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Research Article

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Investigating the Robustness of Process Simulation Tools for Natural Gas Liquefaction Processes

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Abstract The efficiency of liquefied natural gas processing facilities can be determined by recourse to proprietary process simulation tools, whose performance give insight into how plant efficiency can be improved. Notable simulators such as Aspen HYSYS [2], SIMSCI/PRO-II [10] and UniSim [9] are commercially available. This paper investigates the performance of two of such process simulation tools, hereinafter referred to as XTool and YTool, in order to ascertain their respective performance in the simulation of propane precooled, mixed refrigerant natural gas liquefaction process. Results show that the YTool is a more robust simulator with its flowsheet convergence requiring less effort in the reduction of equivalent heat consumption. The YTool process model was, overall, more robust and well suited for optimization and detailed analysis of the LNG production (C3-MR) process.

Keywords Natural gas liquefaction, process simulation; process simulation tools, LNG

1. Introduction

Over the past half century, natural gas (NG) has become one of the most sought after energy source owing to its clean burning characteristics as well as low carbon concentration when compared to other fossil fuels. The market share of NG has grown rapidly from 15.6% of global energy consumption in 1965 to 24% in 2011 [14]. Early transportation of NG was via pipelines to areas of demand which are usually short distances from where it is produced and/or processed. However, with the rapid growth in the NG industry and the increasing demand of NG supplies over long distances and across borders, pipeline transportation has become economically and technically infeasible [22]. As a result, NG liquefaction has become a viable and widely accepted alternative. The economics of NG liquefaction are obtained by reduction of its volume by 600 times at a temperature of -162^{o}C which allows the storage of large quantities. Various processes for liquefaction of NG can be broadly classified into the cascade and the mixed refrigerant (MR) processes. Within the cascade process, the ConocoPhilips Optimized Cascade® uses a single component refrigerant while the Mixed Fluid Cascade (MFC®), developed by Norway's Statoil and Linde LNG technology alliance, uses a mixture of different refrigerants. The PRICO process is an example of a mixed refrigerant process without precooling. Also, a mixed refrigerant process with precooling could either be with a single component refrigerant as in the Propane Precooled Mixed Refrigerant (C3-MR) or with a mixed refrigerant component as with the Shell's Double Mixed Refrigerant (DMR) process [6]. Selection of refrigerant for a typical LNG base-load plant should be such that matches thermodynamically the cooling curve of NG stream (see Figure 1).

There have been studies which compared the simulation performance of a number of software packages for different LNG production configurations. It is of interest to ascertain the accuracy or robustness of their computations for a typical LNG production facility. Studies on process optimization for LNG production have been published [8, 24, 16, 19, 12, 3, 13, 17, 20, 23, 18]. However, there has, in general, been published very few studies comparing simulation performance of different process simulation tools for natural gas liquefaction. In this paper, a proprietary simulation software, YTool, is used to model and optimize a typical three stage propane pre-cooled natural gas liquefaction (C3-MR) process, which will then be compared with the results obtained from an XTool model of a similar facility [8]. Refrigerant composition, e.g., a mixture of hydrocarbons and nitrogen, can be chosen so that it has an evaporation curve that matches the cooling curve of the NG (see Figure 1) with the minimum temperature difference. Small temperature difference reduces entropy generation and, thus, improves thermodynamic efficiency and reduces power consumption.

