

Mixture optimization for mixed gas Joule-Thomson cycle

J Detlor, J Pfothner, and G Nellis

University of Wisconsin-Madison, Department of Mechanical Engineering
Madison, WI 53706, USA

Email: detlor@wisc.edu

Abstract. An appropriate gas mixture can provide lower temperatures and higher cooling power when used in a Joule-Thomson (JT) cycle than is possible with a pure fluid. However, selecting gas mixtures to meet specific cooling loads and cycle parameters is a challenging design problem. This study focuses on the development of a computational tool to optimize gas mixture compositions for specific operating parameters. This study expands on prior research by exploring higher heat rejection temperatures and lower pressure ratios. A mixture optimization model has been developed which determines an optimal three-component mixture based on the analysis of the maximum value of the minimum value of isothermal enthalpy change, Δh_T , that occurs over the temperature range. This allows optimal mixture compositions to be determined for a mixed gas JT system with load temperatures down to 110 K and supply temperatures above room temperature for pressure ratios as small as 3:1. The mixture optimization model has been paired with a separate evaluation of the percent of the heat exchanger that exists in a two-phase range in order to begin the process of selecting a mixture for experimental investigation.

1. Introduction

For a JT cycle, using a suitable mixed gas fluid can provide a more sizable isothermal enthalpy change, Δh_T , at lower temperatures and while operating at lower pressures and pressure ratios than is possible with a pure fluid [1,2]. The performance of the cycle per mass or mole of refrigerant is limited by the value of the minimum Δh_T that occurs over the temperature range. Therefore, one method of optimizing the mixture components and composition is to maximize the value of the minimum Δh_T for the cycle operating temperatures and pressures. By performing this optimization, the mixture with the greatest refrigeration effect for the cycle is determined. This approach ignores other performance metrics such as *COP*, heat exchanger conductance, suction flow rate, etc. that must subsequently be considered during final mixture selection.

2. Mixture optimization model

A Matlab program was developed to determine an optimal three-component mixture based on the analysis of the maximum value of the minimum Δh_T that occurs for each mixture given a list of fluids, load and supply temperatures, and suction and discharge pressures [3]. This is accomplished using three nested functions: the outer, intermediate, and inner functions.



2.1. Outer function

The outer function returns tables of optimal compositions and maximum values of the minimum Δh_T that occur for all of the three-component mixtures that are analyzed by applying the process described below:

1. Generates an array of all possible three-component mixture combinations from the list of fluids.
2. Selects the three-component mixture from the first row of the array.
3. Passes the three-component mixture to the intermediate function with fixed supply and load temperatures and suction and discharge pressures.
4. Stores optimal composition and the associated maximum value of the minimum Δh_T that occurs for the three-component mixture that is returned from the intermediate function in a table.
5. Repeats steps 2-4 for the next row of the array and so on until all the possible three-component mixtures have been analyzed.
6. Sorts the table of results in ascending order according to the maximum value of the minimum Δh_T and prints the results in the command window.
7. Repeats steps 2-6 for the next load temperature in the user-specified load temperature range until all load temperatures have been analyzed.

2.2. Intermediate function

The intermediate function uses nested loops to run through a range of possible molar compositions for the three-component mixture passed from the outer function. Two concentration parameters are passed to the inner function with the specified three-component mixture and fixed values of supply and load temperatures and suction and discharge pressures. The inner function is discussed subsequently; this function returns the mole fractions of each fluid component along with the value of the minimum Δh_T associated with the specified values of the two concentration parameters. The intermediate function assigns these values to a results array. After the nested loop has completed, the intermediate function searches the results array for the maximum value of the minimum Δh_T that is obtained over all compositions and returns this value along with the associated optimal mixture composition.

