Optimization of a simple LNG process using sequential quadratic programming

Per Eilif Wahl[1],
Sigurd Weidemann Løvseth, and
Mona Jacobsen Mølnvik

SINTEF Energy Research, Gas Technology,
NO-7465 Trondheim, Norway

Abstract

The efficiency of using sequential quadratic programming (SQP) for the optimization of a PRICO process for the production of liquefied natural gas (LNG) is demonstrated. Most of the returned objective values have been better, and the execution times much lower, than in most previously published work on similar optimization cases. The optimization runs discussed in this paper require around 5 minutes of execution time.

Keywords

LNG
PRICO
Optimization
Constraints
Minimum temperature difference

1 INTRODUCTION

Liquefied natural gas (LNG) is regarded as the most effective solution for long-distance gas transport. By liquefying the gas, the volume is reduced about 600 times. Hence, transportation by ship typically outperforms pipeline transportation for distances longer than 1500 km. In 1964, the first base load LNG plant was started up in Arzew, Algeria, followed up by the Kenai LNG plant in Alaska in 1969. Both these plants are based on a cascade process. In 1970, the Marsa El Brega plant in Libya, which was based on a single-mixed refrigerant cycle, started up (Bosma and Nagelvoort, 2009). In the following years, various plants based on other processes were introduced. In 1981, Train 40 of the Skikda plant in Algeria, based on the PRICO process from Pritchard, was brought on-line. Previously, this plant had three trains based on the TEAL process, and later two more trains based on the PRICO process were added (Price and Mortko, 1996). Since then, several processes have been developed, and the train size has increased from typically 1 million tonnes per year in the 1970s to the mega-sized trains in Qatar from 2009 producing 7.8 million tonnes of LNG per year (Qatargas, 2013; Karrar, 2009; Tuttle, 2010).

The PRICO process is a simple liquefaction process for natural gas that currently is in use in multiple plants world-wide (Hoffart and Price, 2013). Hence, works where the PRICO process has been the object of optimization have been reported quite frequently in the literature. Remeljej and Hoadley (2006) compared the PRICO process with three other processes. The reported results for the PRICO process were based on work performed by Lee (2001). Relevant parts of this thesis may be found in Lee et al. (2002). Cao et al. (2006) investigated two other LNG processes where they used Aspen HYSYS for evaluation, as well as SQP optimization routines integrated in HYSYS. Jensen and Skogestad (2008) addressed the problems of using the minimum temperature difference as a criterion in process design. They used a simplified total annual cost as a criterion

[1] Telephone number: +47 73 59 38 91
E-mail address: Per.E.Wahl@sintef.no

for the optimization. This objective was also used for several case studies on the PRICO process in Jensen and Skogestad (2009a, 2009b). Other optimization techniques have also been used. Mokarizadeh Haghighi Shirazi and Mowla (2010) used genetic algorithms for the PRICO process. Aspelund et al. (2010) used tabu search combined with Nelder-Mead downhill simplex. Morin et al. (2011) used evolutionary search for similar problems.

Optimization of LNG processes has proven to be a difficult problem, and many methods often fail to converge to a global optimum. In this work, optimization of a PRICO LNG process with the NLPQLP routine from Schittkowski (2006) using Aspen HYSYS® for the process simulations is demonstrated. NLPQLP is an implementation of a sequential quadratic programming method which is very efficient for some types of problems. In this paper, it is shown that NLPQLP is very robust and efficient for the optimization of the PRICO process compressor power consumption. HYSYS is a process simulator that is commonly used among engineers and provides routines that have been thoroughly tested over many years. There are also possibilities to use optimization routines from Aspen Tech in HYSYS. However, in our experience, these routines have not shown to be reliable. One of the alternatives terminates the HYSYS process while the problem is being specified. The other available routine often returns a message stating that the optimal solution has been found although the constraints are severely violated.

In the optimization, the flow rates of each component in the refrigerant and the suction and discharge pressure for the compressor can be varied. Results of the present work will be compared with Aspelund et al. (2010) and Jensen and Skogestad (2008). Aspelund et al. (2010) reported a setup for the PRICO process where the simulations were performed with Aspen HYSYS. The results from this work should be directly comparable with the results from Aspelund et al. (2010) since the same process simulator has been used. Jensen and Skogestad (2008) used a PRICO process with a different framework for the evaluation of the flowsheet, which we do not have available. The main objective for this paper is, however, to demonstrate that optimization of these processes may be performed in a very robust and time efficient way by using an SQP routine.

2 PROBLEM FORMULATION

2.1 The PRICO process

In this work, the PRICO™ process (Stebbing and O'Brien, 1975; Price and Mortko, 1996) has been analyzed. A HYSYS flowsheet of the PRICO process with one compressor and one heat exchanger is provided in Figure 1.

Figure 1 about here

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). Depending on the conditions of the subcooled natural gas, a pressure reduction will normally, but not always, reduce the temperature of the final LNG product. Depending on the specifications, the stream LNG may have a small fraction of vapor. In these cases, the actual LNG product will be the bottom product from a flash unit having the stream LNG as a feed. For the calculations performed here, the flash unit is not needed and is not included in the flowsheet. In the LNG heat exchanger, the mixed refrigerant (stream R1) enters at the same temperature as the natural gas, is condensed, cooled, and subcooled (stream R2). The outlet temperature is for these calculations identical to the outlet temperature of the subcooled natural gas (stream G2). 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 NG and LNG streams are fixed for each case; only parameters for the mixed refrigerant are allowed to vary during the optimization. The variables in the optimization have been indicated in red in the flowsheet and are the compressor suction pressure P_1, compressor discharge pressure P_2, and the vector of flow rates $\underline{F} = \begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ f_i \\ \vdots \\ f_I \end{bmatrix}$ where f_i is the flow rates (molar or mass) for each component *i* of the refrigerant.

2.2 Optimization problem

The objective function is the power consumption of the compressor. The variables P_1, P_2 and f_i defined in the previous have lower and upper bounds. In all cases considered here, the following constraints have been specified:

- 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

Hence mathematically, the optimization problem can be expressed as:

$$\begin{aligned}
&\min W(\underline{F}, P_1, P_2) \\
&\text{subject to} \\
&\Delta T_n(\underline{F}, P_1, P_2) - \Delta T_h \geq 0; \text{ for all intervals n} \\
&T_c(\underline{F}, P_1, P_2) - T_{dew}(\underline{F}, P_1, P_2) - \Delta T_c \geq 0 \\
&f_{i,LB} \leq f_i \leq f_{i,UB}; \text{ for all components i} \\
&P_{1,LB} \leq P_1 \leq P_{1,UB} \\
&P_{2,LB} \leq P_2 \leq P_{2,UB}
\end{aligned} \qquad (1)$$

Here

- W is the compressor power consumption
- ΔT_h is the specified minimum temperature difference allowed for the heat exchanger
- ΔT_n is the calculated temperature difference in interval n of the heat exchanger
- T_c is the calculated inlet temperature for the compressor
- T_{dew} is the calculated dew point temperature of the inlet stream to the compressor
- ΔT_c is the specified minimum temperature difference between T_c and T_{dew}, i.e. the superheating value of the inlet stream to the compressor
- f_i is the molar or mass flow for component i, which is between specified upper (UB) and lower bounds (LB),
- P_1 is the pressure of stream R4, and P_2 is the pressure of stream R5, both with lower and upper bounds.

In addition, two of the cases have a constraint on the maximum UA value for the heat exchanger. The heat transferred in each temperature interval is given by

$$Q = UA\Delta T_{LM} \qquad (2)$$

Here

- Q is the heat transferred between the hot composite curve and the cold composite curve
- U is the overall heat transfer coefficient
- A is the surface area available for heat transfer
- ΔT_{LM} is the log mean temperature difference (LMTD)

$$\Delta T_{LM} = \frac{\Delta T_1 - \Delta T_2}{\ln\left(\frac{\Delta T_1}{\Delta T_2}\right)} \qquad (3)$$

ΔT_1 and ΔT_2 are the temperature differences in the ends of the heat exchanger or the heat exchanger interval.

The heat transfer coefficient and the surface area are often combined into a single variable referred to as UA which is calculated in HYSYS. The returned value is the sum of the UA values for each interval.

None of the expressions for thermodynamic properties or unit operations calculated are available outside HYSYS. The optimization routine only sees the values for the objective and the constraints that are calculated by HYSYS. Hence, there are no possibilities for manipulating the expressions or using analytical derivatives that sometimes may be useful for optimization routines. The function evaluations are thus of a black box type.

3 OPTIMIZATION SET-UP

3.1 Optimization tool

In this work, the NLPQLP routine has been applied for the optimization of LNG processes evaluated with HYSYS. In order to have full control of the optimization, a software tool has been developed that enables the combination of HYSYS for process simulation with optimization routines external to HYSYS like e.g. NLPQLP. The main program is implemented in Microsoft Visual Basic (VB) .NET.

NLPQLP requires that evaluations of the objective and constraints, as well as the corresponding gradients, are performed by user added Fortran code. The user added Fortran code includes a routine that receives a pointer to another routine of the external main program that performs the evaluation by calls to HYSYS. The user-added Fortran code and the source code for NLPQLP is compiled to a dynamic-link library, DLL.

