Formulating the optimization problem when using sequential quadratic programming applied to a simple LNG process

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Abstract

Sequential quadratic programming (SQP) may be very efficient compared with other techniques for the optimization of simple processes for the liquefaction of natural gas (LNG), and can be combined with process evaluation using commercial flowsheet simulators. However, the level of success is dependent on the formulation of the problem. In this work, effects of varying different aspects of the optimization problem formulation is investigated, such as variable selection, formulae for the estimation of derivatives, initial values, variable bounds, and formulation of constraints. Especially the formulation of the constraint for the temperature difference between the hot and cold composite curve is essential. The commonly used minimum temperature difference constraint should generally not be employed in gradient based optimization. Recommendations regarding optimization of simple LNG processes using SQP and flowsheet simulators are provided.

Keywords

LNG
PRICO
Optimization
Sequential quadratic programming
Formulation of constraints

1 INTRODUCTION

Natural gas plays an increasingly important role in the global energy system, and over long distances the most efficient way of transporting this energy carrier is by liquefaction. Hence, during the last decade, the transport and use of liquefied natural gas (LNG) has increased tremendously, driven by large global price differences of natural gas. This trend is expected to accelerate ahead, due for instance to increased focus on carbon footprint of the different energy solutions and opening for shale gas export from the US. Hence, according to the IEA 450 (2°C) scenario, the use of natural gas will increase significantly in the decades ahead, and a large number of LNG carriers are under order (IEA, 2013).

Although LNG is an environment-friendly energy source, the liquefaction process is still costly in terms of investment costs and energy consumption. Hence, improving the effectivity of LNG processes is of great importance and interest, and have been the focus of a number of studies referred to in Lim et al. (2012) and Austbø et al. (2014). However, finding the best operation point of even relatively simple LNG processes in an efficient and rigorous manner remains difficult, due the typically non-linear and non-convex nature of the optimization problem and its high number of variables. To this end, it was shown in an earlier work that optimization of simple

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LNG processes can be performed in a very efficient manner using a combination of a commercial flowsheet simulator and an SQP-routine (Wahl et al., 2013). Later, a study have been performed where a relatively large number of optimization routines have been applied to and compared for the same problem, again with the objective function calculated using a flowsheet simulator.

However, the level of success for any LNG process optimization approach is dependent on careful problem formulation, in particular when using SQP techniques. In this paper, a detailed study of the dependence between the optimization success rate and problem formulation will be presented, pursuing the SQP/flowsheet simulator approach. In order for such an investigation to be reasonable conclusive, the complexity of the problem must be at a manageable level. Hence, the focus has been on the PRICO LNG process, which is a relatively simple natural gas liquefaction process currently used in multiple plants world-wide (Hoffart & Price, 2014). Referring to Austbø et al. (2014), the optimization of single cycle mixed refrigerant processes such as PRICO has previously been discussed in a number of works, and in a handful of these papers SQP techniques have been employed (Skaugen et al., 2010), (Morin et al., 2011), (Khan et al., 2012), (Skaugen et al., 2013), (Wahl et al., 2013). In our experience, the knowledge obtained in the study of relative simple processes like PRICO can also be applied for more complex processes.

As mentioned above, the purpose of the current work is to identify how the problem should be formulated in order to robustly find the optimum operation point of simple LNG processes, using an SQP optimization routine and a commercial flowsheet simulator. The investigation is performed by varying different elements of the formulation and evaluating and comparing the corresponding results. In Section 2, the PRICO process and optimization problem are presented. In Section 3, some further details about the optimization methodology and implementation are provided. Heat exchanger implementation and temperature difference constraint formulation are particularly important for PRICO process optimization and have been given particular attention. In Section 4, the optimization results for different variations of the problem formulation are presented. For each set of formulations, a number of optimization runs are performed with arbitrary initial values within given bounds, and the ratio of successful runs is recorded. A natural place to start is the selection of variables, before investigating formulation aspects such as estimation of derivatives, bounds, effect of non-feasible starting points and the penalty of violating the optimization constraints. The effect of varying these elements are all performed for different implementations of the composite curve heat exchanger and its temperature difference constraint. The results are further analyzed and summarized in the remaining chapters.

2 PROBLEM FORMULATION

2.1 The PRICO process

In this work, the PRICO™ process (Stebbing & O'Brien, 1975), (Price & Mortko, 1996) has been analyzed. The same process was investigated in Wahl et al. (2013) where a more detailed description of the optimization problem is found. An Aspen HYSYS® flowsheet of the PRICO process with one compressor and one heat exchanger is provided in Figure 1.

Natural gas (stream G1) enters the heat exchanger at ambient temperature and at a rather high pressure. The natural gas is condensed, liquefied, and subcooled in the heat exchanger (stream G2) before the pressure is reduced to atmospheric conditions (stream LNG). The mixed refrigerant enters (stream R1) and leaves (stream R2) the LNG heat exchanger at the same temperature as the natural gas. The pressure of stream R2 is reduced (stream R3), and stream R3 is used to reduce the temperature of the high pressure refrigerant and the natural gas. After being heated and vaporized in the LNG heat exchanger (stream R4), the refrigerant is then compressed (stream R5) and cooled (stream R1). The properties of the G1 and LNG streams are fixed for each case; only parameters for the mixed refrigerant are allowed to vary during the optimization.

For the runs provided here, natural gas feed temperature (stream G1) and the refrigerant after external cooling (stream R1) both enters at 25°C, while streams G2 and R2 both leaves at -155°C.

2.2 Heat exchanger calculations

The heat exchanger models used are based on composite curves. All hot streams to be cooled are merged into one pseudo-stream, the hot composite curve, while all cold streams to be heated are merged into the cold composite curve. In this case the hot streams are the natural gas and high pressure refrigerant and the only cold stream is the low pressure refrigerant. One challenge when using a composite curve model is that enthalpy may be transferred from the hot composite stream to the cold composite stream without considering the temperature difference. A positive temperature difference between the two streams is required to avoid that the hot composite stream attains a lower temperature than the cold composite stream at the same location.

2.3 Optimization problem

The objective of the optimization is to minimize the power consumption of the compressor. In all cases considered here, the following constraints have been specified and applied:

- A minimum superheating of the compressor inlet stream above its dew point temperature
- A minimum positive temperature difference between the hot and the cold composite curves in every location of the heat exchanger

The objective function to be optimized is expressed as:

$$\min W\left(\underline{x}, P_{R4,} P_{R5}\right)$$

subject to

$$\Delta T_n\left(\underline{x}, P_{R4,} P_{R5}\right) - \Delta T_h \geq 0; \text{ for all intervals n} \tag{1}$$

$$T_c\left(\underline{x}, P_{R4,} P_{R5}\right) - T_{dew}\left(\underline{x}, P_{R4,} P_{R5}\right) - \Delta T_c \geq 0 \tag{2}$$

$$P_{R4}^{LB} \leq P_{R4} \leq P_{R4}^{UB}$$

$$P_{R5}^{LB} \leq P_{R5} \leq P_{R5}^{UB}$$

$$x_i^{LB} \leq x_i \leq x_i^{UB}; \text{for all components } i$$

where

- W is the compressor power consumption
- ΔT_h is the minimum temperature difference allowed for the heat exchanger
- ΔT_n is the temperature difference in interval number n of the heat exchanger
- T_c is the calculated inlet temperature of the inlet stream (R4) to the compressor
- T_{dew} is the calculated dew point temperature of the inlet stream (R4) to the compressor

- ΔT_c is the specified minimum temperature difference between T_c and T_{dew}
- P_{R4} and P_{R5} are the pressures of stream R4 and R5, respectively
- x_i is variable i relating to the composition and flowrate of the refrigerant, the definition will vary between the formulations
- $\underline{x}$ is a vector of all x_i
- Superscripts LB and UB denote lower and upper bounds, respectively, of the specified variables.

