Optimization of a single expander LNG process

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Abstract

A single expander process with nitrogen as refrigerant has been optimized for liquefaction of natural gas. Comparisons have been made between a simplified process model assuming constant specific heat capacities and ideal gas behavior for the refrigerant, and a rigorous model employing the Soave-Redlich-Kwong equation of state. For the simplified model, equations have been developed that enable an analytical solution to the optimization problem. Quite surprisingly, there is good agreement between the models when the minimum temperature difference is small. For the remaining cases, better solutions are obtained from the rigorous model accounting for the non-ideal behavior of the refrigerant.

Keywords: LNG; Single expander; Optimization; Process modelling

1. Introduction

Liquefied natural gas (LNG) is an energy carrier preferred over pipeline transmission for long transport distances and/or small to moderate gas volumes. By liquefaction at near-atmospheric pressure, the volume of natural gas is reduced by a factor of about 600 compared to standard conditions. This enables overseas transport of large quantities by LNG carriers.

According to BP [1], the global natural gas consumption is projected to grow 1.9 \% per annum from 2012 to 2035. By 2035, LNG is expected to account for 15 \% of the global natural gas consumption and around 46 \% of the total natural gas trade [1]. Since the amount of natural gas resources accessible via existing infrastructure and

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production technology is declining, there has been an increasing interest in remote gas production [2]. However, as marginal resources cannot justify the cost of developing fixed infrastructures [2], offshore floating LNG production has emerged as a cost-effective alternative [3].

Liquefaction of natural gas requires energy intensive cooling over a wide temperature range, and there is a close link between process energy efficiency and operating cost. However, while energy efficiency is arguably the most important criterion for the selection of liquefaction technology in large onshore LNG plants, other properties such as safety, compactness, reliability and simplicity must be taken into account when selecting process concepts for floating LNG [4-5].

Despite lower energy efficiency than other LNG process concepts, nitrogen expander processes possess qualities that are interesting for offshore applications [3]. Since nitrogen is an inert gas, risks associated with flammable refrigerant inventory can be avoided [5]. Problems related to vapor-liquid distribution in heat exchangers are eliminated as the refrigerant is maintained in gas phase throughout the refrigeration cycle [3]. In addition, expander processes are generally simple, reliable and easily operated [3]. In comparison with a single mixed-refrigerant process and a propane-precooled mixed-refrigerant process, Li and Ju [6] found a nitrogen expander process to be a better alternative for offshore LNG production.

Energy efficient low-temperature refrigeration requires small driving forces in heat transfer. With small temperature differences, rigorous thermodynamic models are required for LNG process modelling in order to guarantee practical feasibility of the design. Simplified models may, however, serve as a useful tool in a preliminary phase of the design, for instance by reducing the search space.

The ideal gas equation of state does not apply to real gases. Unlike real gases, the specific enthalpy of an ideal gas depends only on temperature. However, if the pressure is small compared to the critical pressure and/or the temperature is high compared to the critical temperature, the behavior of a real gas approaches ideal gas behavior. In addition, some chemical components behave more ideal than others. Depending on operating conditions, the ideal gas assumption may work well for nitrogen, which has critical temperature \( T_c = 126 \text{ K} \) and pressure \( p_c = 34 \text{ bar} \) [7].

Various studies have been performed on optimization of expander processes for low-temperature applications such as natural gas liquefaction, both using simplified and rigorous thermodynamics. Marmolejo-Correa and Gundersen [8] used a procedure combining pinch analysis and exergy analysis to design a single expander process for liquefaction of natural gas. The nitrogen refrigerant was assumed to behave like an ideal gas with constant specific heat capacity. Wechsung et al. [9] also used the ideal gas model for optimization of an expander LNG process, assuming constant specific heat for the different process streams.

