Development of A Simulation Package of Natural Gas Liquefaction System

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Abstract
Gas liquefaction employs refrigeration process to bring feed gas temperature down to enable it to condense. The refrigeration system for natural gas liquefaction consists of some components combined in several configurations. One of those systems is the reversed-Brayton and its modified cycles. A numerical program package was developed to model and analyze the process of natural gas liquefaction with maximum flow rate 31.7 kg/s. The package was set for the simple 1-stage reversed Brayton cycle and its modified cycle. The process was modelled with assumptions of a steady state condition and natural gas that made of 100% methane. Parameters and variables that may be involved in the simulation are the feed gas flow rate, temperature and pressure, the selection of refrigerants for the cycle, the refrigeration working pressures. The package enable one to calculate the amount of work required for liquefaction process as well as the system’s performance in term of its figure of merit.

Keywords: natural gas, gas liquefaction system, refrigeration, simulator, figure of merit

1 Introduction
Natural gas is a superior energy source in environmental view. Natural gas can reduce carbondioxide (CO2) emission by 20%, sulphur oxide (SOx) up to 100%, nitrogen oxide (NOx) up to 90%, and other particulate up to 99% [1]. In general, natural gas is distributed in liquid form. This is to make the transportation more convenience, since the volume of liquified natural gas is 600 times lower than in its gas form.

Indonesia has huge potential in small-scale natural gas fields such as Ombilih, West Sumatera. The natural gases are non-conventional gas originated from chemical and physical manipulation of coal (Coal Bed Methane). According to Amirullah, et. al [2], natural gas made of 91,81% mole methane are obtained two days after the drill. Liquefaction system with capacity up to 1 MTPA (31,71 kg/s) is needed to utilize such small-scale gas fields. Chang, et. al [3] has researched about the usage of simple 1-stage reversed-Brayton cycle and its modified cycle to liquefy methane gas with nitrogen as refrigerant. Chang also reviewed some cryogenic refrigeration cycles for liquefaction system thermodinamically [4].

With the variety of system configuration that may exist, it will require a long time to analyze the liquefaction process analytically. Therefore, a program package is necessary to solve the problem numerically. In this paper, a simulator is designed to analyze the process of natural gas liquefaction with simple 1-stage reversed-Brayton cycle and its modified cycle.
2 Fundamental Theory

2.1 Refrigeration cycle for natural gas liquefaction

Refrigeration cycle for natural gas liquefaction has different structure than liquefaction cycle for air. This system consist of closed cycle with temperature difference between feed gas and liquefied natural gas as the cooling load. As Chang stated [3], the performance of refrigeration cycle for liquefaction can be determined from its figure of merit (FOM). FOM of a system is defined as the ratio of minimum work required and actual work done for the liquefaction process as stated in equation (1).

\[ \text{FOM} = \frac{\dot{W}_{\text{min}}}{\dot{W}_{C} - \dot{W}_{E}} = \frac{m_{NG}(h_{L} - h_{G}) - T_{0}(s_{L} - s_{G})}{\dot{W}_{C} - \dot{W}_{E}} \]  

(1)

Irreversibility is a difference between actual work done and minimum work required, and it is equal with exergy lost in the system. Exergy indicate the potential of energy that can be used for work. Exergy is defined as multiplication ambient temperature with entropy generation rate in the system. Equation (2) stated the amount of exergy lost in a refrigeration cycle for liquefaction.

\[ (\dot{W}_{C} - \dot{W}_{E}) - \dot{W}_{\text{min}} = T_{0} \times \dot{s}_{\text{gen}} \]  

(2)

2.1.1 Reversed-Brayton cycle

Reverssed-brayton cycle and its modified cycle are some cycles that can be used for natural gas liquefaction. The cycles are shown in figure 2.1. Modification of reversed-Brayton cycle is conducted by Chang [3] to reduce the entropy generation rate in liquefying heat exchanger (LHX) due to large temperature difference between natural gas and refrigerant. However, the modification has consequence of increasing entropy generation rate in recuperative heat exchanger (RHX) instead.

2.2 System components

A liquefaction system consists of several components. Some of the fundamental components are heat exchanger, compressor, aftercooler, and expansion unit such as expander or throttle.

2.2.1 Compressor

Compressor applied in the small-scale natural gas liquefaction system usually is a reciprocating type with pressure ratio no more than three [5]. Reciprocating compressor work for low up to medium mass flow rate at high pressure [6]. There are two ways to determine the compression work, isentropic and polytropic approach. In isentropic approach, entropy of the fluid is ideally constant before and after compression process. Polytropic approach use ideal gas equation to determine the efficiency. Polytropic efficiency is used in this paper and shown in equation (3), while the compression work is shown in equation (4).
Figure 2.1. Schematic of 1-stage reversed-Brayton cycle (a) simple (b) modified.

