Conceptual Process Design and Optimization of Refrigeration Cycles for the Liquefaction of Boil-off Gas

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Improving thermodynamic efficiency for refrigeration cycles is one of the key elements in conceptual process design activities for achieving cost-effective and sustainable production of liquefied natural gas. Various structural and heat recovery options are available for the design of refrigeration cycles, with which shaft power required to drive compressors is attempted to be minimized. Choice of refrigerants to be employed is another important degree of freedoms in a process design of refrigeration cycles. Hence, systematic investigation in a holistic manner is required to screen different liquefaction technologies and evaluate their techno-economic impacts. In this study, the focus is made to gain conceptual understanding in the design of liquefaction processes for boil-off gas. The current study aims to provide guidelines for the selection of the most appropriate technologies for the application of boil-off gas liquefaction as well as for determining optimal design and operating conditions of refrigeration cycles. A heat-integrated design framework is adopted in this work to evaluate energy efficiency in a systematic manner, while optimization methods are applied to systematically determine the most appropriate operating conditions for the liquefaction cycles. From the case study with 1 ton/day of liquefaction capacity, it was found that the power consumption for a single mixed refrigerant cycle is about 12% less than that of an N2 expander cycle.

1. Introduction

Handling of boil-off natural gas is a major design issue in natural-gas-fuelled ships because evaporation of some portion of liquefied natural gas is inevitable during a voyage. Cost-effective and sustainable handling boil-off natural gas becomes important, due to the stricter environmental regulations to be introduced as well as severe competition existing in maritime and shipping businesses. The practical option to deal with boil-off gas is to introduce boil-off gas re-liquefaction systems with which the pressure of the LNG tank is maintained without natural loss. A wide range of processes for boil-off gas liquefaction systems are available and each process is differentiated, based on the choice of refrigerant fluid, methods to generate sub-ambient temperature and/or configuration of refrigeration cycles. Understanding such design issues is important to achieve high energy efficiency of the liquefaction cycle, as shaftpower consumption for the compressor is heavily dependent on cycle configuration and refrigerant fluid.

In addition to structural design options available for the liquefaction cycles, operating conditions is also to be rigorously screened and optimal operating conditions should be selected to minimize thermodynamic inefficiency. Appropriate selection of operating conditions through process design is specific to the given configuration of liquefaction processes and, hence, the selection of cycle configuration and refrigerant fluid should be considered simultaneously with the choice of operating conditions. In order to improve energy efficiency for the refrigeration cycle, heat integration methods have been widely used (Klemes et al., 2014). Exergy analysis has also been used to systematically identify inefficient subsystems (Raei, 2011), while automated approaches based on mathematical optimization techniques (Sharma et al., 2014) have been widely applied for the design of refrigeration cycles.
Considerable efforts have been made to the design and optimization of boil-off gas liquefaction systems, for example reverse Brayton cycle by Romero et al. (2012), N2 expander cycle by Lee et al. (2009), and cascade refrigeration cycle by Tan et al. (2016) and Romero et al. (2015). However, most of the previous studies mainly focused on large shipping applications, for example LNG carriers. This study focused on small-scale applications in which relatively small amount of LNG, as fuel, is used. One recent work on small-scale systems was carried out by Kwak et al. (2018) who developed a process design and optimization framework for boil-off gas re-liquefaction process. However, their study was limited to the nitrogen-based expander cycle. Hence, in this study it is aimed to design and optimize three different processes for boil-off gas liquefaction systems; nitrogen expander cycle, SMR (Single Mixed Refrigerants) cycle and two-level cascaded cycle. Energy efficiency of these three processes will be systematically compared and their techno-economic impact will be discussed in a holistic manner. This study allows new contribution to the knowledge through the case study in which systematic analysis for improving energy efficiency for liquefaction cycles has been made. Also, this study provides conceptual insights and design guidelines in the design of BOG liquefaction systems, with which high sustainability and cost-effectiveness can be achieved.

2. Improving energy efficiency of boil-off gas liquefaction processes

Simple refrigeration cycles using a single refrigerant fluid, as shown in Figure 1a, can be used for liquefying boil-off gas, but achieving high thermodynamic efficiency may be limited because of the limited range of operating conditions. Various design options can be considered: A refrigerant fluid employed in the simple cycle can be replaced by a different fluid with which less shaftpower is consumed. Furthermore, a mixture of refrigerant fluids can be used, with which better match for the heat exchange between boil-off gas to be liquefied and evaporating stream of refrigerant fluids can be obtained (Figure 1b). Selection of working fluids and their compositions is dependent on the operating conditions and the composition of boil-off gas stream, which is typically determined through rigorous process optimization.