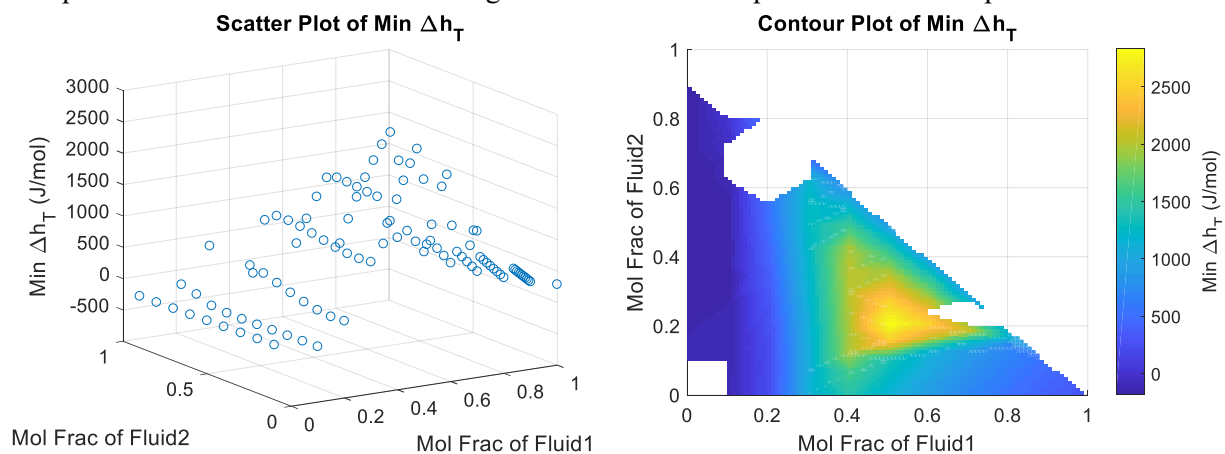


Figure 1. Visualization of the results of the intermediate function run for methane (fluid1), pentane (fluid2), and propane (fluid3) at a load temperature of 140K and with pressures of 22-363 psi.

The scatter plot on the left in figure 1 shows the minimum Δh_T obtained for each molar composition of a three-component mixture consisting of methane, pentane, and propane; examination of the plot shows the maximum value of the minimum Δh_T that can be obtained using this mixture. By interpolating these values to a contour plot that is shown on the right side of figure 1, the optimal mixture composition is evident. In this example, the intermediate function will return 2833 J/mol as the maximum value of the minimum Δh_T that occurs and an associated optimal mixture composition of 50% methane, 20%

pentane, and 30% propane on a molar basis; these results are associated with a load temperature of 140K and suction and discharge pressures of 22 and 363 psi, respectively.

Note that the gaps in the contour plot in figure 1 result from molar compositions that do not return a value of minimum Δh_T . For these mixtures, the property routine REFPROP does not return enthalpy data that spans the entire specified temperature range and thus a minimum Δh_T cannot be estimated [4].

2.3. Inner function

The inner function returns the minimum Δh_T that occurs for a specified composition of the three-component mixture analyzed by the process described below:

1. Converts concentration parameters passed from the intermediate function to mass fractions.
2. For a segmented temperature range larger than specified, calls REFPROP for raw enthalpy data and assigns all enthalpy and temperature data returned to temporary vectors.
3. Removes enthalpy values from temporary vectors that are determined to be outliers.
4. Removes enthalpy values from temporary vectors if they are not thermodynamically consistent (e.g., ones that decrease as temperature rises).
5. Generates enthalpy data for high and low pressure streams by linearly interpolating temporary vectors for specified temperature range and calculates the minimum Δh_T that occurs.