(1) leads to one or more constraints depending on the formulation.

The optimization set-up is similar to the one described in Wahl et al. (2013), using the NLPQLP routine from Schittkowski (2006) for optimization and Aspen HYSYS® V8.2 for process simulation. Most of the basic results presented here are however expected to be relevant also when using other advanced SQP routines or flowsheet simulators.

3 OPTIMIZATION SPECIFICATIONS

3.1 Process flowsheets

Each individual stream in the heat exchanger is divided into a number of intervals, specified as uniformly spaced either in temperature or enthalpy. In this work, the number of intervals has been 10 or 100 for each stream, but 11 or 101 for the natural gas stream when equal temperature step has been used. Since, in our case, the natural gas and the high pressure refrigerant enters and leaves at the same temperature, an additional interval is added for the natural gas stream to avoid identical intervals for these streams. This gives 29 (30) or 299 (300) locations where the temperature difference is calculated in the heat exchanger. Hence, four different flowsheets will be investigated:

- 10 intervals per stream uniformly spaced in temperature
- 100 intervals per stream uniformly spaced in temperature
- 10 intervals per stream uniformly spaced in enthalpy
- 100 intervals per stream uniformly spaced in enthalpy

The pressure drops of the heat exchangers have been ignored in the results presented here. However, similar optimization runs have been performed where fixed pressure drops for each pass in the LNG heat exchanger have been included. These optimization runs generally provide little additional information to the runs without pressure drops and are omitted here.

3.2 Formulation of the temperature difference constraint

The temperature difference constraint within the LNG heat exchanger may be formulated in several ways. The options that have been tested in this work are listed below along with some comments regarding implementations in HYSYS:

- Using the minimum temperature difference (DTmin): This is a scalar that is returned from HYSYS heat exchanger calculations.
- Using all returned heat exchanger temperature differences as constraints (StrPts): The optimization routine requires a fixed number of constraints during each optimization run. Each stream within the heat exchanger is divided into a fixed number of intervals and it is

specified that no additional dew or boiling points are to be calculated. Since each point in the composite curve originates from one of the cold or warm streams, the number of returned temperature differences should be constant. However, this is not the case, and this has to be handled in the main code. HYSYS will occasionally add a point beyond the end of the composite curves that does not correspond to any of the inlet or the outlet streams. These values are simply deleted by the optimization tool. In other situations, the discretization of different streams may return locations that are close to each other, and HYSYS may omit one or more of these locations in order to save execution time. In these cases the optimization tool tries to identify the location and add the value by copying one of the neighboring values. For heat exchangers with many intervals, the error will not be large, and at least it is only one point (one constraint) that is affected.

- Using all temperature differences that originate from the hot streams (HotStrPts): This is identical to the formulation above (StrPts) except that only the temperatures from the hot streams are used. When equal temperature steps are used, this means that each constraint is always evaluated at a fixed hot stream temperature.

- Using linear interpolation (LinInt): A linear interpolation function is made from the returned composite curve points based on the enthalpy transferred and the temperature difference. The number of returned elements from the interpolation is fixed.

- Using spline interpolation (SplineInt): As linear interpolation, but cubic splines are used instead.

- Using known local minima of the temperature difference curve (LocalMin): This formulation requires that a solution that is not far away from the optimal solution has been obtained. If the locations for the minimum temperature differences are distinct, one may use the returned temperature difference curve without the required modifications for StrPts, and instead return only the minimum temperature difference within separate predefined intervals. For the flowsheets investigated here, there are four locations where the minimum temperature difference will be obtained for the best known solution. The following four intervals of the hot composite temperatures will contain one each of these locations:

    - < -120°C
    - -120°C – -70°C
    - -70°C – 0°C
    - 0°C

3.3 Optimization scheme and parameter settings

For each case, 100 optimization runs have been performed. In order to make sure that the initial points are not controlled by the user, random values for each of the variables are created within their lower and upper bounds. If the initial state is feasible, an optimization run is performed, otherwise a new initial state is generated. The bounds for the variables have been selected such that a wide parameter range is covered, while ensuring that it is possible to identify a feasible starting point within a few seconds of execution time.

The feed to the compressor should be superheated at least ΔT_c =10°C above the dew point T_{dew} in all cases. The minimum of the temperature differences ΔT_n should be more than ΔT_h=1.2°C in all cases. This work is a continuation of the work in Wahl et al., 2013 where different values of ΔT_h was selected in order to compare with previous reported work. The largest value for ΔT_h has been used here.

4 RESULTS

In this section, results for different formulations of the optimization problem are presented. The formulation of the optimization problem is varied in terms of the selection of variables, the representation of constraints, different flowsheet representations of the process, and different parameters used during the optimization.

In the following, optimization results using different formulations will be shown. Unless otherwise stated, all temperature differences have been used as constraints for the LNG heat exchanger, forward difference using step lengths of 10^{-3} for all variables has been used for the estimation of the derivatives, the coefficient for the heat exchanger temperature difference constraint has been 10 (left hand side of (1)), and the refrigerant suction and discharge pressure and component molar flow rates have been used as optimization variables.

The returned solutions are compared with the best known solutions for each of the four flowsheets. The percentage of runs that came within different specified deviations from the best known objective is shown in figures for each optimization formulation and flowsheet.

4.1 Selection of optimization variables

Three different combinations of optimization variables have been tested:

- Compressor suction (P_{R4}) and discharge (P_{R5}) pressure and component molar flow rates (8 variables)
- P_{R4}, P_{R5}, component molar fractions, and refrigerant molar flow rate (9 variables)
- P_{R4}, P_{R5}, component molar fractions and refrigerant heat flow rate (9 variables)

The last two sets have one additional variable. Hence, different from the variable selection using component molar flow rates, the variables for the flow rate and the composition of the refrigerant are not independent. Another alternative could have been to use enthalpies or entropies. However, enthalpy and entropy are highly dependent on the composition, and will be difficult to set bounds for, easily leading to conditions where flash calculations are not defined.

4.1.1 P_{R4}, P_{R5}, and component molar flow rates as optimization variables

The variable bounds are provided in Table 1. The minimum flow rate of methane and ethane has been set to 0.1 in order to ensure some flow through the LNG heat exchanger.

In Figure 2, the effects on the optimization of different LNG heat exchanger temperature constraint formulations for the temperature difference within the LNG heat exchanger are illustrated. Heat exchanger models both with 10 and 100 intervals per stream have been used, but the results are clearest for the runs with 100 intervals, at the bottom half of the figure. The conclusions that can be drawn are:

- The minimum temperature difference constraint formulation has lower success ratios than any of the other formulations. The reason is that the minimum temperature difference is found in multiple places of the heat exchangers, depending on the operation point, leading to discontinuities in the derivatives which are difficult to handle for NLPQLP. By inspecting logged values for the estimation of the derivatives, it was often observed that when NLPQLP completed without returning the best solution, two or more locations were found with the minimum temperature difference. Adjusting one variable caused one of the locations with the minimum temperature difference to increase, while the other decreased.
- The version with local minimum points for the temperature difference curve works well when 100 intervals are used, but not with 10 intervals.

- Linear interpolation in general works better than spline interpolation. Visually it seems like both the linear and the spline interpolations fit very well with the original composite curves.

- In general, using all stream points (StrPts) or using all hot stream points (HotStrPts) are the best heat exchanger temperature constraint formulations.

This set of variables has been used in all sections following section 4.1.

4.1.2 P_{R4}, P_{R5}, molar component fractions, and molar refrigerant flow rate as optimization variables

All fractions are used as variables, since the bounds will not allow for any component fractions to be calculated as 1 minus the sum of the rest. Hence, this formulation requires one additional variable compared to the one in Section 4.1.1. HYSYS is normalizing the fractions. The other conditions have been identical to the ones in Section 4.1.1. The bounds of the variables are provided in Table 2.