Li et al. [10] used a genetic algorithm to maximize the exergy efficiency of an expander process with helium as refrigerant. The process, used for liquefaction of different pure substances, was modelled using accurate thermodynamic properties from the National Institute of Standards and Technology (NIST). Thermodynamic data from NIST were also used by Chang et al. [11] when studying the influence of different design parameters on the performance of a single nitrogen expander process for methane liquefaction.
In this work, the net power consumption of a single expander process with nitrogen as refrigerant has been minimized using two different process models for the refrigerant, with different values of the isentropic efficiency and the minimum temperature difference. A simple model assuming perfect gas behavior (ideal gas with constant specific heat capacity) has been optimized analytically, while a rigorous process model has been simulated with the Soave-Redlich-Kwong equation of state and optimized using a sequential quadratic programming method.

2. Problem formulation

A single expander process for liquefaction of natural gas was optimized with the objective of minimizing net power consumption, subject to a minimum temperature difference $\Delta T_{\text{min}}$ in the heat exchangers. The refrigerant used was nitrogen. Constant isentropic efficiencies $\eta_{\text{COMP}}$ and $\eta_{\text{EXP}}$ were assumed for the compressor and expander. The pressure levels were constrained within 1 and 120 bar. Pressure drop in heat exchangers was neglected. The natural gas properties are given in Table 1.

Table 1. Natural gas properties.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Unit</th>
<th>Value</th>
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<tr>
<td>Flow rate $\dot{m}_{\text{NG}}$</td>
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</tr>
<tr>
<td>Feed pressure $p_t$</td>
<td>bar</td>
<td>55</td>
</tr>
<tr>
<td>Feed temperature $T_I$</td>
<td>K</td>
<td>293.15</td>
</tr>
<tr>
<td>Product temperature $T_{\text{III}}$</td>
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<td>Nitrogen</td>
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A process flowsheet is given in Fig. 1. The natural gas is cooled in two stages by a vapor phase refrigerant. In order to obtain the cooling temperature required, the refrigerant itself is precooled in the first heat exchanger, before the refrigerant is expanded to reduce the temperature. By assuming a constant outlet temperature of the cooler ($T_3 = T_I$) and uniform exit temperatures for the first heat exchanger ($T_4 = T_{\text{II}}$), four degrees of freedom were available for the design optimization. An obvious choice of decision variables may be the low and high pressure levels $p_L$ and $p_H$ of the refrigerant, the refrigerant flow rate $\dot{m}_R$ and the stage temperature $T_{\text{II}}$. However, different choices of decision variables were made for the two process models.

Fig. 1. Process flowsheet for a single expander LNG process.
2.1. Simplified model

In the simplified model, the refrigerant was assumed to behave as a perfect gas (ideal gas with constant specific heat \( c_p, R \)). The natural gas was modelled with a constant heat capacity \((m_r c_p)_\text{NG}\) equal to the mean value of the heat capacity in the rigorous model. The simplified model was optimized analytically.

2.2. Rigorous model

The rigorous process model was simulated in Aspen HYSYS\textsuperscript{®} (Aspen Technology Inc., V7.3) using the Soave-Redlich-Kwong equation of state. Optimization was carried out with the sequential quadratic programming algorithm NLPQLP \[12\] using a multi-start approach from random starting points.

3. Simplified model

3.1. Modelling

Figure 2. Composite curves for the simplified model of a single expander LNG process.

The refrigerant flow rate is given by an overall energy balance for the two heat exchangers:

\[
\dot{m}_R = \frac{(m \cdot c_p)_\text{NG} \cdot (T_i - T_{\text{II}})}{c_{p, R} \cdot (T_{\text{II}} - T_{\text{III}} + \Delta T_{\text{cold}} - \Delta T_{\text{hot}})}.
\]