The process is specified in HYSYS independently of the tool. The optimization problem is specified in a text file based on XML (Extensible Markup Language), using either the graphical interface of the tool or any text editor. These optimization specifications include information about variables, constraints, and parameters (the name of the HYSYS case file and names, properties, and units for process streams or process units in HYSYS). The selection of formulae, and step lengths for estimation of derivatives, the bounds for the variables, and some additional parameters for NLPQLP are also specified in the XML file. The values for the superheating, ΔT_c, and the minimum temperature difference between the hot and the cold stream, ΔT_h, are specified in the input file. During execution, the tool reads the specification XML file and launches HYSYS with the specified HYSYS case file. The main program communicates with HYSYS using OLE Automation, which is an inter-process communication mechanism for Microsoft Windows applications. Values for the variables are transferred to HYSYS, and the calculated values for the objective and constraints are retrieved. The optimization DLL then takes control of the execution. During optimization, NLPQLP set values for f_i and P_j which are transferred to HYSYS by the main program. The left hand sides of the temperature constraints in (1) are calculated by calls to HYSYS, and the values are returned to NLPQLP by the main program. When the optimizer has completed, control is handed back to the main program which generates the output files as Excel workbooks. The control relations, represented as solid lines, between the user, the simulation environment, the optimizer, Excel and the main program are illustrated in Figure 2. In this context the control relations includes the communication via the GUIs (Graphical user interfaces) for the user, and function calls between the software components.

Figure 2 about here

3.2 Flowsheet evaluations in HYSYS

3.2.1 Heat exchanger model

The heat exchanger models used are based on composite curves. The hot streams flow in one direction, while the cold streams flow in the opposite direction. All hot streams are merged into one pseudo-stream, the hot composite curve, while all cold streams are merged into the cold composite curve. One challenge when using the composite curves 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. The actual value for the minimum temperature difference may be seen either as a safety margin for the thermodynamic evaluations, or as a trade-off between the heat exchanger area and the operating cost.

In the present work, the values for ΔT_h have been selected to make the optimization cases comparable with selected published studies. If the values had been selected freely, they should be interpreted as a safety margin instead of a tradeoff value between operating and investment cost, since the objective only concerns the power consumption. In that respect the optimization problem only concerns thermodynamic issues without any concern of costs.

More detailed heat exchanger models that include geometric parameters for the heat exchangers normally require additional licenses or user added routines. The use of more detailed heat exchanger models is a subject for future work.

3.2.2 Intervals within the heat exchangers

During the calculations, each individual stream in the heat exchanger is divided into a user specified number of intervals, where each interval either spans over the same difference in temperature or enthalpy. One should be aware that the equal enthalpy difference specification in HYSYS is a bit misleading. It does not mean that the enthalpy differences are identical for all intervals within a stream. Some intervals have almost the same enthalpy difference, but there may be other intervals with substantially different enthalpy differences. The equal temperature difference specification results in intervals with identical temperature differences unless flash calculations fail. In order to have the number of intervals fixed, no additional dew or bubble point calculations have been used in the heat exchanger specifications, since such calculations in some situations will add points to the stream intervals.

3.2.3 The temperature difference between the hot and the cold composite stream

The minimum value of $\Delta T_n(\underline{F}, P_1, P_2)$ is easily available in HYSYS, but using it will cause problems when there is more than one location where this minimum value occurs. Instead, all points returned within the heat exchanger are used as individual constraints in this work. NLPQLP requires that the number of constraints is constant during optimization. However, although the number of intervals within each stream is fixed, it does not mean that the number of points in the composite curves returned from HYSYS is fixed. The temperatures used to evaluate the heat exchanger constraints are therefore based on the points within each individual stream. For each temperature in each hot stream, the index for this temperature is found in the hot composite curve, and this index is used to return the corresponding cold composite temperature. The same is performed for the cold stream. This is a bit awkward, but it is essential to obtain a fixed number of constraints. However, this is not always sufficient. HYSYS will occasionally add a point beyond the end of the composite curves that does not correspond to any of the inlet or outlet streams. These values are simply deleted by the main code. In other situations points may be omitted due to flash problems. In these cases the code 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.

3.2.4 Forced recalculation

If the changes from the last evaluation of the flow parameters associated with a heat exchanger are quite small, HYSYS does not recalculate the heat exchanger. In order to increase the smoothness one may force HYSYS to recalculate the flowsheet by evaluating a totally different set of values. This option is implemented in the tool. Although the number of flowsheet evaluations per iteration step increases, the increased precision normally leads to fewer iterations in NLPQLP, and the overall execution time will not necessarily increase. Forced recalculation is not necessary when pressure drops in the heat exchangers are ignored.

3.2.5 Tolerances of the flow sheet calculations

The precision in the evaluation of the objective and constraints may be important when a gradient based optimization technique is used. There are no possibilities to adjust the tolerance of the internal flash calculations of the thermodynamic packages that have been used here. Only the LNG heat exchanger tolerance parameter, which is a measure for the heat balance error, may be set by the user in HYSYS. The default value of 10^{-4} is not sufficient, but it is not necessary to use the lowest possible value (10^{-15} - 10^{-14}); values around 10^{-10} are normally sufficient. The routines that handle the communication between HYSYS and the optimizer are capable of coping with situations where the specified precision is not reached. The tolerance is relaxed in order to achieve a solution and then increased in order to obtain the best achievable precision.

3.3 Execution conditions

All simulations have been performed with Aspen HYSYS® V7.3 (build 25.0.2.7337) on a Dell Precision M6400 using Windows 7 x64 with 16.0 GB installed memory (RAM) with an Intel® Core™ 2 Extreme Q9300 CPU (four cores, 2.53 GHz). During the runs up to three optimization processes have been run at the same time, in accordance with the maximum number of processes allowed by the HYSYS license. No other CPU demanding operations have been executed during the optimization runs.

4 OPTIMIZATION SPECIFICATIONS

4.1 Investigated PRICO process cases

5 different cases have been defined. The compositions of the natural gas in the cases are shown in Table 1. The remaining fixed condition specifications are given in Table 2. The cases 1 - 2 and 3 - 4 in the present work correspond to cases 1 - 2 and 4 - 5, respectively, in Aspelund et al. (2010). Case 2 and 4 have an additional constraint for the maximum value for UA (48.6 MW/°C) compared with Case 1 and 3, respectively. In Case 5, values from Jensen and Skogestad (2006) have been used.

Three different HYSYS case files have been used for the runs:

- Case 1 and 2: The lean natural gas composition in Aspelund et al. (2010)
- Case 3 and 4: The rich natural gas composition in Aspelund et al. (2010)
- Case 5: The problem from Jensen and Skogestad (2006)

Table 1 about here
Table 2 about here

In this work, the number of intervals for each stream within the LNG heat exchanger was 100. In Jensen and Skogestad (2006) the number of intervals for the whole heat exchanger was 100, while the number of intervals was 25 in Aspelund et al. (2010). In the latter case it is not entirely clear whether this was 25 intervals for each stream or for the heat exchanger as a whole. Aspelund et al. (2010) does not specify the thermodynamic property package used. Some properties have been calculated with both Soave Redlich–Kwong (SRK) and Peng–Robinson (PR) in Table 3 and compared with the results specified in Aspelund et al. (2010). In the table, "Initial" is the initial conditions for optimization in Aspelund et al. (2010). Case 1 and 2 refer to the optimized process parameters in Aspelund et al. (2010). The flowsheets are calculated both with the pressure drops specified (Given ΔP) and when the pressure drops in the refrigerant streams are switched (Switched ΔP) in order to check for a possible error in the reported pressure drops in Aspelund et al. (2010). MITA is the minimum temperature difference. Table 3 shows that in this work SRK gives results comparable to Aspelund et al. (2010). Table 3 also shows that the specified pressure drops in the cold and hot refrigerant streams probably should have been switched in Aspelund et al. (2010). The values for the pressure drops will then correspond to the values in Jensen and Skogestad (2006). The HYSYS versions used in the present work and in the work of Aspelund et al. (2010) are not identical, but the calculations should not differ much between the versions.

Table 3 about here

4.2 Optimization scheme and parameter settings

As discussed in Section 2.2, the variables of the process are the component flow rates of the mixed refrigerant and the suction and discharge pressure of the compressor. For each case, 10 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 minutes of execution time. The bounds for the variables are listed in Table 4 for Case1 to 4 and Table 5 for Case 5. The bounds for the variables have been adapted to the results obtained in this article and will thus differ from the ones in Aspelund et al. (2010).

Table 4 about here
Table 5 about here

The feed to the compressor should be superheated at least ΔT_c =10°C above the dew point T_{dew} in all 5 cases. The minimum of the temperature differences ΔT_n should be more than ΔT_h=0.1°C for Case 1 to 4 and ΔT_h=1.2°C for Case 5. The value of ΔT_h is selected in order to compare with previous work. 0.1°C is a very small value, which will result in a very large heat surface area. As seen from the optimization point of view, any value larger than 0 could be used in order to ensure thermodynamically feasibility. In this context, the value for ΔT_h should not be interpreted as a rule of thumb that balances investment and operating costs. It may, however, be interpreted as a safety margin for the temperature difference.

Aspelund et al. (2010) does not mention any constraint for the compressor inlet stream temperature T_c. In principle, the present study could have obtained better values of the objective without this constraint.