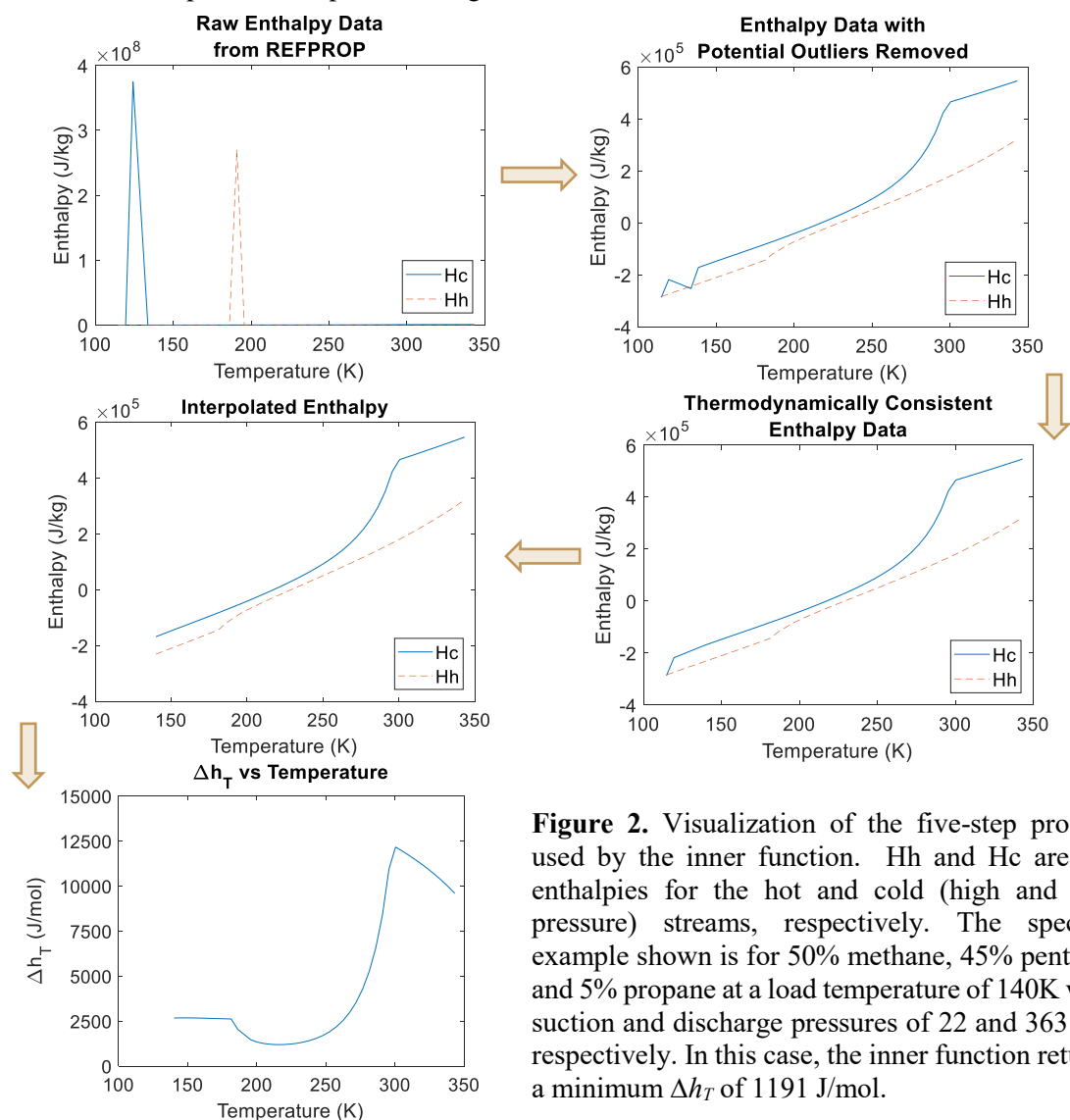


Figure 2. Visualization of the five-step process used by the inner function. Hh and Hc are the enthalpies for the hot and cold (high and low pressure) streams, respectively. The specific example shown is for 50% methane, 45% pentane, and 5% propane at a load temperature of 140K with suction and discharge pressures of 22 and 363 psi, respectively. In this case, the inner function returns a minimum Δh_T of 1191 J/mol.

In figure 2, the first plot displays the enthalpy data obtained from REFPROP corresponding to the high and low pressure streams for the specified composition of the three-component mixture. The dashed and solid lines represent the enthalpy data for the high and low pressure streams (the hot and cold streams), respectively. The large spikes seen in the plot are due to issues of convergence within the property routine REFPROP. These values of enthalpy, along with their corresponding temperatures, are considered to be outliers and removed from the temporary vectors storing the high and low pressure stream data. The enthalpy data obtained from REFPROP with the potential outliers removed is then displayed in the second plot.