The optimization results with this variable selection are shown in Figure 3, and are quite similar to the results using molar flow rates shown in Figure 2. One should be a little careful in comparing the results shown in Figure 3 and Figure 2 since the effect of the bounds may be significant, but it seems like using the component molar flow rates gives a higher percentage of successful runs.

4.1.3 P_{R4}, P_{R5}, molar component fractions, and refrigerant heat flow as optimization variables

In Figure 4, the optimization results when using component fractions plus refrigerant heat flow are summarized. In general, the performance was not good for this selection of variables. One reason may be that the setting of the bounds, shown in Table 3, is difficult since the heat flow depends on the composition.

4.2 Virtual splitting of the LNG heat exchanger

In section 4.1 it was shown that the minimum temperature difference was not useful as a constraint when there are multiple locations where the minimum value may appear. One alternative formulation is to use a set of intervals where the minimum value only appears once. In this section, each interval is replaced by a separate heat exchanger. The exact location for the minimum value may be slightly different from the ones in section 4.1 since the discretization for each pass differs. Within each LNG heat exchanger, the minimum temperature difference is used as the constraint. The results for this formulation are shown in Figure 5 as a function of intervals per LNG heat exchanger. The results are quite good compared to the previous results. For this process, the four locations are clearly distinguishable. In this situation, the minimum temperature difference works very well as the constraint.

One observation is that the number of successful runs does not necessarily increase with the number of intervals. The more intervals that are used, the smoother the temperature difference curve should be, but this does not help for the optimization routine.

It should be noted that this formulation is only feasible if there is some knowledge about the shape of the temperature difference curve for the optimum solution. It is not clear why some runs do not manage to return better solutions. For several of the runs that failed, the conditions for the last combination of variables seem to be good for further progress; almost linear characteristics in the nearby region, but some noise in the evaluations could cause problems.

4.3 Estimation of the derivatives

Estimating the derivatives is important when using a gradient based optimization technique such as NLPQLP. Step lengths for the estimation of the derivatives are normally selected based on the precision of the evaluation of the function and the absolute value of the variable. In this section, step lengths have been varied to see whether they have an impact on optimization success rate. It should be noted that the lower limit of the derivative step length will be dependent on the noise of the process evaluation, and the results here are thus not generally applicable when using other process simulators.

4.3.1 Fixed step lengths for all variables

When only the pressures or the molar flow rates alone are used as variables, the problem becomes too easy to solve in order to check for effects of varying step lengths. When only the molar flow rates are used as optimization variables, at least all step lengths between 10^{-10} and 1 kmol/s may be used. Similarly, for the pressures all step lengths between 10^{-7} and 10^{-1} bar may be used.

Figure 6 shows the optimization success rate as a function of step lengths of the derivative estimators when solving the full problem. The step lengths have had an identical numerical value for all variables, in units of bar and kmol/s for the pressures and component flow rates, respectively. For 100 intervals, step lengths between 10^{-4} and 10^{-3} generally work best for both step types, but the success rate is only marginally reduced for a step length of 10^{-5} for equal enthalpy step. For 10 intervals, the success rates are lower. The step lengths should be larger than 10^{-8} and smaller than 1. A closer inspection of the optimization output data show that the initial conditions that lead to accurate optimization solutions differ for different step length selections, although some initial conditions always lead to failure.

4.3.2 Variable step lengths for each variables

For another set of optimization runs where the step length ϵ for each variable x was calculated by $\epsilon = \min(\varepsilon_{min} + \alpha|x|, \varepsilon_{max})$, performance was comparable to fixed step length of 10^{-4} or 10^{-3} in Figure 6. In this case ε_{min} had the values 10^{-7}, 10^{-6}, 10^{-5}, 10^{-4}, 10^{-3}, α had the values 10^{-4}, 10^{-3} and 10^{-2} while ε_{max} was 0.1. In this case the minimum step length should be between 10^{-5} and 10^{-3}. For this interval the constant α should be smaller or equal to 10^{-3}. For optimization problems using analytical expressions it is often recommended to use a variable step length in order to achieve the highest possible precision in the estimation of the derivatives. For the flowsheet optimizations here, one can as well use a fixed step length.

4.3.3 Formula for the estimation of derivatives

Three different estimators have been tested for the derivatives:

- Forward/backward difference
- Central difference (two sided)
- 4^{th} order difference

There are several bounds that should not be violated in the evaluations for these types of process problems, e.g. flow rates and pressures cannot be negative. Hence, when approaching such bounds, either the step length, the location where the derivative is estimated, or the derivate estimator has to be adjusted. Eight ways of estimating the derivative have been investigated:

- Forward difference with fixed step length (Fw_S): If the upper bound is violated, the value for the variable is adjusted such that the fixed step length may be used.

- Forward difference with fixed location (Fw_L): Performs a forward difference unless the upper bound is violated, then it performs a backward difference.
- Backward difference with fixed step length (Bw_S): If the lower bound is violated, the value for the variable is adjusted such that the fixed step length may be used.
- Backward difference with fixed location (Bw_L): Performs a backward difference unless the lower bound is violated, then it performs a forward difference.
- Central difference with given step length (Cnt_S): If the upper bound for evaluation is violated, the positive part of the step length is reduced to the difference between the value and the upper bound, similarly for the lower bound. Thus the center moves.
- Central difference with fixed location (Cnt_L): If the upper bound for evaluation is violated, a backward difference is used. If the lower bound for evaluation is violated, a forward difference is used.
- Fourth order difference with fixed step length (4th_S): The new value for the variable where the estimation of the derivative is calculated is $x_i = max(\,min(x_i, x_i^{UB} - 2\epsilon), x_i^{LB} + 2\epsilon)$
- Fourth order difference with fixed location (4th_L): The following estimators are used (in prioritized sequence)
- $x_i - 2\epsilon > x_i^{LB} \;\wedge x_i + 2\epsilon < x_i^{UB}$: Fourth order difference
- $x_i - \epsilon > x_i^{LB} \wedge x_i + \epsilon < x_i^{UB}$: Central difference
- $x_i - \epsilon > x_i^{LB}$: Backward difference
- $x_i + \epsilon < x_i^{UB}$: Forward difference

Figure 7 shows the effect of selecting different formulae for the estimation of derivatives. Although there are differences, these are not significant. In general, using a more complicated estimator does not generate more successful runs.

A closer investigation of each run shows that there exists runs that fail to get within the tightest deviation from the best solution independently of the selection of derivation formulae. However, there are some runs that fail for most of the estimators, while it succeeds for some of the others. This implies that if one estimator fails, it may be possible to toggle between other estimators in order to find better solutions. For this simple process, starting from a different location is probably easier, but for more complex processes with lower success rates, switching estimators may be useful.

4.4 **Variable bounds / initial value bounds**

In the optimization formulation discussed above, the bounds for the initial values have been identical to the bounds for the variables. In this section the bounds for the variables and the initial values have been decoupled and varied, but the initial value bounds need to be at least as strict as the variable bounds. Initial values outside the variable bounds would anyway have been rejected by the optimization routine. The bounds have basically been selected based on the best known solutions for each case. The initial value and variable bounds have been set to either of three sets of bounds; tight (T), medium (M) and wide (W). Since the bounds for the initial values must be inside the bounds of the variables, this gives six different combinations. These bounds are provided in Table 4, tabulated together with the best obtained solutions for the heat exchanger formulations with 10 and 100 intervals with constant enthalpy (DH) or temperature (DT) steps. It should be noted that the solution with 10 intervals with fixed temperature steps (10DT) differs significantly from the other solutions.