Most optimization runs of this study have used forced recalculation of the flowsheet evaluations as discussed in Section 3.2.4. The heat exchanger tolerance discussed in Section 3.2.5 has been set to a very low value of 10^{-14}.

5 RESULTS

In this section, the output from the optimization of the 5 cases are presented and compared with previously published results. In addition, the execution times are reported in order to give an idea of the efficiency of the SQP routine compared with the reported execution times of Aspelund et al. (2010). As discussed above, all initial conditions of the present work have been created randomly in the feasible solution domain.

The percentage levels in the following figures showing either execution times or the number of evaluations indicate when a solution better than the specified percentage has been obtained. This means that the top of the green area indicates when a solution within 0.01% of the currently best known solution was obtained. The top of the red area indicates when NLPQLP has completed.

The execution time per evaluation is dominated by the flowsheet evaluation, but it also includes the execution time for the optimizer. Note that all of the curves shown below are produced using forced recalculation for each evaluation, but optimization runs have also been performed without using forced recalculation.

5.1 Case 1

The best objective value achieved for Case 1 was 106.1 MW. This value was obtained for several runs using step lengths for the derivative estimations of either 10^{-3}, 10^{-2} or 10^{-1}. For all step lengths the best value was achieved both with and without forced recalculations. The solution obtained here is compared to the solution from Aspelund et al. (2010) in Table 6. In short, the solution of Aspelund et al. (2010) had a smaller flow rate, but a larger compressor pressure increase. Note that the present solution does not contain any propane.

Table 6 about here

The current optimized objective was roughly 4% better than the one returned in Aspelund et al. (2010). In some of the present solutions with this objective value the constraints for the inlet conditions for the compressor were active, which means that better solutions could exist if this constraint is either relaxed or removed. The initial and optimized objectives are shown in Figure 3, while the execution time and the number of evaluations are shown in Figures 4 and 5.

A step length of 10^{-1} was used for the estimation of the derivatives for all variables, and the flowsheet was forced to recalculate. In all ten optimization runs the solutions were better than in Aspelund et al. (2010). One of the runs returned a solution that was within 0.01 % of the currently best known solution, 8 were within 0.1 % and all 10 runs were within 1 %. For most of these runs, the execution time was roughly around 2 - 3 minutes, and a solution within 1% of the currently best known solution was normally found in roughly 1 minute. The execution times reported in Aspelund et al. (2010) were around 4 hours for one optimization run. One should be careful in comparing execution time under different executing conditions, but there should be no doubt; using NLPQLP is much more efficient and gives better solutions for this case than tabu search combined with Nelder-Mead downhill simplex method. Note that since the flowsheet was forced to recalculate, the actual number of flowsheet evaluations was twice the number of function evaluations shown in the Figure 5. The execution time per evaluation was similar in all the runs; between 0.24 and 0.27 seconds. Since the number of evaluations scales very well with the execution time in all the cases presented in this paper, only the execution times will be presented for the other cases.

Figure 3 about here
Figure 4 about here
Figure 5 about here

The objective value was very similar for all the 10 runs in Figure 3. The values for the variables of the solutions were very similar as well.

5.2 Case 2

This case corresponds to Case 2 in Aspelund et al. (2010). The best solution obtained here was 143.0 MW for step lengths for the derivative of either 10^{-4}, 10^{-3} or 10^{-2}, all with forced recalculation. This was only 1% better than the solution in Aspelund et al. (2010) which was 144.5 MW. Compared with the results from Case 1, the power consumption has increased from 106.1 to 143.0 MW, while the UA value has decreased from 835.5 to the specified value of 48.6 [MW/°C]. The execution times are shown in Figure 6. 9 of the runs returned a solution that was within 0.01% of the currently best known solution. The remaining run was within 1 % of the currently best known solution and thus also better than the one in Aspelund et al. (2010). Most optimization runs completed in 3 to 5 minutes compared to 12 hours in Aspelund et al. (2010). The execution time per evaluation for the runs was between 0.26 and 0.28 seconds.

Figure 6 about here

The returned objective values were very similar in all runs for this case. The returned values for the variables were quite similar, except for the run that only came within 1% of the currently best known solution. The solution is compared with the solution from Aspelund et al. (2010) in Table 7. In short, this solution has lower flow rates for the lightest components, a larger flow rate for n-butane, lower pressure levels, but a slightly larger pressure ratio for the compressor. For both this solution and the solution from Aspelund et al. (2010), the pressure ratios for the compressor is so large that the compression should take place in two stages in a physical realization of the case. This would of course also affect the obtained solution. One may observe that also this solution does not contain any propane.

Table 7 about here

5.3 Case 3

This case corresponds to Case 4 in Aspelund et al. (2010). The best solution obtained here was 90.3 MW, while it was 91.4 MW in Aspelund et al. (2010). The execution time is shown in Figure 7. All of the runs returned a solution that was within 0.01% of the currently best known solution, and thus better than the solution of Aspelund et al. (2010). Most runs completed in 1.5 minutes or less compared to 4 hours in Aspelund et al. (2010). The execution time per evaluation is almost identical in all the runs; around 0.23 seconds.

Figure 7 about here

In this case there was no variation at all between the runs in the variables. The present solution is compared with the solution of Aspelund et al. (2010) in Table 8. The variables were not reported in Aspelund et al. (2010), but the calculated values are quite similar, except for the UA value, which was much larger in the current solution. One may observe that this was the only case in the present work where the solution contains propane; however the fraction is small.

Table 8 about here

5.4 Case 4

Case 4 corresponds to Case 5 in Aspelund et al. (2010). The best objective value obtained in the present work is 125.5 MW, which was actually worse than the 122.7 MW objective obtained by Aspelund et al. (2010). The reason is not known. Aspelund et al. (2010) do not report the variables for this case. Hence, it is difficult to verify if their solution is feasible. The execution time is shown in Figure 8. 7 of the runs returned a solution that was within 0.01% and the remaining runs were within 1 % of the currently best known solution. Most runs completed in less than 6 minutes, but there were also some runs that needed more time. The execution time per evaluation is similar in all the runs; between 0.24 and 0.26 seconds.

Figure 8 about here

Except for the runs that only came within 1% of the currently best known solution all variables were quite similar. The solution is compared to the solution from Aspelund et al. (2010) in Table 9. The variables were not reported in Aspelund et al. (2010), but the calculated values are identical, except for the compressor power, which is slightly larger in the present work. One may observe that this solution does not contain propane. One may also observe that this solution was very similar to the solution in Case 2, where the natural gas had a different composition.

Table 9 about here

5.5 Case 5

The results shown here are for step lengths of 10^{-4} for all variables. The execution times for the runs are shown in Figure 9. In this case all 10 returned solutions are for all practical purposes identical; both with respect to the objective and the variables. None of the runs needed more than 6 minutes to return the optimal solution, and most of them completed in around 3 minutes. Hence, for this case NLPQLP is both very accurate and efficient. It should be noted that the number of intervals for each stream is 100 for this case compared to 25 for the other cases. This means that the execution time is longer for each flowsheet evaluation, between 0.43 and 0.54 seconds. However, the total execution time is still low.

Figure 9 about here

This case was taken from Jensen and Skogestad (2006), where the SRK thermodynamic equation of state was used. However, HYSYS was most likely not applied for the evaluation. A table showing the results from the present work and Jensen and Skogestad (2006) are shown in Table 10, but the comparison should be performed with care since the environment used for the evaluations differ. Case 5 of the present work is based on the same assumptions as the design case of Jensen and Skogestad (2006). Some of the values for the variables were not legible in their article, but at least the results they obtained for their Case 2, where all values were legible, give a significant temperature crossover in HYSYS. In the present work the optimized power consumption of the case was 18.7 MW while it was 17.4 MW in Jensen and Skogestad (2006). If Peng Robinson is used, the returned objective value of the present work is 18.0 MW. The pressures obtained here are higher than the ones obtained in Jensen and Skogestad (2006). The amounts of nitrogen and methane are slightly higher in the present case. In both cases no propane is present in the refrigerant. Although the results differ a little, the solutions are comparable, and the differences are most likely due to the equations used for evaluation of the flowsheet. The execution time in Jensen and Skogestad (2006) is not known.

Table 10 about here

A plot of the temperatures of the cold (blue) and hot (red) composite curves and a plot of the temperature difference between these (green) are shown in Figure 10. The figure illustrates that the returned solution has composite curves that are very close to each other except for the warm part of the heat exchanger. These curves are very similar for the rest of the cases as well.

Figure 10 about here

6 CONCLUSIONS

6.1 Robustness

In all of the optimization runs reported here, the assumed optimal solution is returned within a margin of 1%. Since the optimal solution is not known analytically, better solutions could exist, but since so many optimization runs starting from different and random initial conditions return the same solution, it is assumed that the optimal solution has been found. In the optimization framework presented here, NLPQLP is very robust in returning the same solution. One should be aware that the robustness is sensitive to the bounds of the variables. When the bounds are widened, the performance of the optimizer is reduced. There are still situations where the optimizer will fail, even for this simple process. However, the present work illustrates that gradient based optimization is very efficient when it is applicable.