In the second plot, there can be seen an enthalpy value that decreases as temperature rises for the low pressure stream. As this is not thermodynamically consistent, this value of enthalpy, along with its corresponding temperature, is considered to be an outlier and removed from the temporary vectors storing the low pressure stream data. The thermodynamically consistent enthalpy data is then displayed in the third plot.

Now that the enthalpy data obtained from REFPROP for the segmented temperature range has been checked for outliers and thermodynamic consistency, the inner function linearly interpolates the temperature and enthalpy vectors for the desired temperature range. The linearly interpolated data is shown in the fourth plot. Finally, the inner function calculates the Δh_T that occurs for the desired temperature range from the high and low pressure stream enthalpy vectors and displays the results in the fifth plot. In the fifth plot, the minimum Δh_T that occurs can be seen for the specified composition of the three-component mixture.

3. Mixture optimization results

The Matlab program described in Section 2 has been ran for both hydrocarbon and synthetic refrigerant mixtures (with argon). The fluids analyzed for the hydrocarbon mixture optimization included argon, butane, ethane, methane, nitrogen, pentane, and propane. The fluids analyzed for the synthetic refrigerant mixture optimization included argon, R14, R23, R32, R116, R134a, and R218.

The hydrocarbon and synthetic refrigerant mixture optimizations were performed for three sets of suction and discharge pressures: 100-300 psi, 100-400 psi, and 22-363 psi. All mixtures were analyzed for load temperatures ranging from 110-180K in increments of 10K while the supply temperature remained constant at 343.15K.

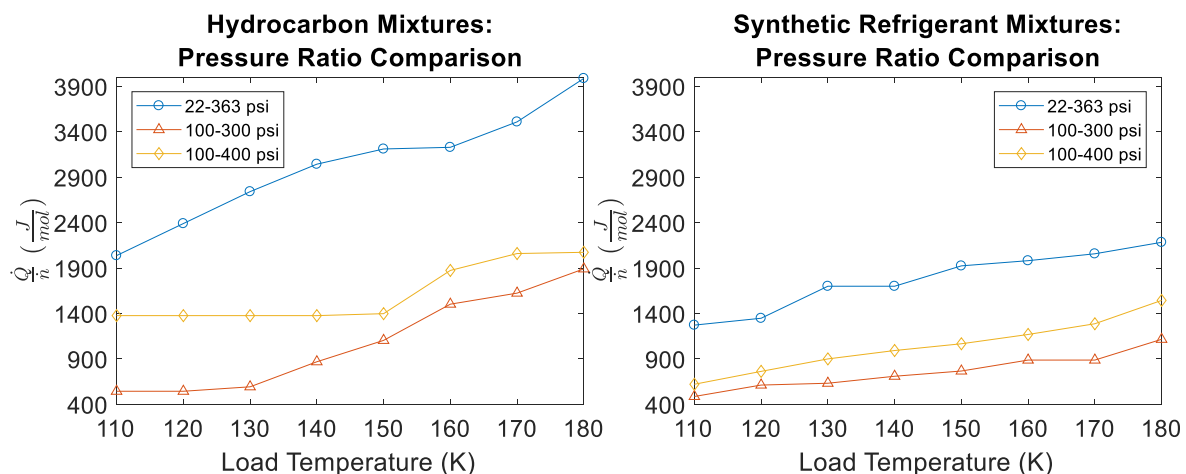


Figure 3. Refrigeration per molar flow, \dot{Q}/\dot{n} (J/mol), as a function of load temperature (K) for suction and discharge pressures of 100-300 psi, 100-400 psi, and 22-363 psi. Each marker represents the maximum value of the minimum \dot{Q}/\dot{n} that occurs for the optimal combination of three fluids and composition selected specifically for that load temperature.

As shown in figure 3, for both the hydrocarbon and synthetic refrigerant optimal composition mixtures, suction and discharge pressures of 22-363 psi produce the greatest values of \dot{Q}/\dot{n} while pressures of 100-300 psi produce the lowest values. There is also a notable increase in the value of \dot{Q}/\dot{n} for the hydrocarbon mixtures when compared to the synthetic refrigerant mixtures.