This can further be used to calculate the expansion power from an energy balance for the expander, given that \(\Delta h = c_p \cdot \Delta T\) for a perfect gas:

\[
\dot{W}_\text{EXP} = (m \cdot c_p)_\text{NG} \cdot (T_i - T_{\text{III}}) \cdot \frac{T_{\text{II}} - T_{\text{III}} + \Delta T_{\text{cold}}}{T_{\text{II}} - T_{\text{III}} + \Delta T_{\text{cold}} - \Delta T_{\text{hot}}}.
\]
From the definition of isentropic efficiency for an expansion process, the isentropic expansion temperature (expander discharge temperature in the case of isentropic expansion) may be formulated as

$$T_{s,\text{EXP}} = \frac{T_{\text{II}} \cdot (\eta_{s,\text{EXP}} - 1) + T_{\text{III}} - \Delta T_{\text{cold}}}{\eta_{s,\text{EXP}}}.$$  \hspace{1cm} (3)

For a perfect gas, the entropy change between two states 1 and 2 is given by

$$\Delta s_{1 \rightarrow 2} = c_p \cdot \ln \frac{T_2}{T_1} - R \cdot \ln \frac{p_2}{p_1}.$$  \hspace{1cm} (4)

Hence, the pressure ratio of the refrigerant can be expressed as

$$\frac{p_\text{II}}{p_\text{L}} = \left( \frac{T_{\text{II}} \cdot (\eta_{s,\text{EXP}} - 1) + T_{\text{III}} - \Delta T_{\text{cold}}}{T_{\text{II}} \cdot (\eta_{s,\text{EXP}} - 1) + T_{\text{III}} - \Delta T_{\text{cold}}} \right)^{\frac{c_p R}{R}}.$$  \hspace{1cm} (5)

where $p_\text{L}$ and $p_\text{II}$ are the low and high pressure levels of the refrigerant, respectively. When the refrigerant pressure ratio is known, the isentropic compressor discharge temperature may be calculated from the definition of the entropy change:

$$T_{s,\text{EXP}} = \frac{(T_{\text{I}} - \Delta T_{\text{heat}}) \cdot (T_{\text{II}} - T_{\text{III}} + \Delta T_{\text{cold}} - \Delta T_{\text{heat}} \cdot \eta_{s,\text{EXP}} - 1)}{(T_{\text{II}} - T_{\text{III}} + \Delta T_{\text{cold}} - \Delta T_{\text{heat}} \cdot \eta_{s,\text{EXP}} - 1)}.$$  \hspace{1cm} (6)

Further, the compression power can be calculated from an energy balance for the compressor:

$$W_{\text{COMP}} = \frac{(m \cdot c_p)_{\text{NG}} \cdot (T_{\text{II}} - T_{\text{III}}) \cdot (T_{\text{II}} - T_{\text{III}} + \Delta T_{\text{cold}})}{\eta_{s,\text{COMP}} \cdot (T_{\text{II}} - T_{\text{III}} + \Delta T_{\text{cold}})} \left( \frac{T_{\text{II}} \cdot (\eta_{s,\text{EXP}} - 1) + T_{\text{III}} - \Delta T_{\text{cold}}}{(T_{\text{II}} - T_{\text{III}} + \Delta T_{\text{cold}}) \cdot (\eta_{s,\text{EXP}} - 1) + T_{\text{III}} - \Delta T_{\text{cold}}} - 1 \right).$$  \hspace{1cm} (7)

The net power consumption is then given as the difference between the compression and expansion power:

$$W_{\text{NET}} = \frac{(m \cdot c_p)_{\text{NG}} \cdot (T_{\text{II}} - T_{\text{III}}) \cdot (T_{\text{II}} - T_{\text{III}} + \Delta T_{\text{cold}})}{T_{\text{II}} - T_{\text{III}} + \Delta T_{\text{cold}} - \Delta T_{\text{heat}}} \left( \frac{T_{\text{II}} \cdot (\eta_{s,\text{EXP}} - 1) + T_{\text{III}} - \Delta T_{\text{cold}}}{(T_{\text{II}} - T_{\text{III}} + \Delta T_{\text{cold}}) \cdot (\eta_{s,\text{EXP}} - 1) + T_{\text{III}} - \Delta T_{\text{cold}}} - 1 \right).$$  \hspace{1cm} (8)