![Diagram of single and mixed fluids for a simple refrigeration cycle](image)

Figure 1: Use of single and mixed fluids for a simple refrigeration cycle

Working fluids used in the refrigeration cycle may be selected such that the refrigeration cycle is operated below critical conditions and the evaporation of refrigerant enables sub-ambient cooling (i.e. the compressed refrigerant gas after the compressor is condensed below critical conditions and becomes saturated or subcooled liquid before expanding it through an expander or a valve.). However, the whole refrigeration cycle can be operated in gaseous conditions, in which the heat of boil-off gas stream to be cooled is removed by low-temperature refrigerant gas through sensible heat transfer. Nitrogen is a typical working fluid for such cycles operating in gaseous conditions and, in general, the expander is used for expanding high pressure nitrogen gas.
to generate low-temperature conditions. The power is also recovered through the expander, which is utilized in the compressor. The provision of cooling for boil-off gas may be done either with a single stage or double stages configuration (Figure 2a).

Another option for improving energy efficiency of the refrigeration cycle is to consider multi-level cascaded cycles (Figure 2b). It is not energy-efficient to cover a wide range of sub-ambient conditions using a single working fluid for the refrigeration cycle, because of the lengthy thermodynamic path for the compression between evaporation level and condensation level. As discussed in Smith (2016), thermodynamic efficiency of the refrigeration cycle is fluid dependent due to the difference in location of the critical point and shape of the phase diagram for each candidate refrigerant fluid. This implies that working fluids should be selected based on operating temperature to be cooled. Hence, refrigeration cycles can be designed such that the operating range is divided, and a single working fluid is adequately selected for each cycle as illustrated in Figure 2b. For maximizing energy efficiency (i.e. minimizing shaftpower requirements), a number of cycles are necessary by having small temperature range for each refrigeration cycle, at the expense of system complexities and heavy capital investment. Hence, balance should be sought between energy efficiency and system complexity when the number of refrigeration cycles are determined.

Figure 2: Design options for a simple refrigeration cycle (Smith, 2016)

As discussed above, various structural options are available for the design of boil-off gas liquefaction systems and different processes are being offered. Hence, it is required to evaluate different liquefaction systems in a common design basis and evaluate their technical benefits and shortcomings in a holistic manner. In order to systematically assess energy efficiency of various liquefaction processes, heat integration techniques are used in this study. Energy composite curves and grand composite curves are constructed for cycles, with which thermodynamic differences in cooling methods can be effectively compared and any inefficient elements/options in the design can be rigorously examined (Kwak et al., 2012).

3. Case Study: Process Modeling, Simulation and Design

1 ton/day of boil-off gas to be liquefied is selected, which is a typical capacity for on-board small-scale boil-off gas liquefaction systems. Boil-off gas feed to be liquefied is taken from Ryu et al. (2016). The molar composition is 95.5% of methane, 1% of ethane and 3.5% of nitrogen, while the feed is supplied at 510 kPa and 100 °C. The cycle is designed for saturated liquid conditions the product gas stream at the pressure of 110 kPa. The process is designed to minimize shaftpower requirement for compressors used for the refrigeration cycle and boil-off gas compression. Minimum approach temperature for heat exchange is assumed to be 3 °C. Isentropic efficiency for the compressor is taken as 75%, while gas streams after intercoolers of multi-stage compression is assumed to be at 40 °C. Aspen HYSYS® is used for modelling and simulation of refrigeration cycles, in which the Peng-Robinson EOS (Equation of State) is selected for thermodynamic calculations. Three processes modelled and simulated in the case study are presented in Figure 3.

The two-level cascaded cycle in this study is designed with ethylene for the lower temperature cycle and propylene for the higher temperature cycle. It should be noted that the choice of working fluids for cascaded cycles is a degree of freedom in the design of the refrigeration cycle. Also, this two-level cascaded cycle is designed for liquefying boil-off gas to be in the temperature range of -100 °C, while the N2 expander cycle and the SMR cycle are designed to cool the gas to around -160 °C.
Process design for the liquefaction systems is carried out with an optimization framework developed by Kwak et al. (2018), in which the process simulator is strategically linked and interacting with a GA (genetic algorithms) solver available in MATLAB® optimization toolbox. The decision variables for the liquefaction process are generated with MATLAB® which are then simulated with Aspen HYSYS®. With simulation results, MATLAB® evaluates the objective function and suggests new decision variables for the simulation. This iterative procedure continues until optimal designs are identified.