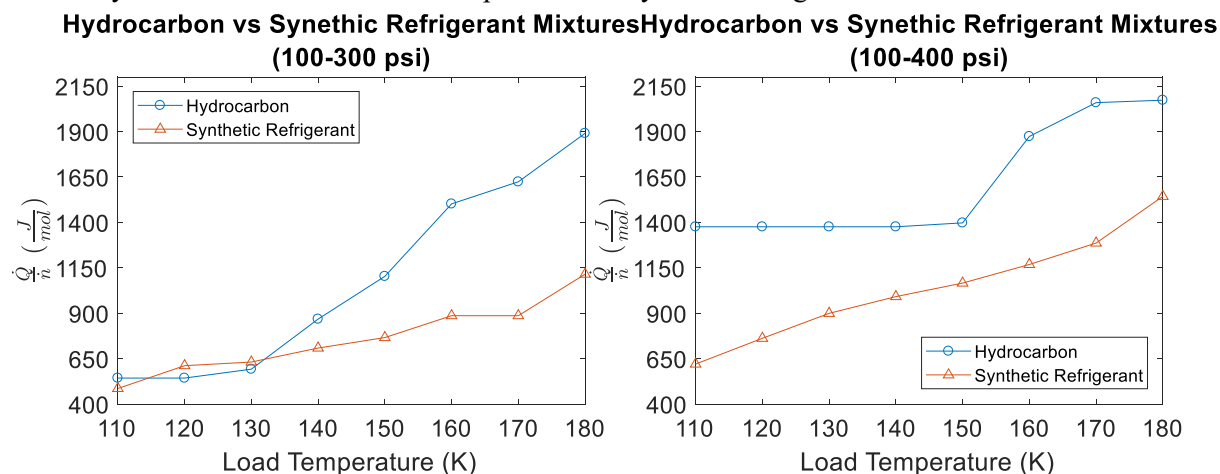


Figure 4. Refrigeration per molar flow, \dot{Q}/\dot{n} (J/mol), as a function of load temperature (K) for pressures of 100-300 psi (left) and 100-400 psi (right). Each marker represents the maximum value of the minimum \dot{Q}/\dot{n} that occurs for the optimal mixture composition at each load temperature.

The plot on the left in figure 4 displays that for low load temperatures of 110-130K and pressures of 100-300 psi, the optimal mixtures made of synthetic refrigerants perform similarly to the optimal mixtures for hydrocarbons. However, as the load temperature increases, the hydrocarbon mixtures begin to outperform the synthetic refrigerant mixtures. The plot on the right in figure 4 shows that the hydrocarbon mixtures outperform the synthetic refrigerant mixtures for the entire load temperature range of interest when the suction and discharge pressures are 100-400 psi. A similar trend was observed for pressures of 22-363 psi.

The plots in figures 3 and 4 displayed the thermodynamic performance of the optimal mixture appropriate at each load temperature. In order to generate these plots, a new optimization was run for each load temperature resulting in a new optimal mixture and \dot{Q}/\dot{n} associated with each plotted point. In addition to being displayed in figures 3 and 4, the results for pressures of 100-300 psi are highlighted in figure 5 as the dashed line. The plots in figure 5 are different from those in figures 3 and 4 in that they show how an optimal mixture selected for a particular load temperature will perform across the entire load temperature range. Figure 5 demonstrates that some optimal mixtures produce positive values of \dot{Q}/\dot{n} over a large load temperature range while the performance of other mixtures quickly drops when they are operated below the temperature that they were optimized for. The hydrocarbon optimal mixtures have a greater tendency to plummet in performance than the synthetic refrigerant optimal mixtures. Similar trends were observed for pressures of 100-400 psi.