Fig. 3. (a) Refrigerant flow rate (blue) and pressure ratio (red) plotted as functions of the stage temperature in the simplified process model; (b) Net power consumption plotted as a function of the stage temperature in the simplified process model.
In Fig. 3 (a), the refrigerant flow rate \( \dot{m}_R \) and the pressure ratio \( p_H/p_L \) are given as functions of the stage temperature \( T_{II} \) for the case with \( \Delta T_{\text{hot}} = \Delta T_{\text{cold}} = \Delta T_{\text{min}} = 2 \) K and \( \eta_{\text{s,COMP}} = \eta_{\text{s,EXP}} = 0.80 \). The stage temperature is assumed equal to the temperature of the refrigerant after precooling in the first heat exchanger. With decreasing stage temperature, the cooling load induced by refrigerant precooling increases, hence the refrigerant flow rate increases. As the stage temperature approaches the target temperature of the natural gas \( (T_{III}) \), the refrigerant flow rate goes to infinity, as can be seen from Eq. (1) for the case where \( \Delta T_{\text{cold}} = \Delta T_{\text{hot}} \).

The refrigerant pressure ratio is given by the temperature drop required in the expander, and thereby decreases with decreasing stage temperature. As increasing pressure ratio and decreasing refrigerant flow rate have opposite effects on the net power consumption, the optimal stage temperature is given as a balanced trade-off between these two effects. The net power consumption is given as a function of the stage temperature in Fig. 3 (b).

### 3.2. Optimization

From thermodynamic principles it is given that the heat transfer irreversibilities and thereby the process power consumption is minimized when the heat transfer driving forces are minimized. Hence, the temperature differences \( \Delta T_{\text{hot}} \) and \( \Delta T_{\text{cold}} \) should be equal to the minimum required. For reasonable values of the process parameters, this can be confirmed mathematically.

From basic calculus, the optimal stage temperature \( T_{II} \) can be derived analytical as a function of the minimum temperature difference and the isentropic efficiencies for the compressor and expander. Since the final expression is rather complex, the optimization results are only given graphically. As can be observed in Eq. (8), the net power consumption is independent of the specific heat capacity of the refrigerant and proportional to heat capacity flow rate of the natural gas. Hence, the optimal stage temperature is independent of these variables.

In Fig. 4 (a), the optimal stage temperature is plotted as a function of the minimum temperature difference \( (\Delta T_{\text{hot}} = \Delta T_{\text{cold}} = \Delta T_{\text{min}}) \) and the isentropic efficiency \( (\eta_{\text{s,COMP}} = \eta_{\text{s,EXP}} = \eta_s) \). The resulting net power consumption is given in Fig. 4 (b). The optimal stage temperature increases with both increasing \( \Delta T_{\text{min}} \) and \( \eta_s \). As one would expect, increasing temperature driving forces in the heat exchangers leads to increased irreversibilities in heat transfer and thereby increased power consumption. With increasing isentropic efficiency for the compressor and expander, the net power consumption is reduced.

With increasing minimum temperature difference, the heat transfer driving forces will increase. Hence, in order to reduce the power consumption, the design should shift to a smaller refrigerant flow rate and a higher pressure ratio. As illustrated in Fig. 3 (a), this is done by increasing the stage temperature. This is confirmed by the results given in Fig. 5, where the optimal refrigerant flow rate \( \dot{m}_R \) and the optimal pressure ratio \( p_H/p_L \) are plotted as functions of \( \Delta T_{\text{min}} \) and \( \eta_s \). For increasing values of \( \Delta T_{\text{min}} \), the optimal flow rate is reduced while the optimal pressure ratio is increased.
Thermodynamic analysis suggests that with increasing isentropic efficiency, the compression/expansion processes become more efficient, hence the optimal balance between pressure ratio and refrigerant flow rate should be shifted towards decreasing flow rate and increasing pressure ratio. This relation is confirmed by the results in Fig. 5, as the optimal refrigerant flow rate decreases with increasing isentropic efficiency while the optimal pressure ratio increases. As can be observed in Fig. 4 (a), increased isentropic efficiency leads to increasing optimal stage temperature.