6.2 Execution time

For the optimization runs performed here, the execution time is typically a few (2 - 6) minutes. In Aspelund et al. (2010) the execution time was 4 or 12 hours typically with lower accuracy. In Morin et al. (2011) the execution time for a similar problem with two compressors was around 22 hours and 40,000 flowsheet evaluations. In the work reported here, most runs completed in less than 2,000 evaluations. The optimization runs performed here are most likely performed on a faster PC, so the execution times should be compared with care. However, the difference is much larger than can be explained by a faster CPU. Hence, it can be concluded that NLPQLP can be very efficient and that one should definitely consider gradient based optimization methods for these types of problems.

6.3 Complexity of the process

These runs are performed on a very simple LNG process. Although NLPQLP works very well here, more complex processes will be more difficult for all optimization strategies.

7 SUMMARY

In this paper the efficiency of an SQP routine (NLPQLP) for the optimization of a simple LNG process represented in HYSYS has been illustrated. For the runs that can be compared to previous work (Aspelund et al., 2010), most of the returned objective values have been better in this work. The runs presented in this paper require around 5 minutes of execution time, while the runs of Aspelund et al. (2010) required either 4 or 12 hours. Some of this difference is explained by a faster processor, but the SQP routine will still be more efficient than non-gradient based methods. Care must be taken regarding how the problem is formulated, and some effort must be made with respect to how HYSYS calculates the flowsheet. One should be aware that these results are obtained for a very simple process. When the complexity of the processes increases, optimization using both gradient based and other routines is expected to be more difficult. In addition to LNG liquefaction, the framework presented here is applicable to other processes implemented in HYSYS.

8 ACKNOWLEDGEMENTS

This publication has been funded by the project "Enabling low emission LNG systems", performed under the strategic Norwegian Research program Petromaks. The authors acknowledge the partners; Statoil, GDF SUEZ and the Research Council of Norway (193062) for support.

9 REFERENCES

Aspelund, A., Gundersen, T., Myklebust, J., Nowak, M. P., & Tomasgard, A. (2010). An optimization-simulation model for a simple LNG process. Computers & Chemical Engineering, 34, 1606-1617.

Bosma, P., & Nagelvoort, R. K. (2009). Liquefaction Technology; Developments through History. In A. H., R. G. V & E.-H. M.M. (Eds.), 1st Annual Gas Processing Symposium: Elsevier

Cao, W. S., Lu, X. S., Lin, W. S., & Gu, A. Z. (2006). Parameter comparison of two small-scale natural gas liquefaction processes in skid-mounted packages. Applied Thermal Engineering, 26, 898-904.

Hoffart, S. D., & Price, B. C. (2013). Producing LNG from Coal. http://bv.com/Home/news/thought-leadership/energy-issues/producing-lng-from-coal

Jensen, J. B., & Skogestad, S. (2006). Optimal operation of a simple LNG process. In ADCHEM 2006: International Symposium on Advanced Control of Chemical Processes (pp. 241-246). Gramado, Brazil.

Jensen, J. B., & Skogestad, S. (2008). Problems with specifying Delta T-min in the design of processes with heat exchangers. Industrial & Engineering Chemistry Research, 47, 3071-3075.

Jensen, J. B., & Skogestad, S. (2009a). Single-cycle mixed-fluid LNG process Part I: Optimal design, In H. Alfadala, G. V. Reklaitis & M. M. El-Halwagi (Eds.), 1st Annual Gas Processing Symposium. Qatar, Elsevier

Jensen, J. B., & Skogestad, S. (2009b). Single-cycle mixed-fluid LNG process Part II: Optimal Operation, In H. Alfadala, G. V. Reklaitis & M. M. El-Halwagi (Eds.), 1st Annual Gas Processing Symposium. Qatar, Elsevier

Karrar, T. (2009). Qatargas Inaugurates Trains 4 and 5. http://downstreamtoday.com/news/article.aspx?a_id=15942&AspxAutoDetectCookieSupport=1

Lee, G. C. (2001). Optimal design and analysis of refrigeration systems for low temperature processes. PhD, UMIST, University of Manchester, UK.

Lee, G. C., Smith, R., & Zhu, X. X. (2002). Optimal synthesis of mixed-refrigerant systems for low-temperature processes. Industrial & Engineering Chemistry Research, 41, 5016-5028.

Mokarizadeh Haghighi Shirazi, M., & Mowla, D. (2010), Energy optimization for liquefaction process of natural gas in peak shaving plant, Energy, Volume 35, Issue 7, 2878-2885, (http://www.sciencedirect.com/science/article/pii/S0360544210001374)

Morin, A., Wahl, P. E., & Molnvik, M. (2011). Using evolutionary search to optimise the energy consumption for natural gas liquefaction. Chemical Engineering Research & Design, 89, 2428-2441.

Price, B. C., & Mortko, R. A. (1996). PRICO - A simple, flexible proven approach to natural gas liquefaction. In Gastech 96: The 17th International LNG/LPG/Natural Gas Conference. Vienna, Austria.

Qatargas. (2013). http://www.qatargas.com/English/AboutUs/Pages/CurrentOperationsD.aspx

Remeljej, C. W., & Hoadley, A. F. A. (2006). An exergy analysis of small-scale liquefied natural gas (LNG) liquefaction processes. Energy, 31, 2005-2019.

Schittkowski, K. (2006). NLPQLP: A Fortran Implementation of a Sequential Quadratic Programming Algorithm with Distributed and Non-Monotone Line Search. User's Guide Version 2.2.

Stebbing, R., & O'Brien, J. (1975). An up-dated report on the PRICO (TM) process for LNG plants. In Gastech '75, 6th International LNG/LPG Technology Conference. Paris.

Tuttle, R. (2010). Qatar's RasGas Starts Producing LNG From Train 7 (Update2). http://www.bloomberg.com/apps/news?pid=newsarchive&sid=a.w3CDgJKONY

List of figures

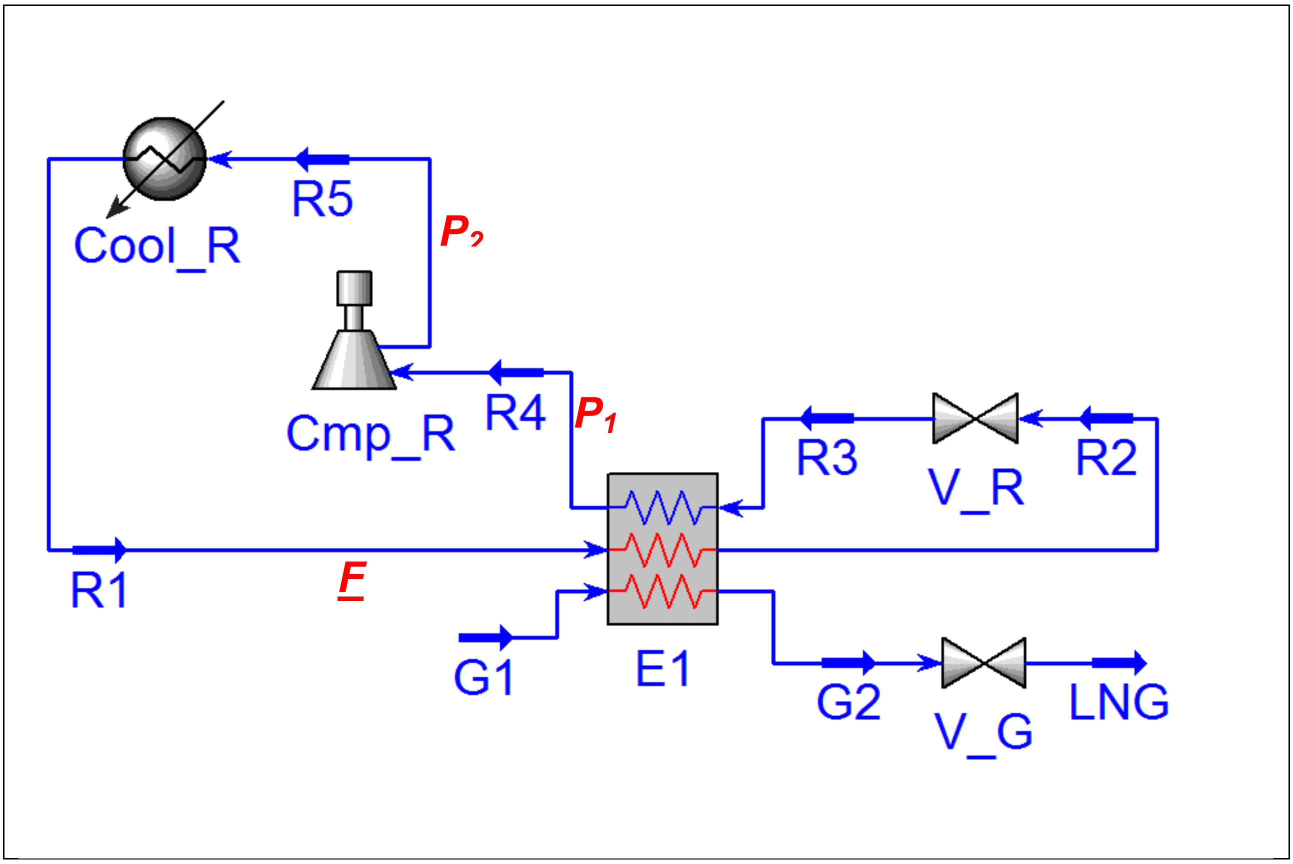

Figure 1. HYSYS flowsheet used in this work. Letters in red have been added to the flowsheet and indicate the variables.