The optimization results for the different bounds are shown in Figure 8. For the labels, the first letter indicates the bounds for the variables and the second the bounds for the initial values. This means the label "W/T" means wide bounds for the variables and tight bounds for the initial values. In most situations, narrowing the bounds for the variables improves the likelihood of finding the best solution. In the same way, starting with a set of variables that are closer to the solutions increases the success rate. The effect seems to be more pronounced with crude 10 interval heat exchangers.

4.5 Feasible start

For simple processes like the PRICO process, finding feasible initial values for the variables by random generations within their bounds is quite easy. Finding a feasible set of variables leading to a process state within the constraints is more difficult for complex processes. Hence, the effect of starting from non-feasible starting points has been investigated. In Figure 9, the four results to the right in each plot are identical to the ones in Figure 2. The four results to the left are started from initial conditions that not necessarily fulfil the constraints; some do, but not all. Not surprisingly, for all four flowsheets, the optimization runs that started from only feasible initial points perform best on average. This trend is especially clear when more intervals are used in the heat exchanger model. This implies that ensuring feasibility for the starting points could be essential when using this optimization routine.

4.6 Coefficient for the temperature difference constraint

Each term in the optimization problem may have a factor that is multiplied to the term in order to make sure that all evaluated results, i.e. objective and constraint functions, are within comparable orders of magnitude of each other. The factor in front of the temperature constraint for the LNG heat exchanger is varied in this section, while the factor for the objective function and the dew point deviation is fixed to 1. The step length for the estimation of the derivatives has in this case been 10^{-4} and every returned element in the composite curve (StreamPoints) has been used as the constraint for the LNG heat exchanger.

Variables have been defined in such a way that they are roughly in the same order of magnitude (between 0 and 20). The objective typically is between 1 and 100, while the temperature differences will is between -100 and 100 without any scaling. When close to the best solution the objective will be around 15 and the temperature difference around 1.

The results are shown in Figure 10. In general it seems like coefficients around 10 to 20 gives the best performance. Coefficients below 1 and above 50 significantly reduce the number of successful runs.

4.7 Execution times/flowsheet evaluations

Execution time has not been the focus in this work. Typically, to get within 0.1 % deviation from the best known solution or closer required 450 – 800 flowsheet evaluations for the case using 100 intervals distributed on temperature. The formulation using the local minimum temperature difference formulation required the least; the one using temperature differences based on the hot stream points required slightly less than 700, the two types of interpolation required a bit more than 700 evaluations, and finally the one using all temperature differences required around 800 evaluations. The execution time was typically slightly above 1 min, with one flowsheet evaluation requiring less than 0.1 second. When the distribution was on enthalpy, the same pattern was observed; the only difference was a 10 % increase in the execution time per flowsheet evaluation. When 10 intervals were used, the execution time per flowsheet evaluation was reduced by a factor of 2.

5 CONCLUSIONS

Mathematical optimization of LNG processes has proven to be a difficult task due to the high number of variables, and typical non-linearity and non-convexity of the problem. In a previous work (Wahl et al., 2013) it was shown that the optimization of a single-cycle mixed refrigerant LNG liquefaction process can be performed efficiently using a combination of a commercial flowsheet simulator such as HYSYS and a widely used SQP routine such as NLPQLP. However, the success rate of this approach is highly dependent on how the optimization problem is formulated and implemented. In this work, a study of the effect of the problem formulation of the single cycle mixed refrigerant PRICO process has been presented. Aspects of the formulation which have been investigated includes optimization variables selection and bounds, composite curve heat exchanger implementation and minimum temperature difference, derivative estimation formulae and step lengths, and feasibility of initial values.

Three selections of variables have been investigated. In all sets, the refrigerant compressor suction and discharge pressure were used as variables. The additional variables characterized the refrigerant flow. Using the component molar flow rates performed slightly better than using the molar fractions and total molar flow, while using the heat flow had less success.

Of higher importance is the implementation of the minimum temperature constraint in the heat exchanger. As long as there is more than one location within the LNG heat exchanger where the minimum temperature difference could be achieved during optimization, the minimum temperature difference should not be used as a constraint. Using all values returned from the composite curve as minimum temperature constraints is a better solution. Alternatively, if the initial value is reasonably good, the heat exchanger can be divided up in such a way that each section only has one minimum temperature location.

Another important result is that there is no gain in using a more complex and accurate formula than first order expressions for the derivative estimation for a sufficiently detailed heat exchanger model. This is important because process evaluation is the computational expensive part of LNG process optimization. The step lengths for the estimation of the derivatives must be selected with care. For the runs performed here, where the variables were roughly between 0 and 20, step lengths around 10^{-4} – 10^{-3} showed the best performance.

NLPQLP performs much better if the initial point produced a feasible solution. For a simple process like PRICO, a random combination of variables will quickly return a feasible solution. For more complex processes, where tight variable bounds have not been identified, random initial value generation will not work. In this case, a routine or possibly just a simple algorithm to find a feasible solution might be required.

As with most optimization problems, tightening the bounds improves the performance of the optimization routine. This also includes the set of values for the initial variables. However, it is not necessarily true that the tightest bounds give the best performance.

This work has been investigating a relatively simple LNG process. Depending on the formulation, this work has shown that NLPQLP performs well. It is believed the results here can be generalized to most similar gradient based, and in particular SQP based local search routines. However, more complex processes will pose new challenges, and the optimization of more advanced LNG liquefaction processes are currently under progress.

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Nomenclature

α	Constant for the absolute value of variable x_i
ϵ	Step length
P	Pressure
T_c	Calculated inlet temperature of the inlet stream to the compressor
ΔT_c	Specified minimum temperature difference between T_c and T_{dew}
T_{dew}	Calculated dew point temperature of the inlet stream to the compressor
ΔT_h	Minimum temperature difference allowed for the heat exchanger
ΔT_n	Temperature difference in interval number n of the heat exchanger
x_i	Variable i
W	Compressor power consumption
$\underline{x}$	Vector of all x_i

Superscripts

LB	Lower bounds of the specified variables
UB	Upper bounds of the specified variables

