
G.add_node('8', node_color= '#0df2ec')
G.add_node('9', node_color= '#0d79f2')
G.add_node('C1', node_color= '#0d28f2')
G.add_node('R1', node_color= '#2c0df2')
G.add_node('C2', node_color= '#710df2')
G.add_node('R2', node_color= '#d90df2')
G.add node('C3', node color= '#f20d98')
G.add_node('R3', node_color= '#f20d52')
G.add_node('W', node_color= '#f20d52')
G.add_node('V', node_color= '#f20d52')
G.add node('S', node color= '#f20d52')
G.add_edge('1', '2', weight = 465.2252 + 10.978 + 510.6)
G.add_edge('2', 'R3', weight = .16726)
G.add_edge('W', '4', weight = .2763)
G.add_edge('W', '8', weight = 1.7582 + 7.062)
G.add_edge('W', '5b', weight = .847 + 1.2)
G.add_edge('W', '9', weight = 1.9012 + 3.8182)
G.add_edge('W', '2', weight = 13.439)
G.add edge('W', 'C2', weight = 48.5793 + 118.54)
G.add_edge('2', '3', weight = .448)
G.add_edge('3', '7', weight = 42.65177)
G.add_edge('S', '7', weight = 42.51344)
G.add_edge('W', '7', weight = 55.11)
G.add_edge('W', '5a', weight = 22.6)
G.add edge('W', '6',
                    weight = 34.509)
G.add edge('V', '6', weight = 22.891)
G.add_edge('V', '7', weight = 196.0251)
G.add edge('V', '8', weight = 16.3955)
G.add\_edge('C3', 'R1', weight = 95)
G.add edge('W', 'C3', weight = 2.883)
color map = []
for node in G:
   if node == '1':
       color_map.append('#05dfff')
    if node == '2':
       color_map.append('#e13622')
    if node == '3':
        color map.append('#05dfff')
    if node == '4':
       color map.append('#e13622')
    if node == '5a':
       color_map.append('#e13622')
    if node == '5b':
       color_map.append('#e13622')
    if node == '6':
       color_map.append('#e13622')
    if node == '7':
        color map.append('#e13622')
    if node == '8':
       color_map.append('#e13622')
    if node == '9':
       color_map.append('#e13622')
    if node == 'C1':
       color_map.append('#fd0000')
    if node == 'R1':
       color_map.append('#0998f0')
    if node == 'C2':
       color_map.append('#fd0000')
    if node == 'R2':
        color_map.append('#0998f0')
    if node == 'C3':
       color map.append('#fd0000')
    if node == 'R3':
       color_map.append('#0998f0')
    if node == 'W':
       color map.append('#00b8ff')
    if node == 'S':
```

```
color_map.append('#90c4d8')
if node == 'V':
    color map.append('#d2d2d2')
```

#### import matplotlib.pyplot as plt

```
nx.draw_circular(G,node_color = color_map,with_labels = True, font_weight='bold')
plt.show()
```

```
EC = nx.eigenvector_centrality(G)
print(EC)
print()
ECW = nx.eigenvector_centrality(G, max_iter=100, tol=1e-02, weight = 'weight')
print(ECW)
```



{'1': 0.06698449238761839, '2': 0.24325102068509669, '3': 0.15333991736577712, '4': 0.1641343596669508, '5a': 0.1641343596669508, '5b': 0.1641343596669508, '6': 0.24759309681177238, '7': 0.3135979384319429, '8': 0.24759309681177238, '9': 0.1641343596669508, 'C1': 2.909283080721106e-15, 'R1': 0.08036737752710574, 'C2': 0.1641343596669508, 'R2': 0.08036737752710574, 'C3': 0.2918539561092076, 'R3': 0.06698449238761839, 'W': 0.5960543690891199, 'V': 0.30308174340111277, 'S': 0.08635542497816165}

```
{'1': 0.025685992371378627, '2': 0.025436759991558335, '3': 0.0012645215193602972, '4':
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0.0071313984601447805, '7': 0.06068672449786642, '8': 0.005079345968489468, '9':
1.0240451106845926e-05, 'C1': 2.6574779989223003e-14, 'R1': 0.0313112901962263, 'C2':
0.00029922317312500434, 'R2': 0.09442825938119732, 'C3': 0.6825299132706437, 'R3':
4.353693938423002e-06, 'W': 0.0031145665844965016, 'V': 0.7205390620858562, 'S':
0.0012487969752413418}
```

# In [506]:

print(['%s %0.4f'%(node,EC[node]) for node in EC])
print()
print(['%s %0.4f'%(node,ECW[node]) for node in ECW])

['1 0.0670', '2 0.2433', '3 0.1533', '4 0.1641', '5a 0.1641', '5b 0.1641', '6 0.2476', '7 0.3136', '8 0.2476', '9 0.1641', 'C1 0.0000', 'R1 0.0804', 'C2 0.1641', 'R2 0.0804', 'C3 0.2919', 'R3 0.067 0', 'W 0.5961', 'V 0.3031', 'S 0.0864']

['1 0.0257', '2 0.0254', '3 0.0013', '4 0.0000', '5a 0.0000', '5b 0.0000', '6 0.0071', '7 0.0607', '8 0.0051', '9 0.0000', 'C1 0.0000', 'R1 0.0313', 'C2 0.0003', 'R2 0.0944', 'C3 0.6825', 'R3 0.000 0', 'W 0.0031', 'V 0.7205', 'S 0.0012']