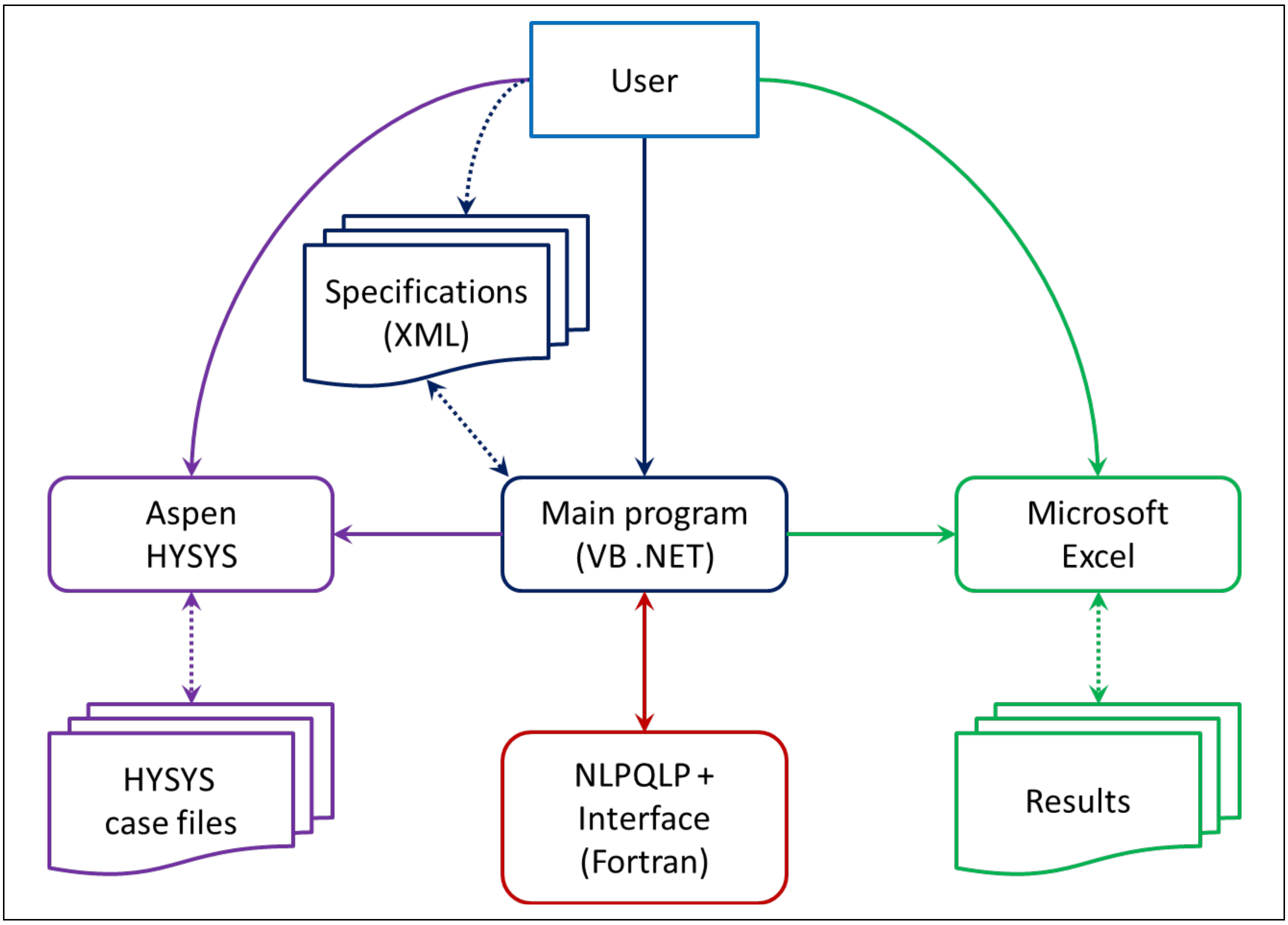

Figure 2. Control relations between the user and the different modules prior to and during optimization. The solid arrows indicate direction of control, while the dotted arrows indicate creation and reading of files.