4. Rigorous model

For the rigorous process model, both the heat capacity of the natural gas and the refrigerant are assumed to be functions of temperature and pressure. In this case, it is not necessarily given that the smallest temperature differences will be observed in the end points of the composite curves.

For the rigorous process model, refrigerant flow rate $\dot{m}_R$, stage temperature $T_{II}$, pressure ratio $p_H/p_L$ and one of the pressure levels ($p_L$ or $p_H$) were used as decision variables. By employing the pressure ratio as a variable, opposed to using both pressure levels, wide bounds can be used for both pressure levels without risk of crossover ($p_H < p_L$).
For the different cases studied, two different noticeable local solutions were observed in the multi-start approach; one with the low pressure level at the lower bound \( (p_L = 1 \text{ bar}) \) and one with the high pressure level at the upper bound \( (p_H = 120 \text{ bar}) \). The two different solutions are plotted in Fig. 6 for different values of the minimum temperature difference and the isentropic efficiency. As can be observed, the solutions with \( p_L = 1 \text{ bar} \) are slightly better for low values of both \( \Delta T_{\text{min}} \) and \( \eta_s \). However, since the power consumption of the solutions with \( p_H = 120 \text{ bar} \) grow less with increasing temperature difference, these solutions are better for high values of \( \Delta T_{\text{min}} \).

### 5. Comparison

As can be observed in both Fig. 4 and Fig. 6, the net power consumption is very sensitive to the isentropic efficiency of the compressor and the expander. With reduced isentropic efficiency, for the same inlet temperatures and pressure ratios, the compressor consumes more power while the expander produces less. Hence, the ratio of expander power to compressor power is significantly reduced. Assuming the stage temperature (inlet temperature of the expander) is the same, the pressure ratio must be increased in order to obtain the required outlet temperature when the isentropic efficiency is reduced. Only small changes will be observed for the actual expansion power (for the simplified model it will remain exactly the same) since both inlet and outlet temperatures of the expander remain the same. Increased pressure ratio will, however, lead to increased compression power as the compressor discharge temperature increases. These two effects (reduced ratio of expansion power to compression power and increased pressure ratio for the same stage temperature) both contribute to increased net power consumption. The effects of reduced isentropic efficiency are somewhat compensated in the optimal design by reducing the stage temperature and thereby also the pressure ratio, but a significant increase in net power consumption is still observed.

<table>
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<tr>
<th>( \Delta T_{\text{min}} ) (K)</th>
<th>( \eta_s ) (-)</th>
<th>Simplified</th>
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<th>Rigorous</th>
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In Table 2, the best results obtained for the rigorous process model are compared with results from the simplified model. For all except four cases, the solution with \( p_H = 120 \text{ bar} \) is best for the rigorous model. In general, the solutions with \( p_H = 120 \text{ bar} \) are characterized by a small refrigerant flow rate and a high pressure ratio, when
compared to the solutions with $p_L = 1$ bar. As discussed for the simplified model, high refrigerant flow rate and low pressure ratio is beneficial for small values of both $\Delta T_{\text{min}}$ and $\eta_r$.

As can be observed in Table 2, for the best solutions obtained with the rigorous model, the temperature differences in both ends of the composite curves are equal to the minimum required for all cases except $\eta_r = 1$. This means that the assumption of a constant heat capacity for the natural gas in the simplified model does not affect the results. For the theoretical case of $\eta_r = 1$, the temperature difference in the hot end is higher than the minimum required. In this case, the best solution is obtained for $T_H = T_L$. Hence, there is no refrigerant precooling and natural gas cooling makes up the cold composite curve.