2.2.2 After cooler

After cooler is used to lower the refrigerant’s temperature after compression process by rejecting its heat to ambient. The amount of heat released is calculated with equation (5).

\[ Q_h = \dot{m}_{Refr} (h_{AC,in} - h_{AC,out}) \]  \hspace{1cm} (5)

2.2.3 Heat exchanger

Heat exchanger is the main component in natural gas liquefaction system where heat is transferred from natural gas to refrigerant. In heat exchanger, energy conservation law as shown in equation (6) came into effect. The minimum temperature approach in heat exchanger according to Tianbiao [5] should be higher than 3°C.

\[ \sum(\dot{m}_{HE,in} \times h_{HE,in}) = \sum(\dot{m}_{HE,out} \times h_{HE,out}) \]  \hspace{1cm} (6)
2.2.4 Expander

Expander is a mechanical engine to lower the pressure of a fluid and produce work [7]. The process in expander can also be determined in two ways, isentropic and polytropic approach. Polytropic efficiency and work produced by expander is calculated with equations (7) and (8).

\[
\eta_{p,E} = \frac{y_E}{y_E - 1} \times \ln\left(\frac{T_{E,\text{out}}}{T_{E,\text{in}}}\right) \quad (7)
\]

\[
W_{\text{EXP}} = \dot{m}_{\text{REF}}(h_{E,\text{out}} - h_{E,\text{in}}) \quad (8)
\]

3 Methodology

3.1 Natural gas: composition and thermal properties

Natural gas has different components in different gas fields. Generally, methane has the highest mole percentage in a natural gas. For example, Coal Bed Methane in Ombilih, West Sumatera, 2 days after drilling, natural gas that had been found contains 91% mole of methane [2]. After demineralization and purification processes which are not included in the program package design, compound with more than 98% mole methane is obtained. The compound can be approached by pure methane properties. In the program design, CoolProp is used to determine the thermal properties of pure fluid. Pure methane is set by default to enter the liquefaction process at 1 atm (101325 Pa) and 25°C (298 K). According to methane saturation curve, methane will start to condense around 161°C (111 K) at 1 atm and thus is set as the output temperature of natural gas. However, user can change the default setting as they pleased.

3.2 Refrigerant: composition and thermal properties

Refrigerant used for liquefaction process must have working condition in cryogenic temperature and should retain in its gas form when the natural gas condensed. In the simulator design, five refrigerants are chosen as they meet the criteria: nitrogen (N2), Helium (He), Oxygen (O2), Argon (Ar), and low pressure methane (CH4). However, O2 and CH4 is flammable substance and must be used with caution in real plant. He and Ar is not flammable but their working pressure is relatively high, therefore N2 is set as default refrigerant in the simulator [8-12].

3.3 Simulator design

Simulator is designed using MATLAB R2012A. The design consists of three parts: graphical user interface, calculation program, and output display. Interface is made using GUIDE (Graphical User Interface Development Environment) feature from MATLAB. The purpose of interface is for users to easily input the parameters involved. Calculation program is designed to determine the thermodynamic properties of refrigerant and natural gas in every point in the cycle, entropy generation rate, and efficiency of cycle in terms of FOM. In the
output display, the calculation result is shown and the liquefaction process is presented in T-s diagram.

4 Data and Analysis

4.1 Validation

Output of simulator is compared with manual calculation to test its validity. Parameters is set as shown in Table 4.1, and result with error less than 5% is obtained for every dependent variables.

4.2 Parametric analysis

Parametric analysis is performed to identify the effect of changing the value of each parameters to the system performance and mass flow rate of refrigerant required. In simple 1-stage reversed-Brayton cycle as shown in Figure 2.1(a), parametric analysis is performed in four quantities: mass flow rate of natural gas \( \dot{m}_{NG} \), pressure of point 1 (P1), temperature of point 5 (T5), and temperature of point 3 (T3).

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Dependent variable</th>
<th>Analytic result</th>
<th>Simulator output</th>
<th>Error (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \dot{m}<em>{NG} = 0.01 \text{ kg/s,} ) ( T</em>{NG} = 298 \text{ K,} ) ( P_{NG} = 101325 \text{ Pa,} ) ( T_{LNG} = 111,667 \text{ K,} ) ( PR = 3, ) ( P_{1} = 300000 \text{ Pa,} ) ( T_{S} = 105 \text{ K,} ) ( T_{3} = 301 \text{ K,} ) ( T_{1} = 295 \text{ K} ) ( \eta_{c} = 0.85 ) ( \eta_{E} = 0.85 )</td>
<td>FOM</td>
<td>0.378</td>
<td>0.369</td>
<td>2.381</td>
</tr>
<tr>
<td>( \dot{W}_{\text{Comp}} ) (kJ/s)</td>
<td>39.908</td>
<td>39.770</td>
<td>1.734</td>
<td></td>
</tr>
<tr>
<td>( \dot{W}_{\text{exp}} ) (kJ/s)</td>
<td>10.519</td>
<td>10.520</td>
<td>0.010</td>
<td></td>
</tr>
<tr>
<td>( S_{\text{gen}} ) (kW/K.s)</td>
<td>0.060</td>
<td>0.062</td>
<td>3.333</td>
<td></td>
</tr>
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</table>