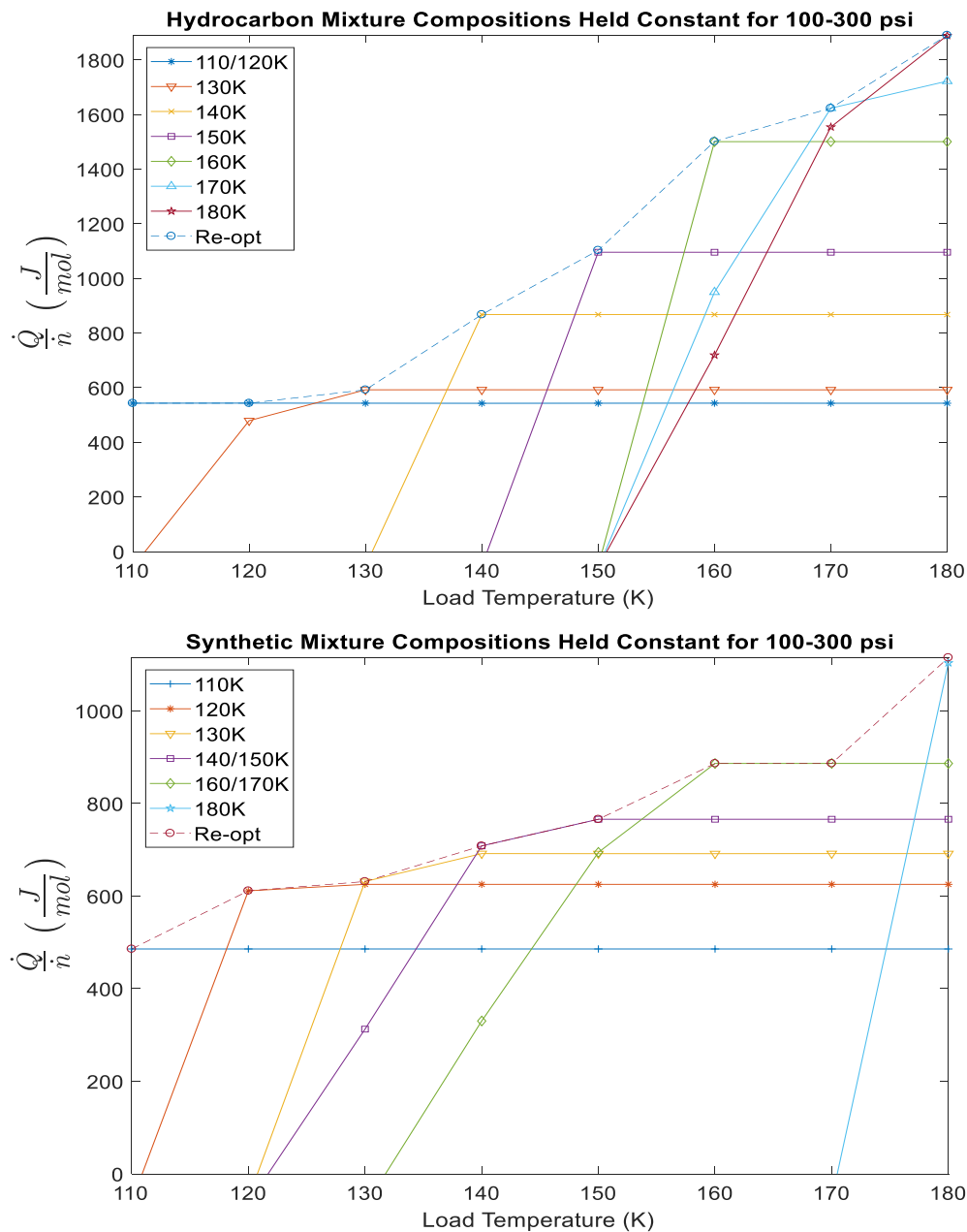


Figure 5. Refrigeration per molar flow rate, \dot{Q}/\dot{n} (J/mol), as a function of the load temperature (K) for optimal mixtures with the composition held constant over the entire load temperature range. The optimal hydrocarbon and synthetic refrigerant mixtures are displayed on the top and bottom figures, respectively. Both figures are for pressures of 100-300 psi. For lines labeled with two load temperatures, the composition of the optimal mixture was the same for both load temperatures. The dashed line displays the thermodynamic performance when a new optimization is run at each load temperature, resulting in a new optimal mixture and \dot{Q}/\dot{n} for each plotted point.