For the cases where $p_L = 1$ bar provides the best design, the stage temperature of the rigorous model is close to the optimal value for the simplified model, with a slightly higher net power consumption. In the cases where the solution with $p_H = 120$ bar is found to be best for the rigorous model, the optimal stage temperature is significantly different for the two models. In these cases, the net power consumption is smaller for the rigorous model.

In the solutions for the rigorous model where $p_L = 1$ bar, the specific heat capacity of the nitrogen refrigerant is near constant throughout the cycle and the compressibility factor is close to unity. Hence, the assumptions of the simplified process model are close to fulfilled, confirming the similarity of the results. Even closer resemblance with the perfect gas model is observed if a smaller low pressure level is allowed. For the case with $p_H = 120$ bar, both the specific heat capacity and the compressibility factor vary significantly in the different unit operations. Due to considerable deviation from ideal behavior, large differences are observed in the results obtained for the two models.

Since the rigorous model accounts for the non-ideality of the refrigerant, significantly better solutions are found for the cases where $p_H = 120$ bar provides the best result.

6. Conclusions

A single expander process for liquefaction of natural gas has been modelled and optimized using both a simplified (perfect gas) and a rigorous (cubic equation of state) thermodynamic model. In the case of the simplified model, equations have been derived for net power consumption and optimized analytically without need of iteration or search procedures. Optimization of the rigorous process model has been performed using a sequential quadratic programming method.

For small values of the minimum temperature difference in the heat exchangers and low to moderate values of the isentropic efficiency for the compressor and expander, the optimization results for the simplified model are in close agreement with the rigorous model, and the behavior of the refrigerant is close to ideal. This suggests that a simplified thermodynamic model could be a useful tool for early stage screening of nitrogen expander processes. For the majority of the cases studied, however, the best results obtained for the rigorous model are significantly different from the optimal solution found for the simplified model. The non-ideality of the refrigerant is taken into account and a solution with considerable savings in net power consumption is found. The results indicate that the simplified model gives a good estimate of the best solution when the trade-off between refrigerant flow rate and accou}

driving forces, the total cooling load and thereby the heat exchanger size is significantly larger for solutions with $p_L = 1$ bar than for solutions with $p_H = 120$ bar. The compressor investment cost would also be affected, as the volumetric flow rate of the compressor suction stream is significantly higher. A design operating at low pressure is also more prone to be affected by pressure drop in heat exchangers.

Methane and nitrogen-methane mixtures are alternative refrigerants in expander processes for liquefaction of natural gas. The simplified process model is general and would therefore apply to any refrigerant behaving like a perfect gas under the given operating conditions. While the refrigerant flow rate and pressure ratio will change if the specific heat capacity is different (see Eqs. (1) and (5)), the optimal stage temperature will remain the same irrespective of the refrigerant. Methane has a higher critical temperature ($T_c \approx 191$ K [7]) than nitrogen, suggesting that methane or a nitrogen-methane mixture is less likely to fulfill the prerequisites of the simplified process model than a pure nitrogen refrigerant. The critical pressure ($p_c \approx 46$ bar [7]) is, however, also higher than for methane.
In this work, compression is assumed to take place in a single stage. For many of the cases studied, the pressure ratio of the refrigerant would require compression in two or more stages. Multi-stage compression with intercooling will necessarily lead to different solutions. For future work, the process model should also be extended to a dual expander cycle, as this is more relevant for industrial applications. Dual expansion provides better matching of the composite curves, which leads to improved energy efficiency and stricter requirements on the accuracy of the thermodynamic models. With closer matching of the composite curves, it is more likely that the assumption of a constant heat capacity flow rate for the natural gas will affect the results. In the simplified model, this could be accommodated by dividing the cooling curve of the natural gas stream in segments with constant heat capacity, like in the approach presented by Marmolejo-Correa and Gundersen [8].

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