Subscripts

Max	Maximum value
Min	Minimum value
R4	Stream R4
R5	Stream R5

List of figures

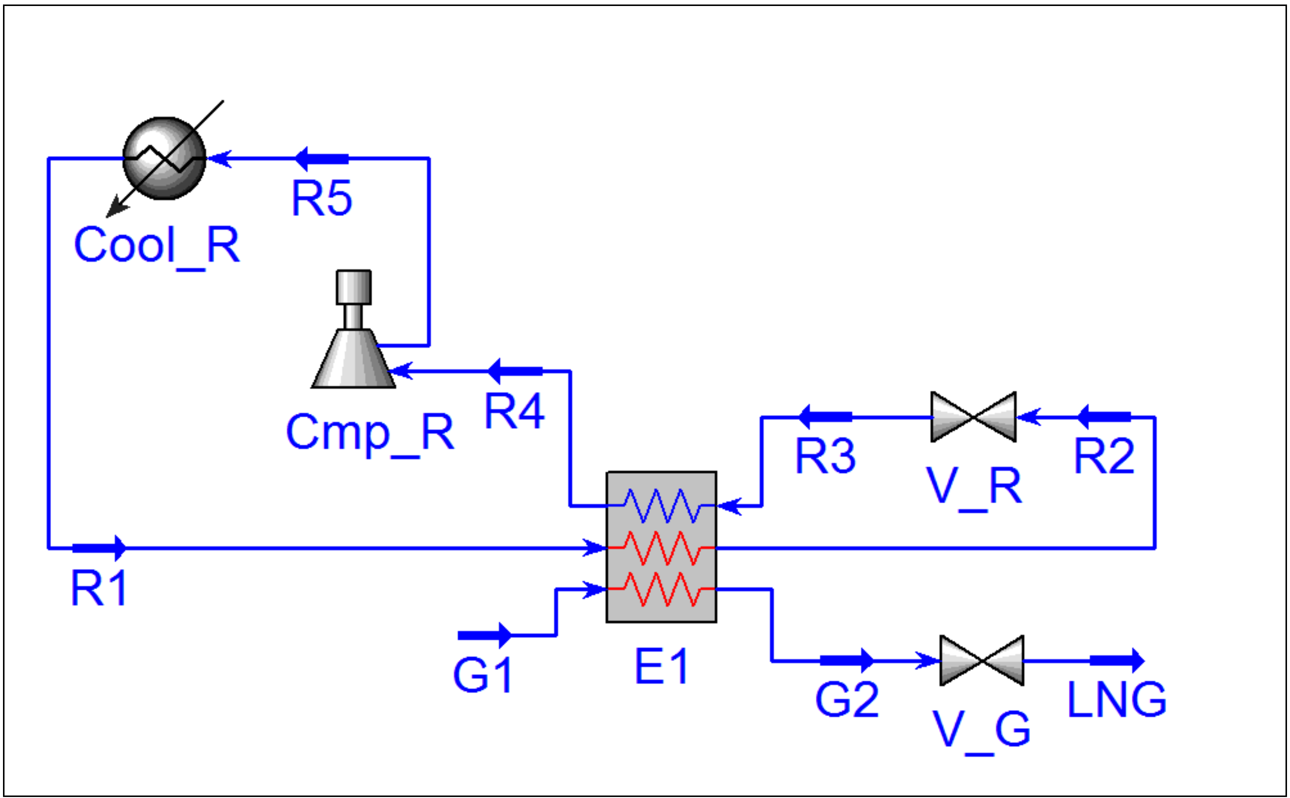

Figure 1. Flowsheet for the LNG process to be optimized. The cycle consists of one mixed refrigerant (R) and a natural gas stream (G).

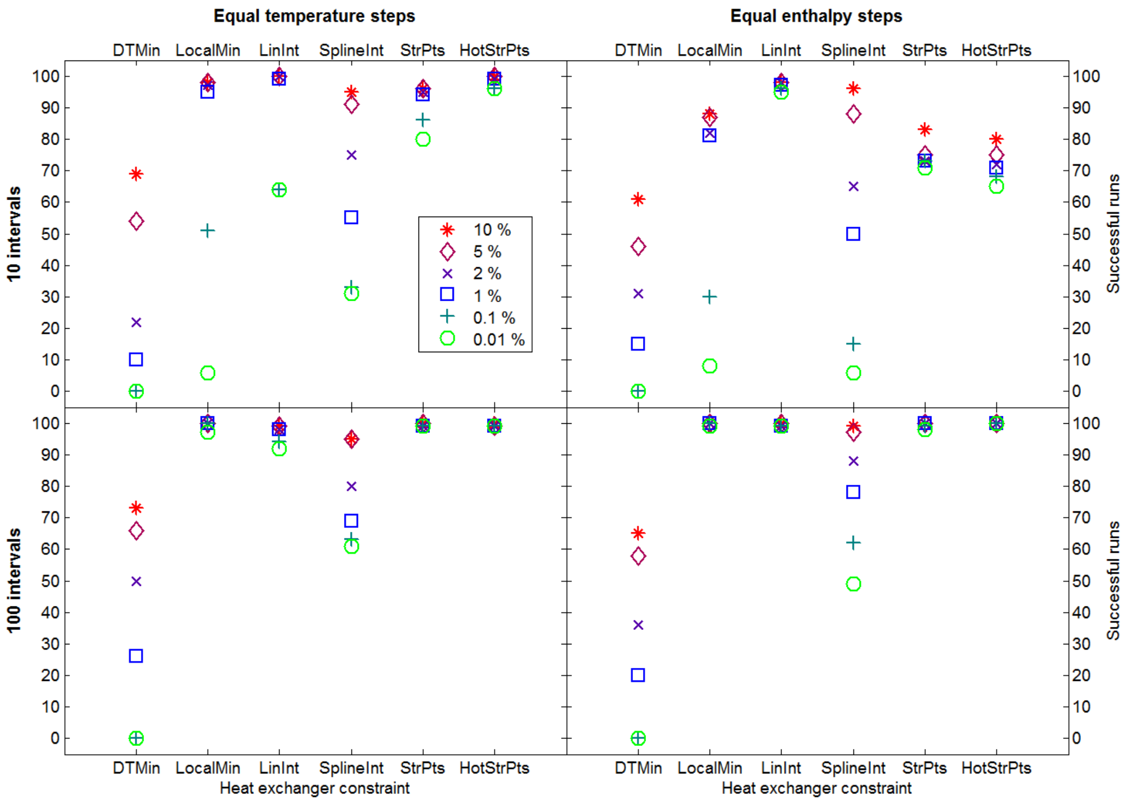

Figure 2. Number of successful optimization runs for various formulations of the LNG heat exchanger constraints when molar flow rates have been used as variables. Legend indicates deviation from best known solutions.

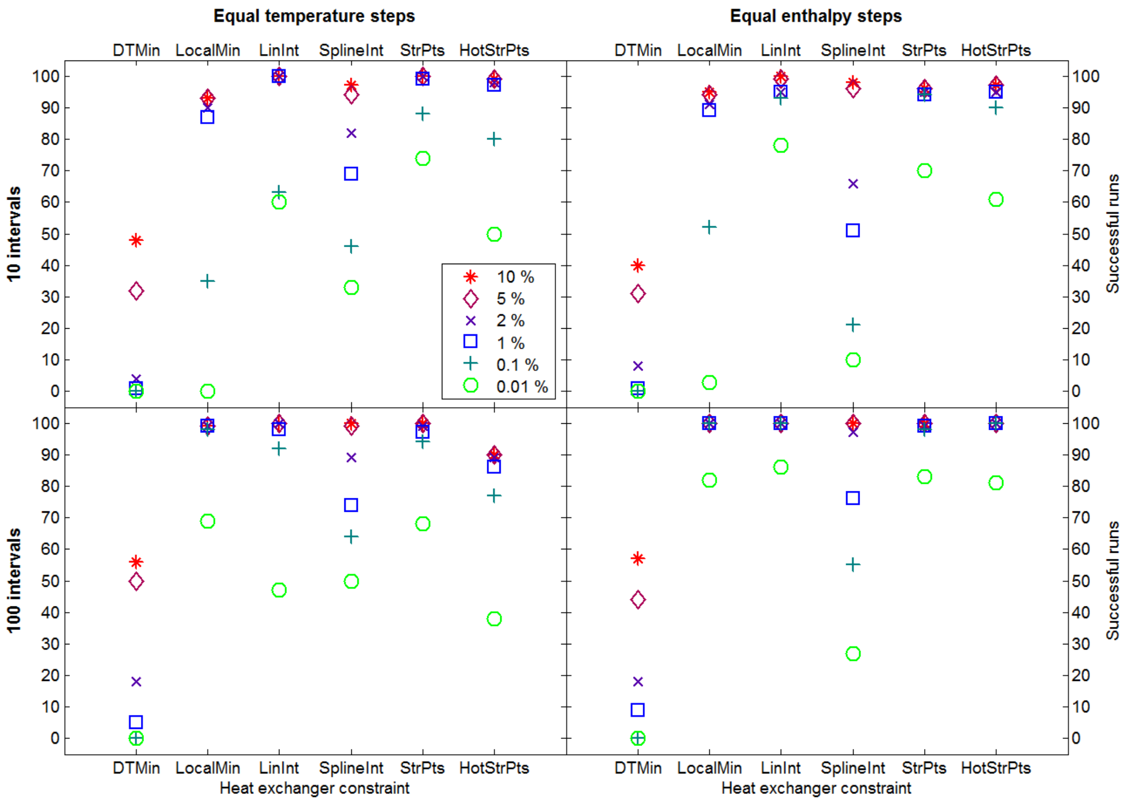

Figure 3. As Figure 2, but using molar fractions and total flow rate as variables.