4. Percent Two-Phase

The percent of the temperature range of the recuperator where the mixture is in the two-phase region is one metric that can be used to further distinguish between candidate mixtures. The heat transfer coefficient associated with a two-phase state is much larger than a single phase state, as reported by Barraza et al. [5]. Therefore, given the same thermodynamic performance, represented by Δh_T , a mixture that is two phase over a larger fraction of the temperature range will be practically superior as a smaller recuperator can be employed. The percent of the recuperator in a two-phase state was calculated using the bubble and dew points for the optimal mixtures and comparing them to the load and supply temperatures.

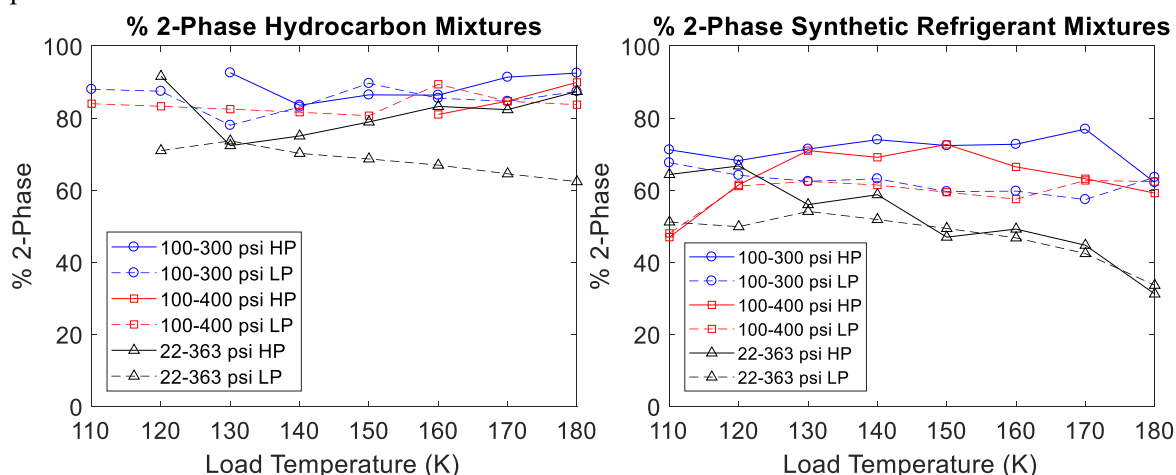


Figure 6. Plot of the percent of the temperature range that is two-phase as a function of the load temperature (K) for the optimal hydrocarbon (left) and synthetic refrigerant (right) mixtures with pressures of 100-300 psi, 100-400 psi, and 22-363 psi. The percent two-phase for the high and low pressure streams (HP and LP) are shown as solid and dashed lines, respectively.

It follows from figure 6 that the optimal hydrocarbon mixtures are in the two-phase region for a greater percentage of the temperature range than the optimal synthetic refrigerant mixtures. For the three sets of suction and discharge pressures compared, the JT cycle with pressures of 100-300 psi has the greatest percentage of the temperature range in the two-phase region for both hydrocarbon and synthetic mixtures.

For the hydrocarbon mixtures, data for the bubble and dew points was not always returned from REFPROP, especially at load temperatures below 130K. For these mixtures and load temperatures, the percent two-phase was unable to be calculated and has been left blank in the plot on the left of figure 6.

5. Maximum Temperature Gap

In step 2 of the five-step process described previously for the inner function, the mixture optimization model calls REFPROP in order to obtain enthalpy data and assigns all enthalpy data returned from REFPROP to temporary vectors before outliers are removed and interpolation is used to analyze the mixture. However, enthalpy data is not always available from REFPROP for the desired temperature range and mixture.

Figure 7 shows that the optimal hydrocarbon mixtures below about 130K in particular might have large gaps in the temperature range where enthalpy data is not available. The optimal synthetic refrigerant mixtures consistently have a minimum temperature gap that is consistent with the temperature segmentation used to call REFPROP indicating that enthalpy data is consistently returned from REFPROP for the synthetic refrigerant mixtures.