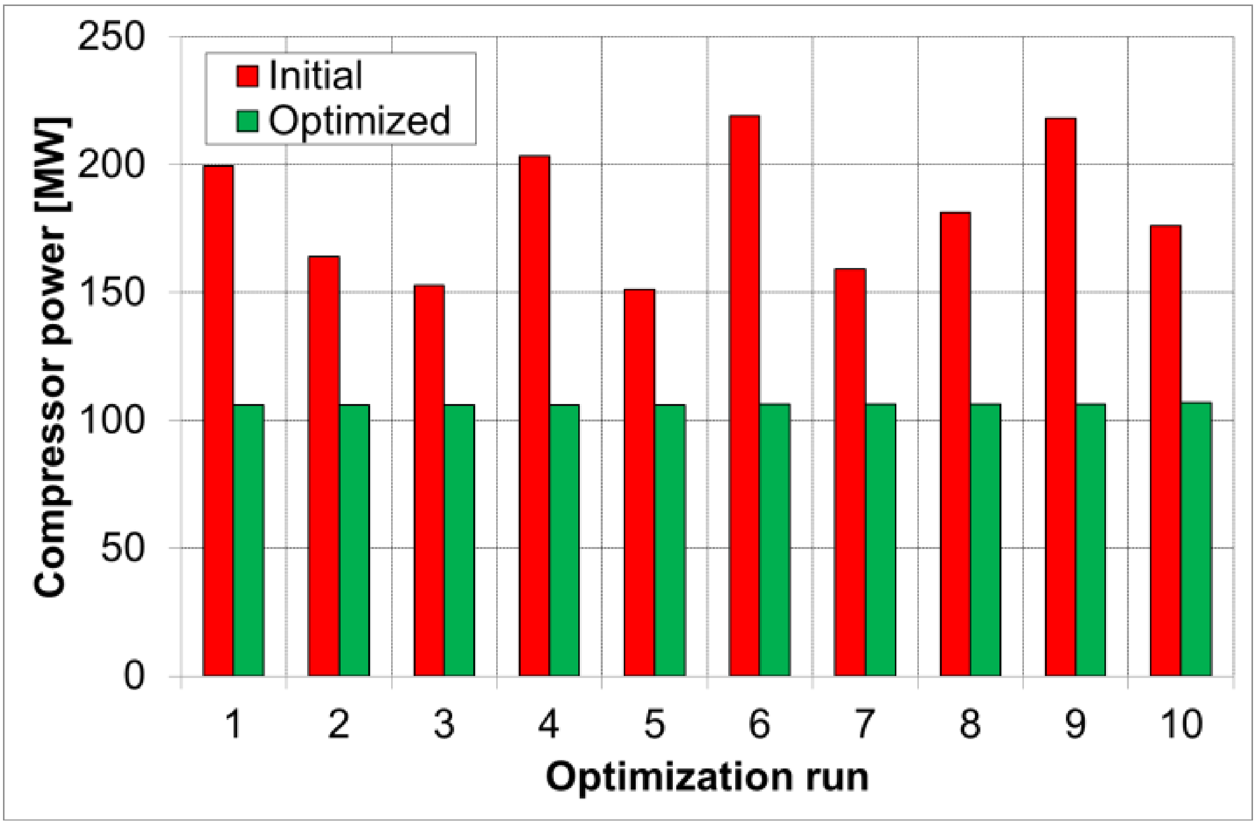

Figure 3. Initial and optimized objective for Case 1

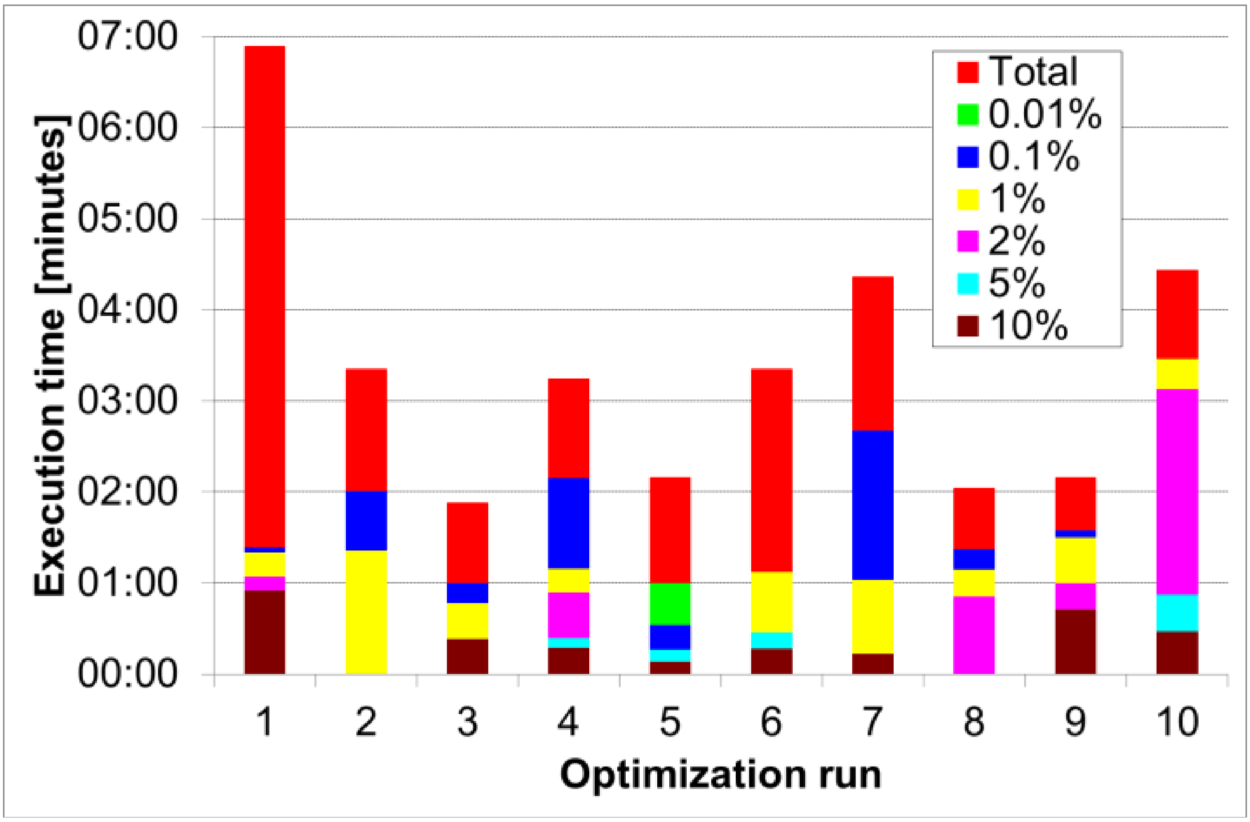

Figure 4. Execution times for Case 1 as a function of obtained precision.

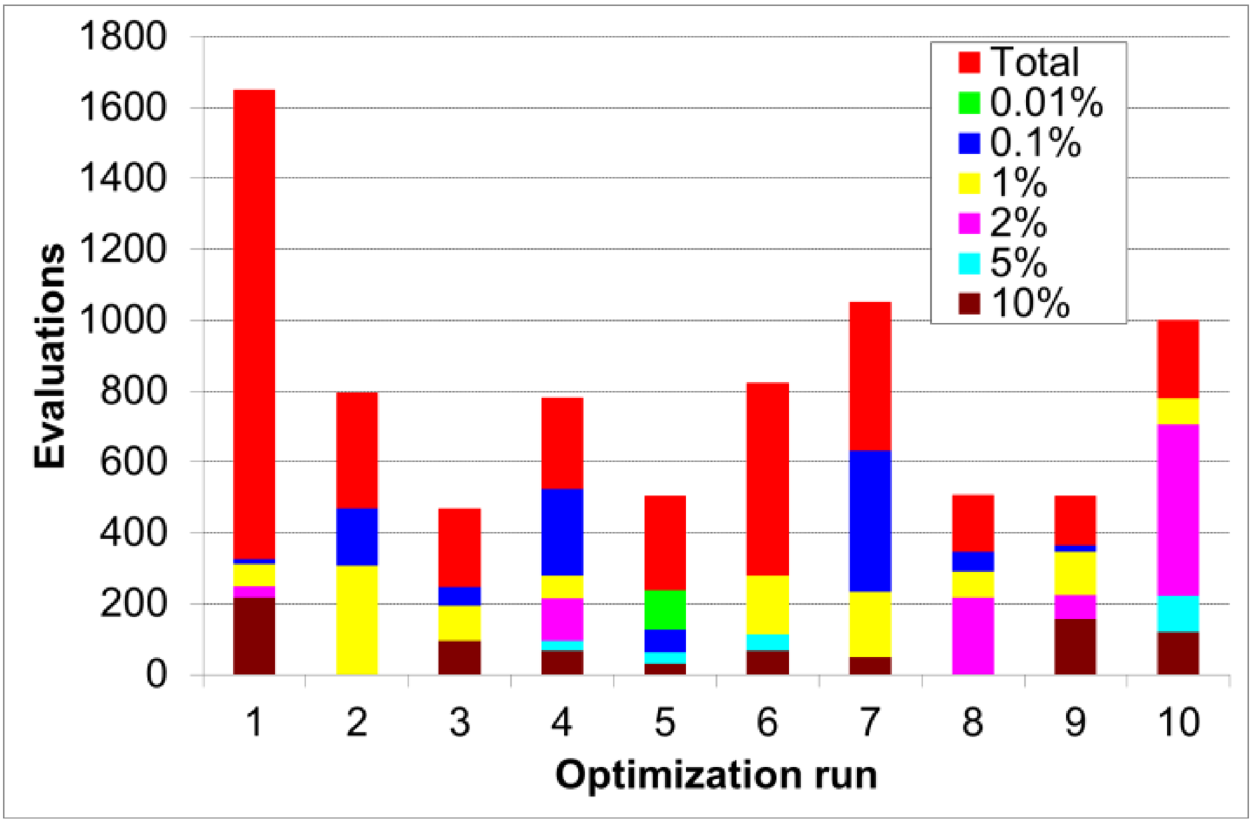

Figure 5. Number of evaluations for Case 1 as a function of obtained precision.

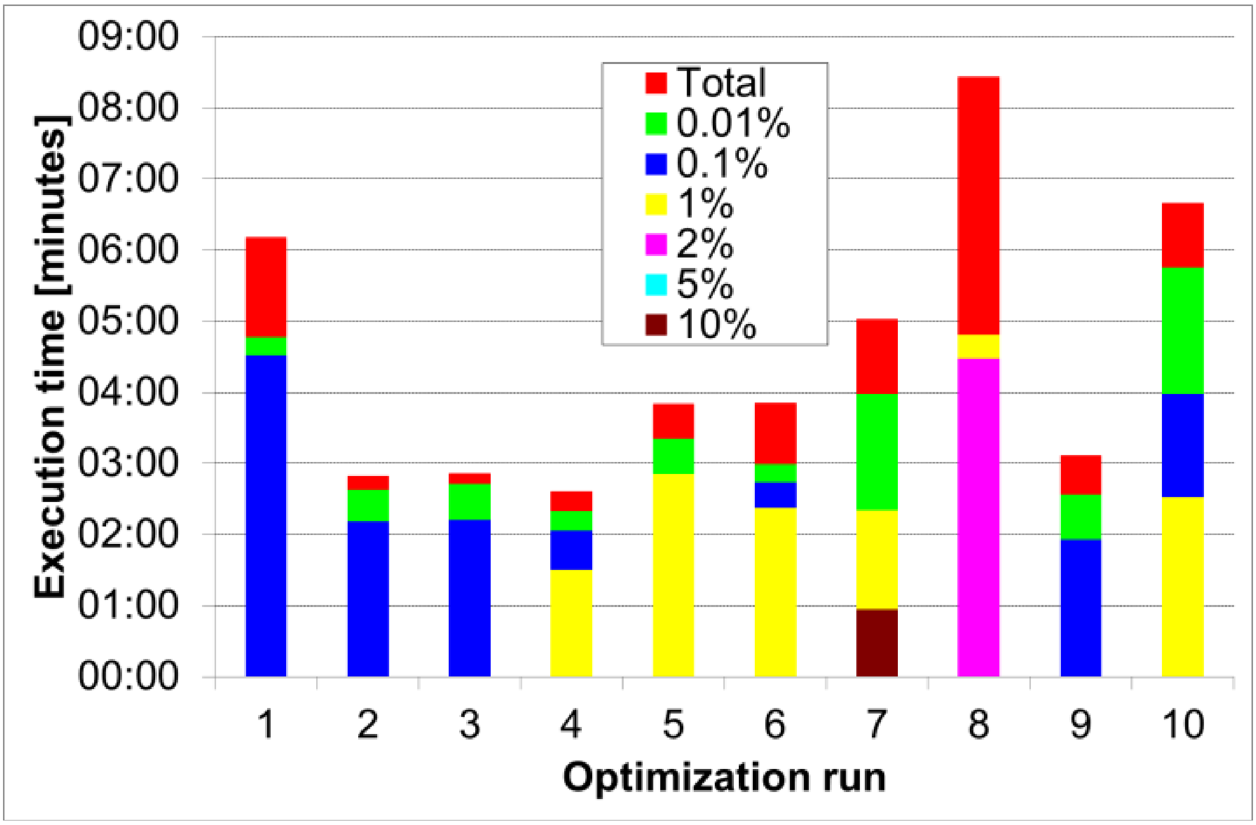

Figure 6. Execution times for Case 2 as a function of obtained precision.