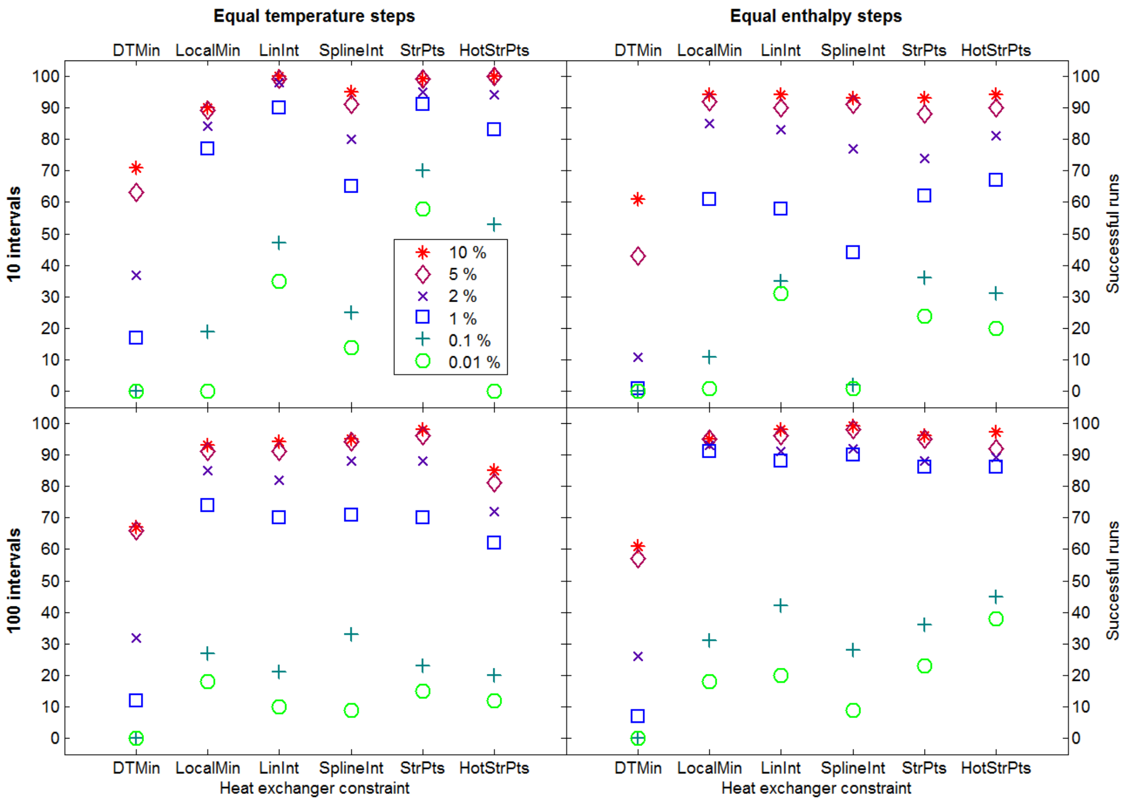

Figure 4. As Figure 2, but using heat flow and molar fractions as variables.

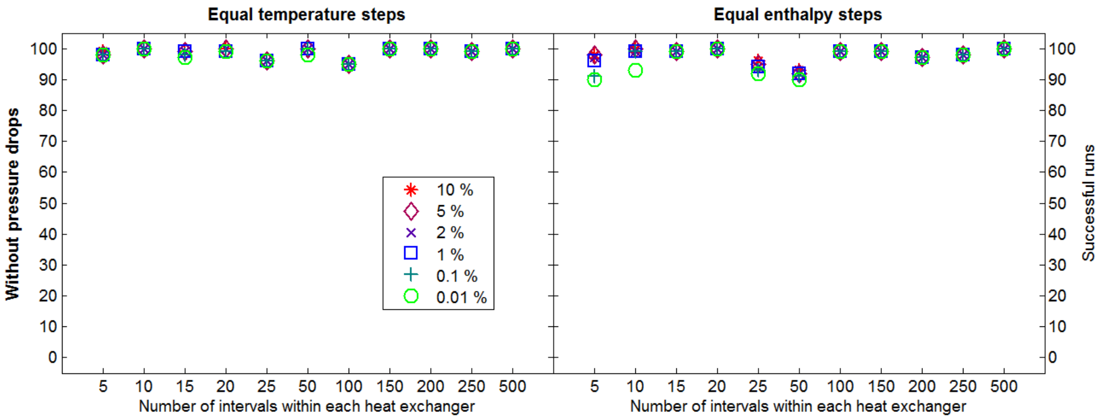

Figure 5. Number of successful runs when the physical LNG heat exchanger has been represented in the flowsheet by a series of heat exchangers, each with a single local minimum location. The minimum temperature approach is used for each flowsheet heat exchanger. Legend indicates deviation from best known solutions.

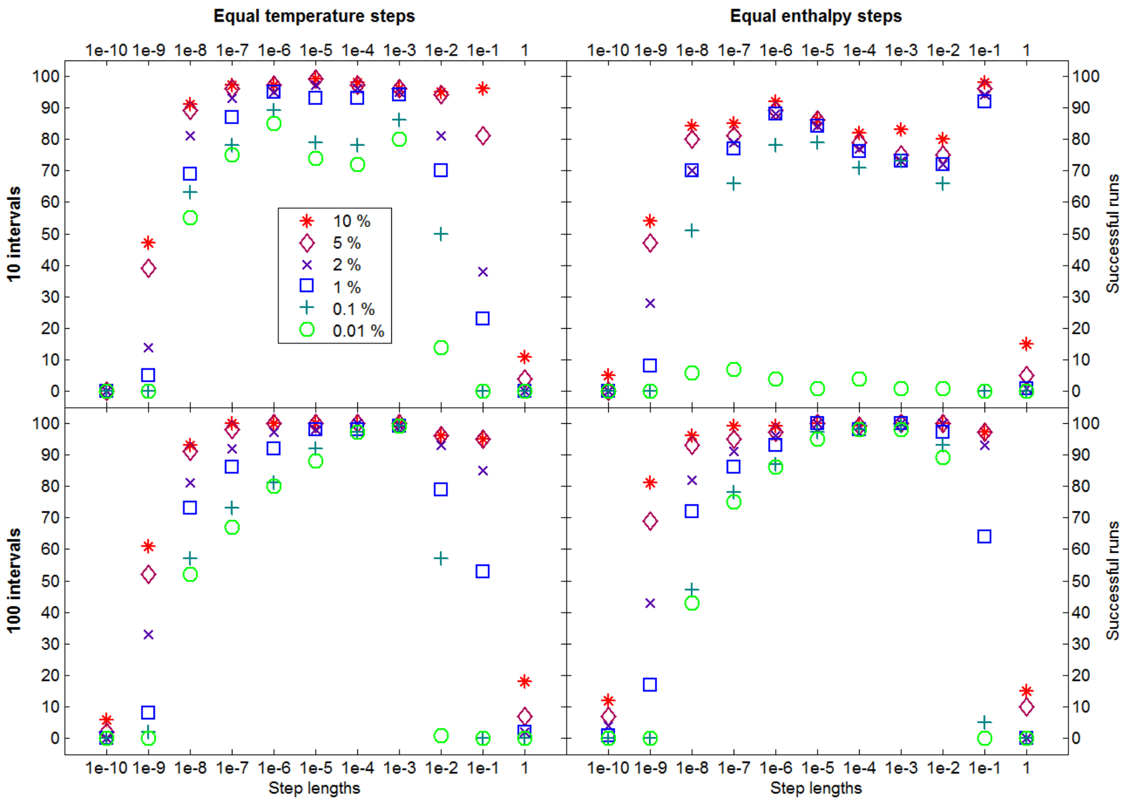

Figure 6. As Figure 2, but where the step length of the derivative estimator has been varied instead of the heat exchanger temperature constraint implementation