Pressure of point 1 is varied from 20,000 - 366,846 Pa while other parameters are retained. The simulation resulting in higher FOM as the pressure is increased. This is bound to happen as the change in pressure will also affect other thermodynamic properties of the refrigerant, resulting in higher thermal capacity \( (C_{p}) \). Thus, it will require less amount of refrigerant to receive same amount of heat from natural gas if the working pressure is higher as shown in Figure 4.2. Less refrigerant’s flow rate means less work is required, and the efficiency of the cycle is increased. However, if the pressure is higher than 366,846 Pa, it will results in negative entropy generation rate in expander and violate the second law of thermodynamic. This is happened because the polytropic efficiency of expander is set at 0.85 in this simulation. It may be possible that the efficiency of expander should be higher to make the system work in higher pressure.

Next parameter to be varied is the temperature of point 5, started with 108 K as the minimum temperature approach in heat exchanger and gradually lowered the value until 98 K. The simulation showed that lower temperature of refrigerant in point 5 will result in
higher amount of refrigerant needed to liquefy the natural gas and lower FOM as shown in Figure 4.3. It is happened because the temperature difference in heat exchanger between refrigerant and natural gas is widen, resulting in less heat exchanger effectiveness. Thus, mass flow rate of refrigerant needed to liquefy same amount of natural gas is higher. However, when temperature at point 5 is lower than 98 K, it will result in negative entropy generation rate in expander since lower temperature usually followed with lower entropy of the refrigerant.

The last parameter is temperature at point 3 which is the output of after cooler. The result of the simulation show that having higher temperature in point 3 will affect to lower FOM of the cycle. This is expected since the effectiveness of after cooler will be lower. The temperature range for the simulation is 301 – 318 K, to prevent having FOM lower than 0.15 when the temperature is higher. The mass flow rate of refrigerant needed is increasing in quadratic trend as shown in Figure 4.4. It is happened because to keep the energy conservation law in RHX, temperature at point 6 bound to get lower when the temperature at point 3 increasing. However, the difference in pressure between the two points made the temperature change inequally.

![Figure 4.1. Required mass flow rate of refrigerant as a function of mass flow rate of natural gas.](TNG = 298 K; PNG = 101,325 Pa; TLNG = 111.67 K; PR = 3; P1 = 300,000 Pa; T5 = 105 K; T3 = 301 K; T1 = 295 K)

![Figure 4.2. Required mass flow rate of refrigerant as a function of pressure of point 1.](TNG = 298 K; PNG = 101,325 Pa; TLNG = 111.67 K; PR = 3; \( m_{NG} = 0.01 \) kg/s; T5 = 105 K; T3 = 301 K; T1 = 295 K)
5 Conclusion

A program package is designed to analyze and simulate a liquefaction process using simple 1-stage reversed-Brayton cycle and its modified cycle. The simulator output is compared with manual calculation and results with error less than 5% are obtained. Parametric analysis is also performed using the program package. Higher mass flow rate of natural gas will only affect the amount of refrigerant needed to condense it and FOM of the cycle remain constant. Higher working pressure will result in higher FOM, but only until a point when the process will result in negative entropy generation. Similar trend also happened when the temperature of point 5 is higher. The increase of temperature in point 3 will result in lower FOM due to lower after cooler effectiveness.

6 Reference


Nomenclature

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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<tbody>
<tr>
<td>FOM</td>
<td>figure of merit</td>
</tr>
<tr>
<td>h</td>
<td>specific enthalpy</td>
</tr>
<tr>
<td>ṁ</td>
<td>mass flow rate</td>
</tr>
<tr>
<td>P</td>
<td>pressure</td>
</tr>
<tr>
<td>Q</td>
<td>heat transfer rate</td>
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<tr>
<td>s</td>
<td>specific entropy</td>
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<tr>
<td>Š_gen</td>
<td>entropy generation rate</td>
</tr>
<tr>
<td>T</td>
<td>temperature</td>
</tr>
<tr>
<td>W</td>
<td>power or work rate</td>
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<table>
<thead>
<tr>
<th>Subscripts</th>
<th>Description</th>
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</thead>
<tbody>
<tr>
<td>0</td>
<td>ambient</td>
</tr>
<tr>
<td>AC</td>
<td>after-cooler</td>
</tr>
<tr>
<td>C, Comp</td>
<td>compressor</td>
</tr>
<tr>
<td>E, Exp</td>
<td>expander</td>
</tr>
<tr>
<td>F</td>
<td>natural gas feed</td>
</tr>
<tr>
<td>HE</td>
<td>Heat exchanger</td>
</tr>
<tr>
<td>L</td>
<td>LNG or liquefied natural gas</td>
</tr>
<tr>
<td>min</td>
<td>minimum</td>
</tr>
<tr>
<td>Refr</td>
<td>Refrigerant</td>
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<tr>
<td>p</td>
<td>polytropic</td>
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Greek letters

<table>
<thead>
<tr>
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<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>η</td>
<td>Efficiency</td>
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ratio calor specific