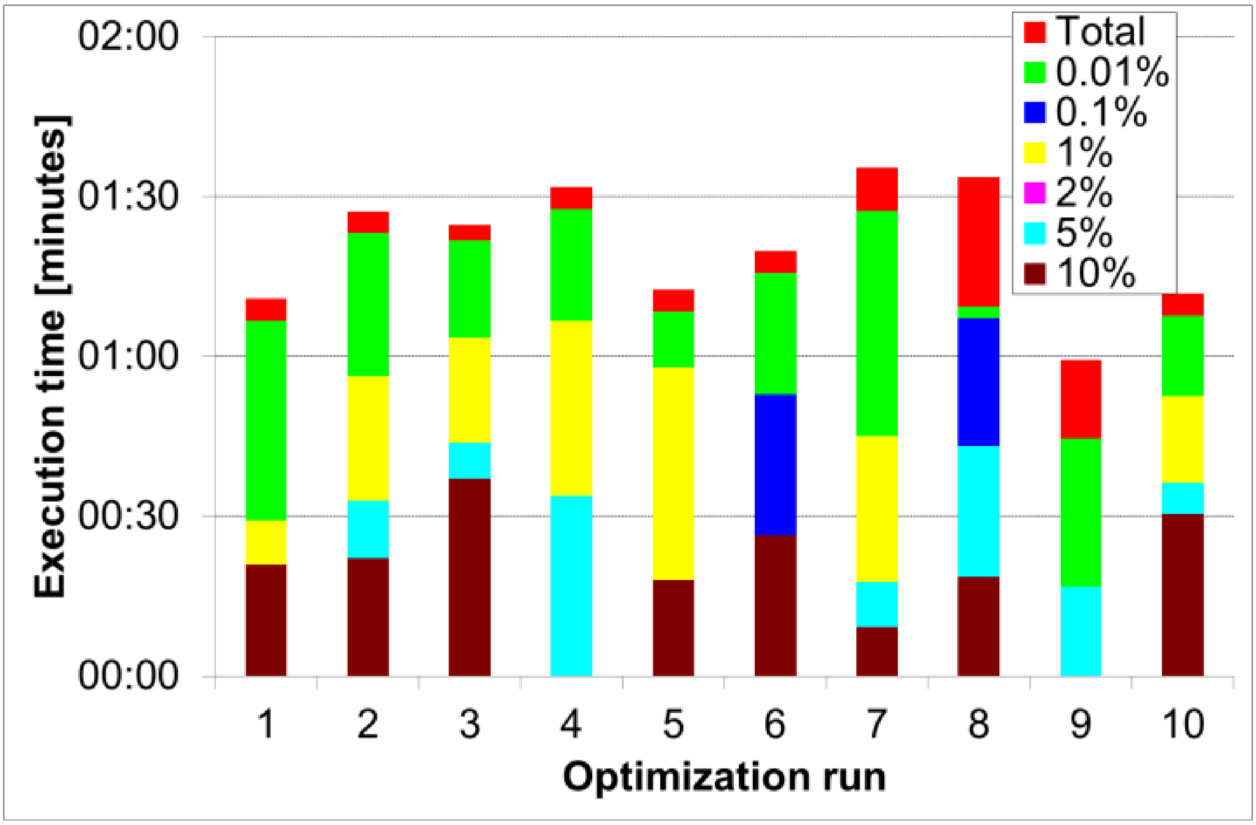

Figure 7. Execution times for Case 3 as a function of obtained precision

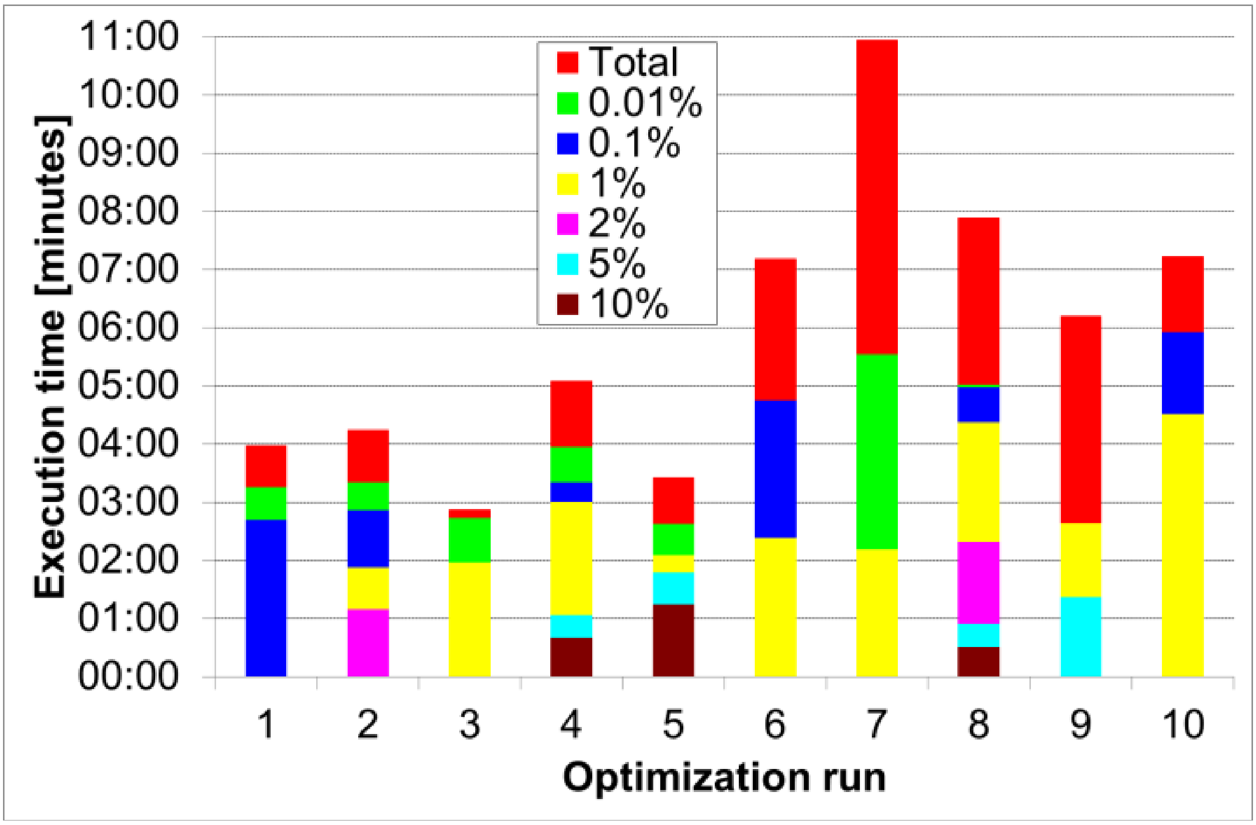

Figure 8. Execution times for Case 4 as a function of obtained precision

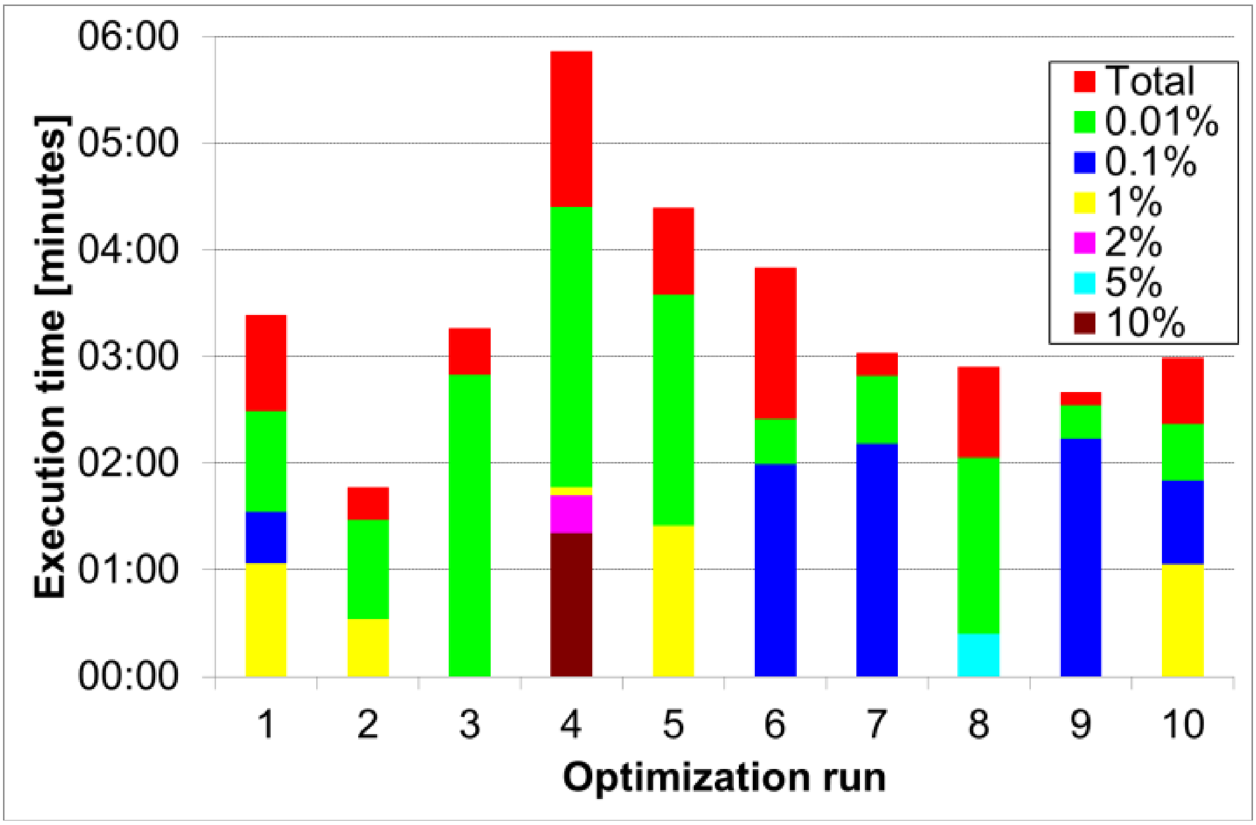

Figure 9. Execution times for Case 5 as a function of obtained precision

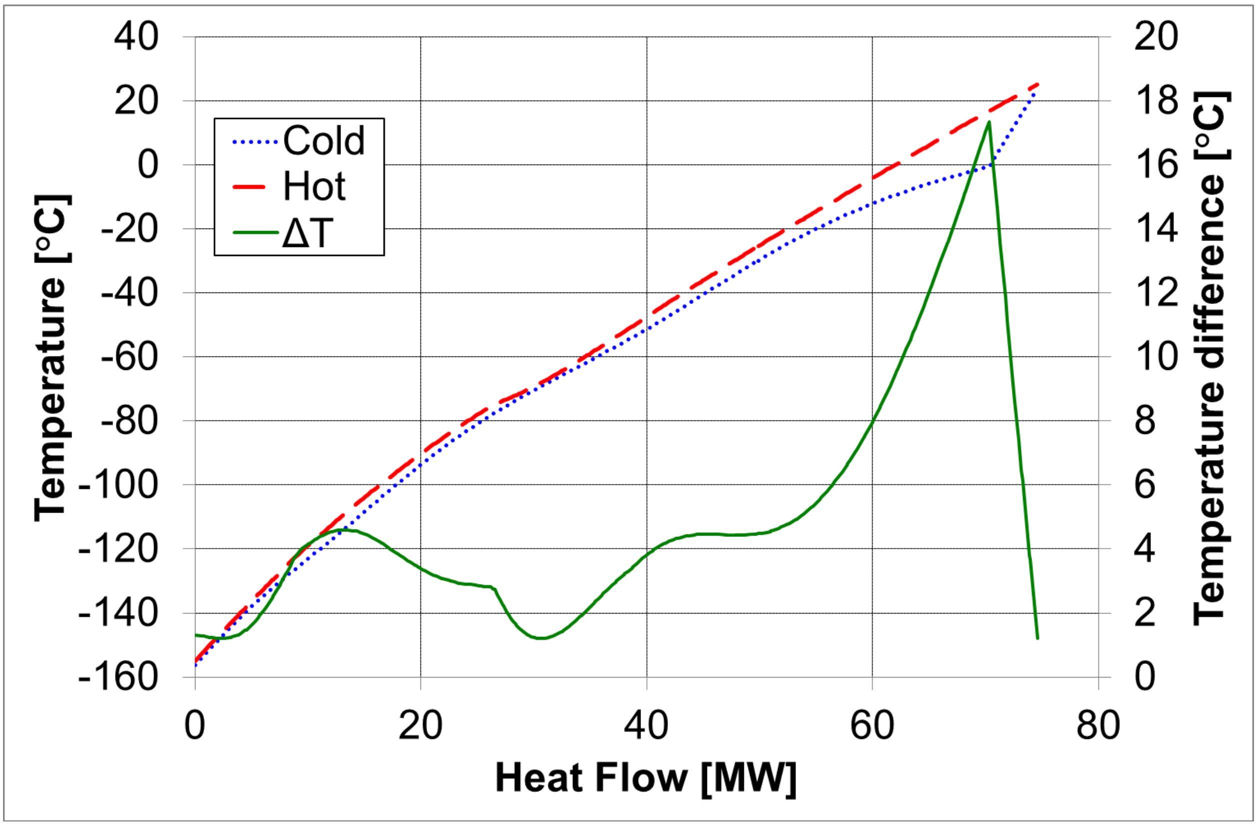

Figure 10. Temperature profile for Case 5

List of Tables

Table 1. Natural gas composition (mole percentage)

Component	*Case 1/Case 2*	*Case 3/Case 4*	*Case 5*
Nitrogen	0.37	0.00	2.80
Methane	95.89	88.80	89.79
Ethane	2.96	5.60	5.51
Propane	0.72	3.70	1.80
n-Butane	0.06	1.90	0.10

Table 2. Other conditions

Property	*Case 1 – Case 4*	*Case 5*
Natural gas feed temperature	20°C	25°C
Natural gas feed pressure	60 bar	55 bar
Natural gas feed flow rate	100 kg/s	1 kmol/s
Vapor fraction in LNG stream	0.0	-
Natural gas temperature after LNG heat exchanger	-	-155°C
High pressure refrigerant temperature after LNG heat exchanger	Equal to natural gas temperature after heat exchanger	
Pressure drop LNG heat exchanger: Natural gas	5 bar	5 bar
Pressure drop LNG exchanger: High pressure refrigerant	4 bar	4 bar
Pressure drop LNG exchanger: Low pressure refrigerant	1 bar	1 bar
Pressure drop external cooler	1 bar	1 bar
LNG product pressure	1.05 bar	1.1 bar
Adiabatic efficiency compressor	80%	80%

Table 3. Results from Aspelund et al. (2010) compared with simulations from this work in order to select thermodynamic system.

			Given ΔP			*Switched ΔP*		
	HX outlet temp [°C]	Compressor power [MW]	UA [MW/°C]	LMTD [°C]	MITA [°C]	UA [MW/°C]	LMTD [°C]	MITA [°C]
Initial								
Aspelund	-163.7	145.5	73.0	5.30	1.67	73.0	5.30	1.67
SRK	-163.8	144.7	18401.8	0.02	-2.17	74.0	5.23	1.63
PR	-164.0	142.8	-	-	1.47	60.3	6.26	2.41
Case 1								
Aspelund	-163.7	110.5	376.9	0.85	0.10	376.9	0.85	0.10
SRK	-163.8	110.4	2052.8	0.18	-4.66	574.8	0.65	0.02
PR	-164.0	108.8	661.0	0.55	-4.35	235.7	1.53	0.16
Case 2								
Aspelund	-163.7	144.4	48.6	6.80	2.93	48.6	6.80	2.93
SRK	-163.8	144.5	-	-	-0.64	49.0	6.76	2.88
PR	-164.0	142.2	263.1	1.23	0.10	43.4	7.42	3.26