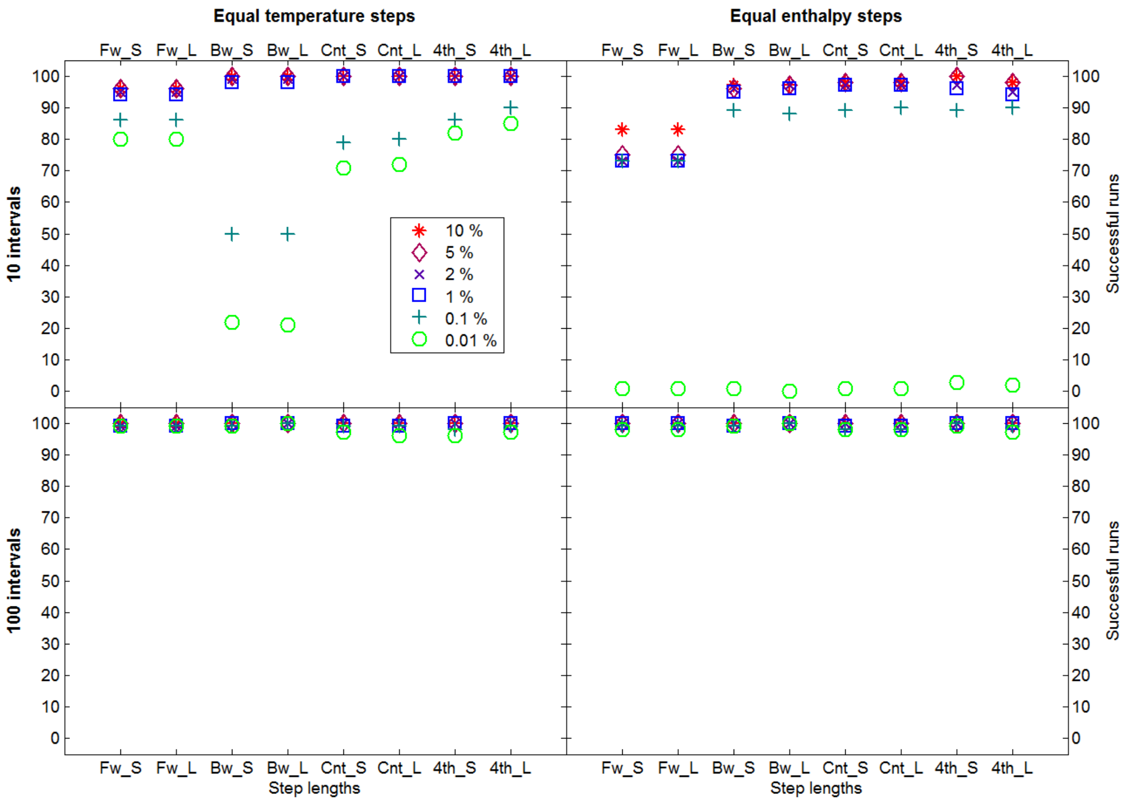

Figure 7. As Figure 2, but for different derivative estimator implementations.

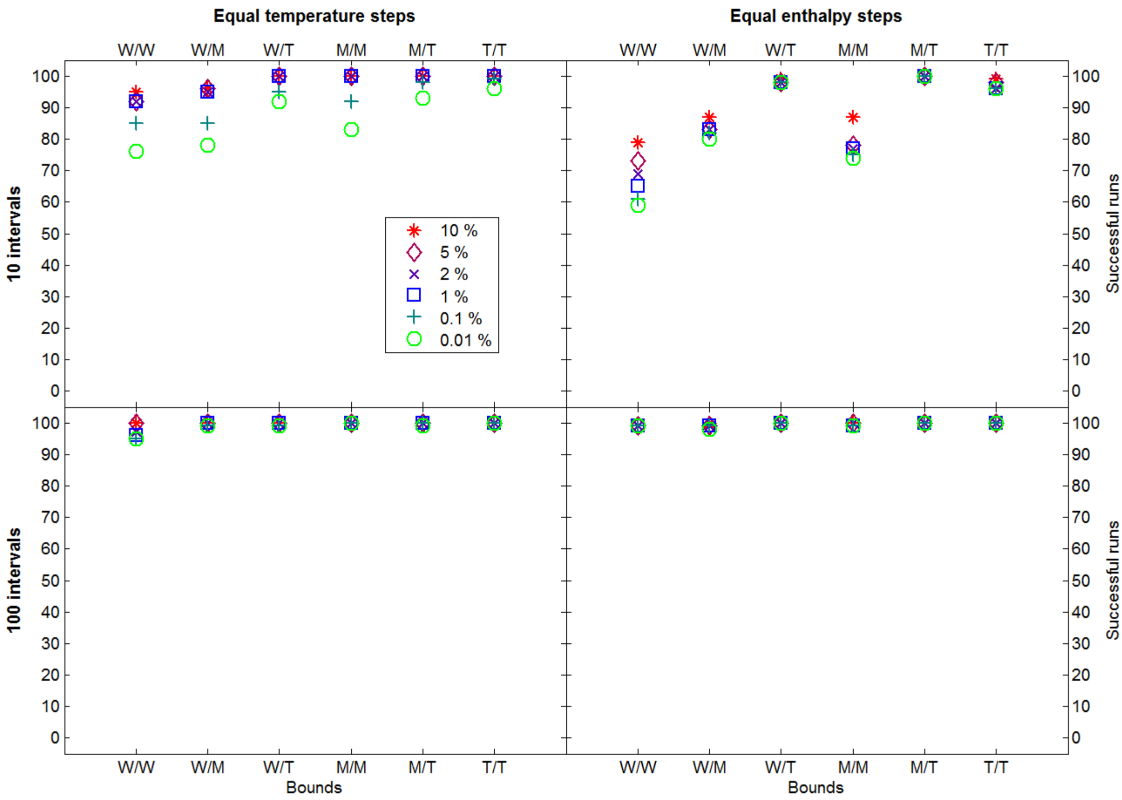

Figure 8. As Figure 2, but for different bounds for the variables and initial values for the variables, with reference to Table 4.