With the aid of an optimization solver, a wide range of key design variables can be evaluated and the most appropriate values for the design variables can be selected. The decision variables to be optimized in this study include operating conditions of refrigeration cycles (e.g. refrigerant flowrate and suction and discharge pressures of the refrigeration compressor) and operating conditions of the boil-off gas stream (e.g. discharge pressure of boil-off gas compressor). For SMR cycles, composition of refrigerant fluids is also important design variables, of which optimal values are selected together with other operating variables.

(a) N2 expander cycle

(b) SMR cycle

(c) Two-level cascaded cycle

*Figure 3: Modeling and simulation of three liquefaction cycles considered in the case study*

### 4. Results of process design

Process design is carried out for three cycles considered in this study. Results are summarized in Tables 1-3 which include optimal values of the key decision variables and overall power requirements. Power requirement for the N2 expander cycle is larger than for the SMR cycle. This is because the usage of mixed refrigerants for SMR cycles is well fitted to the temperature-enthalpy profile of a boil-off gas stream to be cooled, with which
thermodynamic inefficiency can be effectively minimized, leading to better energy efficiency. Direct comparison of the N2 cycle and the SMR cycle with the cascaded cycle cannot be made, as the cascaded cycle is designed for providing cooling up to -100 °C.

Table 1: Results of process design for an N2 expander cycle

<table>
<thead>
<tr>
<th>Optimization variables</th>
<th>Optimization results</th>
</tr>
</thead>
<tbody>
<tr>
<td>Refrigerant mass flow [kg/h]</td>
<td>Compressor discharge pressure [kPa]</td>
</tr>
<tr>
<td>892</td>
<td>3547</td>
</tr>
</tbody>
</table>

Table 2: Results of process design for a SMR cycle

<table>
<thead>
<tr>
<th>Refrigerant mass composition [kg/h]</th>
<th>Optimization variables</th>
<th>JT valve outlet temperature [°C]</th>
<th>Optimization results</th>
</tr>
</thead>
<tbody>
<tr>
<td>C1 63</td>
<td>Compressor discharge pressure [kPa]</td>
<td>5,029</td>
<td>-172.5</td>
</tr>
<tr>
<td>C2 59</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C3 217.7</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C4 76.2</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>N2 149.8</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 3: Results of process design for a two-level cascaded cycle

<table>
<thead>
<tr>
<th>Optimization variables</th>
<th>Optimization results</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ethylene mass flow [kg/h]</td>
<td>Propylene mass flow [kg/h]</td>
</tr>
<tr>
<td>49</td>
<td>52.5</td>
</tr>
</tbody>
</table>

Figure 4: Energy composite curves for the SMR cycle

The effectiveness of the process design and optimization framework used in this study is illustrated with Figure 4, in which comparison is made before and after the optimization. Through the systematic optimization, close match between hot and cold composite curves can be obtained.

5. Conclusions and future work

Process integration techniques are used to assess inefficient heat recovery, and to identify design options for minimizing power consumption for the refrigeration cycles. Such investigation is made in a system-wide manner,
with which local optimal performance of refrigeration cycles should be avoided. The process optimization method is also applied with the aid of a process simulator integrated with a stochastic optimization solver. The case study is given to demonstrate how process integration and optimization can be effectively utilized for the conceptual design of boil-off gas liquefaction processes in practice.

The design and optimization framework presented in this work can be further extended to complex refrigeration cycles, for example dual N2 expander cycle, 3-stage pure-refrigerant cycle, etc. Also, the economic trade-off between capital cost and energy cost can be further explored to provide cost-effective solutions to boil-off gas liquefaction. This study only focuses on the design and optimization of the liquefaction cycle, although the use of boil-off gas for the propulsion system should be investigated in a holistic manner. Such integration between the refrigeration cycle and propulsion systems should be systematically evaluated as future work.

Acknowledgments
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Raei B., 2011, Optimization in energy usage for refrigeration systems using combined pinch and exergy analysis, Chemical Engineering Transactions, 25, 135-140.