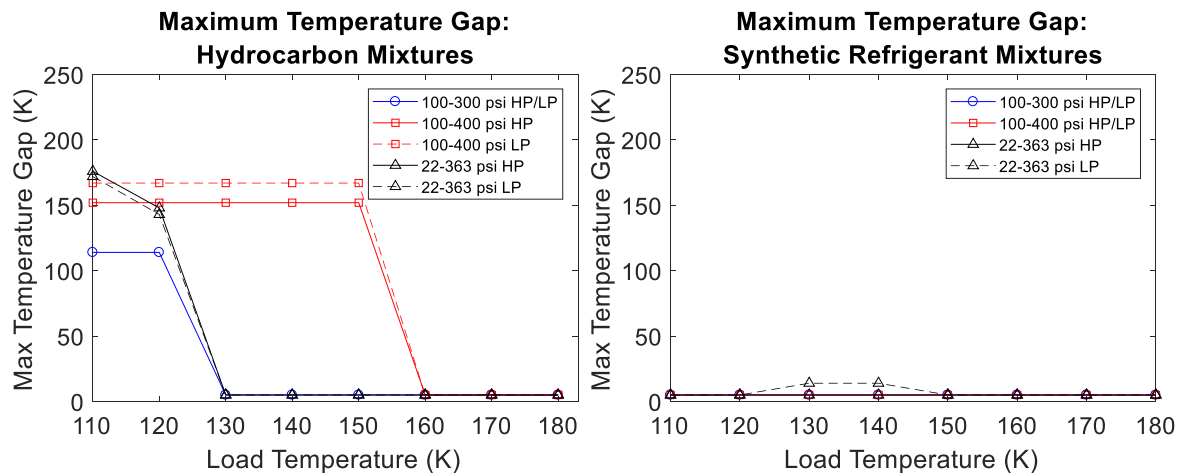


Figure 7. Plot of load temperature (K) vs. maximum temperature gap (K) for optimal hydrocarbon (left) and synthetic refrigerant mixtures (right) with pressures of 100-300 psi, 100-400 psi, and 22-363 psi. The maximum temperature gap is the largest range of temperature where enthalpy data is not available from REFPROP for the desired mixture. The maximum temperature gap for the high and low pressure streams (HP and LP) are shown as solid and dashed lines, respectively.

6. Conclusions

This paper describes initial work in a project that will identify attractive candidate mixtures for mixed gas Joule-Thomson applications. From analysis of the maximum value of the minimum Δh_T and the percent of the temperature range that is two-phase, the optimal hydrocarbon mixtures appear to provide the greatest refrigeration effect for the specified JT cycle parameters. However, for load temperatures below 130K the large gaps in temperature where REFPROP is unable to return enthalpy data increases uncertainty that the maximum values of the minimum Δh_T are accurate suggesting that other mixtures should be considered.

The optimal synthetic refrigerant mixtures appear to provide lower refrigeration effect for the specified JT cycle parameters due to lower maximum values of the minimum Δh_T and also a smaller percent of the temperature range in the two-phase regime. However, the consistency in enthalpy data returned from REFPROP allows for greater confidence in the accuracy of the results.

References

- [1] Hinze J Thermodynamic optimization of mixed refrigerant Joule-Thomson cycle with heat transfer considerations (Madison: Univ. of Wisc. Madison) MS [thesis] Available from: UW Madison Library System
- [2] Hinze J F, Klein S A, and Nellis G 2015 Thermodynamic optimization of mixed refrigerant Joule-Thomson systems constrained by heat transfer considerations *IOP Conf. Ser.: Mater. Sci. Eng.* **101** 012133
- [3] MATLAB release R2017a, The MathWorks, Inc., Natick, Massachusetts, United States.
- [4] Lemmon E W, Huber M L, McLinden M O. NIST Standard Reference Database 23: Reference Fluid Thermodynamic and Transport Properties-REFPROP, Version 9.1, National Institute of Standards and Technology, Standard Reference Data Program, Gaithersburg, 2013.
- [5] Barraza R 2015 Thermal-fluid behavior of mixed refrigerants for cryogenic applications (Madison: Univ. of Wisc. Madison) PhD [dissertation] Available from: UW Madison Library System