Table 4. Lower and upper bounds for Case 1 to 4. The locations for the pressures are shown in Figure 1.

Component flow rates [kg/s]	*Lower*	*Upper*
Nitrogen	25.00	100.00
Methane	50.00	150.00
Ethane	100.00	250.00
Propane	0.00	100.00
n-Butane	150.00	300.00
Pressures [bar]		
P_1	2.00	5.00
P_2	20.00	50.00

Table 5. Lower and upper bounds for Case 5

Component flow rates [kmol/s]	*Lower*	*Upper*
Nitrogen	0.00	1.00
Methane	0.10	2.00
Ethane	0.10	2.00
Propane	0.00	2.00
n-Butane	0.00	2.00
Pressures [bar]		
P_1	2.00	6.00
P_2	10.00	30.00

Table 6. Solution for Case 1 (SRK) compared with Aspelund et al. (2010)

Case 1	*SRK*	*Aspelund*
Component flow rates [kg/s]		
Nitrogen	53.5	45.65
Methane	80.7	66.98
Ethane	234.5	175.47
Propane	0.0	15.74
n-Butane	265.0	204.77
Pressures [bar]		
P_1	4.1	3.55
P_2	23.6	31.26
Work [MW]	106.1	110.5
UA [MW/°C]	835.5	376.9
LMTD [°C]	0.56	0.85
MITA [°C]	0.10	0.10

Table 7. Solution for Case 2 (SRK) compared with Aspelund et al. (2010)

Case 2	*SRK*	*Aspelund*
Component flow rates [kg/s]		
Nitrogen	50.9	64.67
Methane	61.4	68.81
Ethane	148.5	154.50
Propane	0.0	14.45
n-Butane	181.8	164.47
Pressures [bar]		
P_1	2.3	3.2
P_2	44.7	52.4
Work [MW]	143.0	144.4
UA [MW/°C]	48.6	48.6
LMTD [°C]	6.6	6.8
MITA [°C]	2.6	2.9

Table 8. Solution for Case 3 (SRK) compared with Aspelund et al. (2010)

Case 3	*SRK*	*Aspelund*
Component flow rates [kg/s]		
Nitrogen	48.3	-
Methane	70.8	-
Ethane	175.6	-
Propane	2.7	-
n-Butane	226.2	-
Pressures [bar]		
P_1	4.5	-
P_2	26.8	-
Work [MW]	90.3	91.4
UA [MW/°C]	1022	538
LMTD [°C]	0.4	0.7
MITA [°C]	0.1	0.1

Table 9. Solution for Case 4 (SRK) compared with Aspelund et al. (2010)

Case 4	*SRK*	*Aspelund*
Component flow rates [kg/s]		
Nitrogen	50.1	-
Methane	55.9	-
Ethane	138.5	-
Propane	0.0	-
n-Butane	180.1	-
Pressures [bar]		
P_1	2.7	
P_2	44.2	-
Work [MW]	125.5	122.7
UA [MW/°C]	48.6	48.6
LMTD [°C]	6.2	6.2
MITA [°C]	2.6	2.6

Table 10. Optimized values for Case 5 compared with Jensen and Skogestad (2006)

Component flow rates [kmol/s]	*Optimized*	*Jensen and Skogestad*
Nitrogen	0.29	0.24
Methane	0.91	0.74
Ethane	1.21	?
Propane	0.00	0.00
n-Butane	0.71	?
Pressures [bar]		
P_1	4.34	3.23
P_2	25.97	?