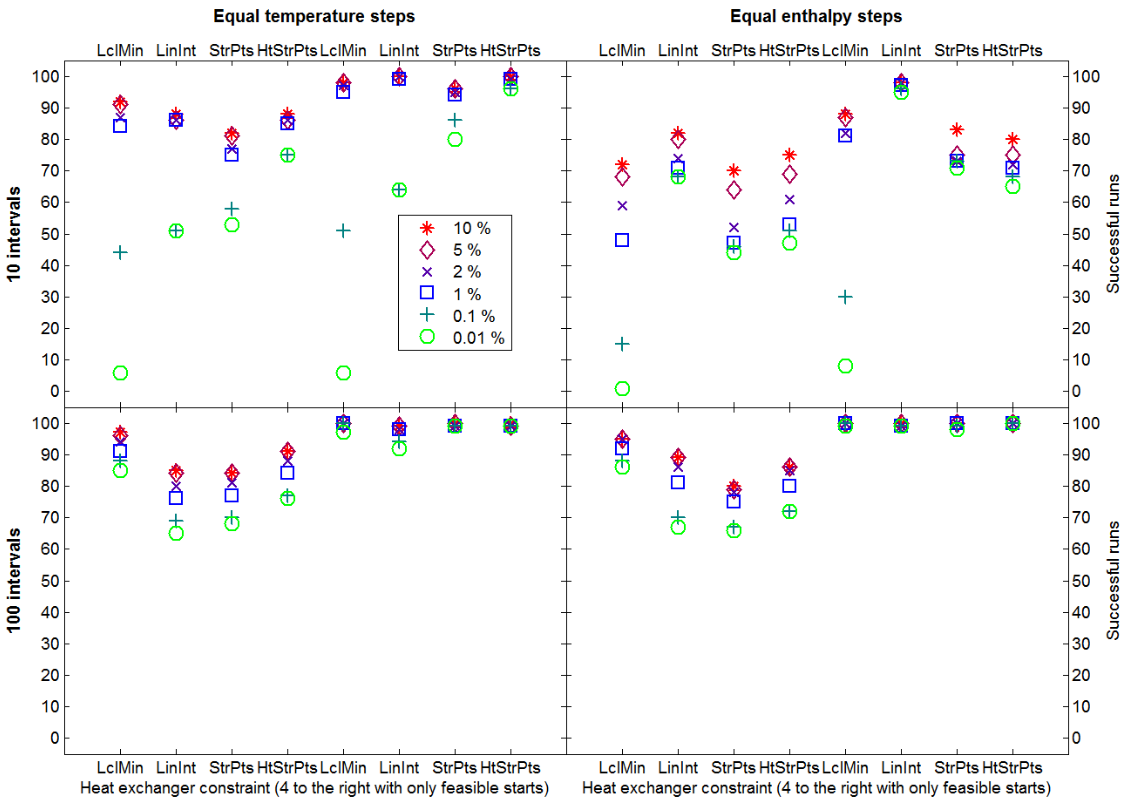

Figure 9. As Figure 2, but showing the dependence on the feasibility of the optimization starting point.

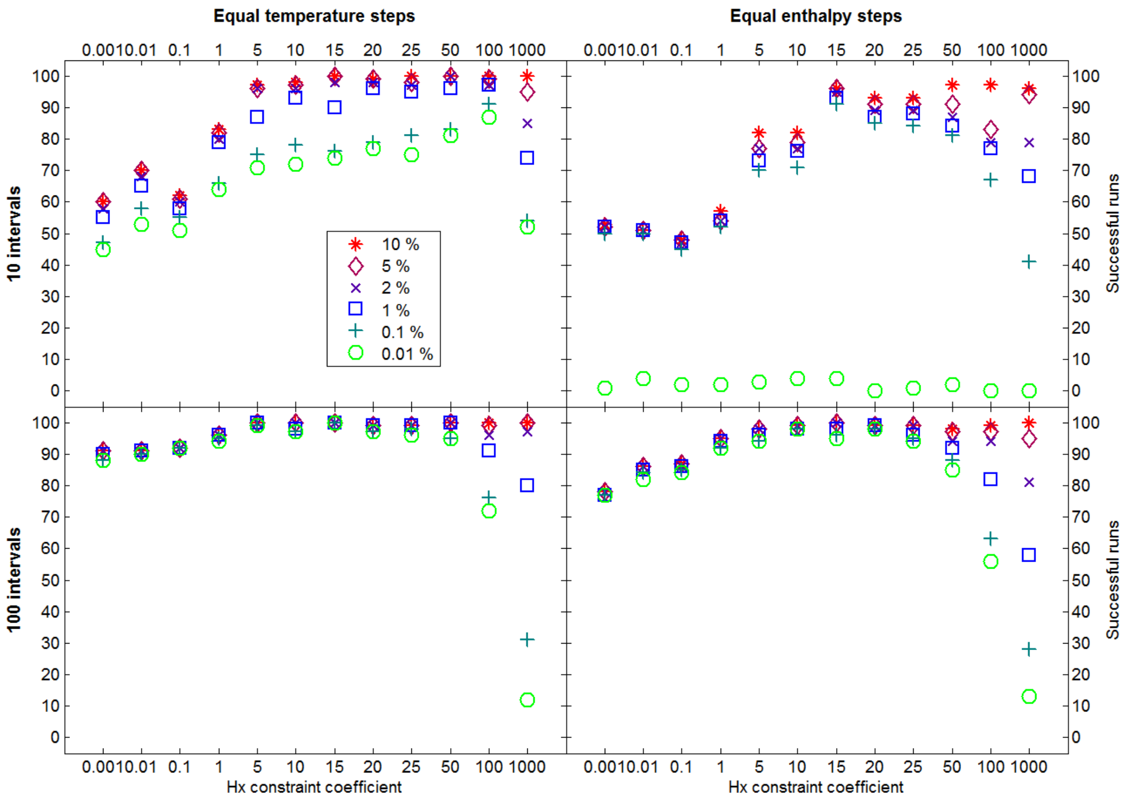

Figure 10. As Figure 2, but varying the coefficients for the temperature difference constraint

List of Tables

Table 1: Bounds when using the refrigerant component molar flow rates

Variable	*Unit*	*LB*	*UB*
R4: Pressure	bar	2.0	6.0
R5: Pressure	bar	10.0	20.0
R1: Nitrogen	kmol/s	0.0	1.0
R1: Methane	kmol/s	0.1	2.0
R1: Ethane	kmol/s	0.1	2.0
R1: Propane	kmol/s	0.0	2.0
R1: i-Butane	kmol/s	0.0	2.0
R1: n-Butane	kmol/s	0.0	2.0

Table 2: Bounds when using the refrigerant component molar fractions and the total refrigerant molar flow rate

Variable	*Unit*	*LB*	*UB*
R4: Pressure	bar	2.0	6.0
R5: Pressure	bar	10.0	20.0
R1: Molar flow	kmol/s	0.1	6.0
R1: Nitrogen	mol/mol	0.0	0.2
R1: Methane	mol/mol	0.1	0.5
R1: Ethane	mol/mol	0.1	0.5
R1: Propane	mol/mol	0.0	0.5
R1: i-Butane	mol/mol	0.0	0.5
R1: n-Butane	mol/mol	0.0	0.5

Table 3: Bounds when using the refrigerant component molar fractions and the total refrigerant heat flow rate

Variable	*Unit*	*LB*	*UB*
R4: Pressure	bar	2.0	6.0
R5: Pressure	bar	10.0	20.0
R1: Heat flow	GJ/h	-1500.0	-500.0
R1: Nitrogen	mol/mol	0.0	0.2
R1: Methane	mol/mol	0.1	0.5
R1: Ethane	mol/mol	0.1	0.5
R1: Propane	mol/mol	0.0	0.5
R1: i-Butane	mol/mol	0.0	0.5
R1: n-Butane	mol/mol	0.0	0.5

Table 4: Bounds and best known values for the variables.

Variable	*Unit*	*LBW*	*LBM*	*LBT*	*10 DH*	*10 DT*	*100 DH*	*100 DT*	*UBT*	*UBM*	*UBW*
R4: Pressure	bar	1.0	2.0	3.0	3.1	5.1	3.1	3.1	6.0	6.0	9.0
R5: Pressure	bar	10.0	10.0	12.0	12.1	14.7	12.3	12.4	15.0	20.0	30.0
R1: Nitrogen	kmol/s	0.0	0.0	0.1	0.2	0.3	0.2	0.2	0.4	1.0	2.0
R1: Methane	kmol/s	0.1	0.2	0.6	0.7	1.1	0.7	0.7	1.2	1.2	2.0
R1: Ethane	kmol/s	0.1	0.8	1.2	1.3	1.7	1.3	1.3	1.8	1.8	2.0
R1: Propane	kmol/s	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.2	1.0	2.0
R1: i-Butane	kmol/s	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.2	1.0	2.0
R1: n-Butane	kmol/s	0.0	0.5	0.9	1.1	1.1	1.1	1.1	1.3	1.5	2.0

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