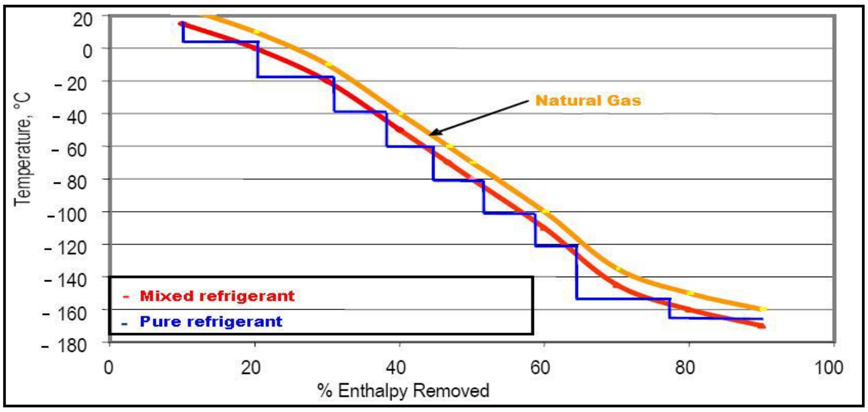


Figure 1: Cooling curves of pure refrigerant and mixed refrigerant (MR) versus NG [8]

2. Methodology and Modelling Considerations

2.1.Process Configuration

A standard natural gas liquefaction process has a propane precooling loop, a mixed refrigerant loop and NG-LNG path, with a traditional configuration shown in Figure 2. Natural gas passes through the high medium and low pressure evaporators (HX-X) before entering the main cryogenic heat exchanger where liquefaction and subcooling to LNG occurs The propane refrigerant precools both the natural gas and the mixed refrigerants passing through the evaporators. The mixed refrigerant exiting the third evaporator enters the separator, thus splitting into light and heavy mixed refrigerants streams both of which enters the main cryogenic heat exchanger where they help in liquefying and sub-cooling the already precooled natural gas to -162 ^{o}C. Thereafter, the spent mixed refrigerant which is vaporized during the process of liquefaction and subcooling in the main cryogenic heat exchanger (MCHE) exits the MCHE and re-enters the compressor suction where the mixed refrigerant vapour is compressed back through the evaporators. The precooling cycle uses the propane refrigerant at three pressure levels to exchange heat with the mixed refrigerant (MR) and the hot, dry NG stream. As a result of this heat exchange, the NG and the MR are initially cooled to a temperature of -35 ^{o}C.

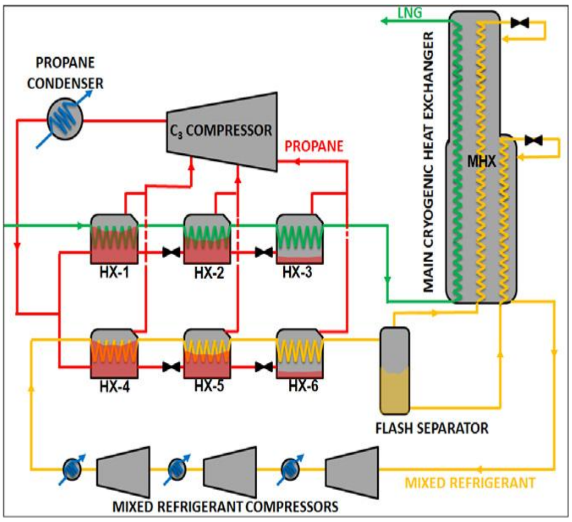


Figure 2: C3-MR process flow diagram [5]

2.2. Modelling in YTool

We set up a simulation of the LNG production process in YTool software using the same conditions and parameters as used for the XTool Simulator [8] and also selectedPeng-Robinson thermodynamic fluid package for the simulation. Tables 1 and 2 list the composition of natural gas (NG) and mixed refrigerant (MR) streams as well as other process and cycle parameters used in the simulation of the natural gas liquefaction process. The feed rate of the dry NG was 60,000 Kgmol/h which corresponds to a LNG production capacity of 8.4 million tons per year. It is assumed that the NG-feed has been conditioned and pretreated before entering the liquefaction unit of the baseload facility.

Table 1: Composition and Parameters

Component	Fraction (%)		Parameter	Value		
	NG	MR		NG	C3	MR
Methane (C1)	89.7	45.0	Inlet Pressure (bar)	40	10.81	47.90
Ethane (C2)	5.5	45.0	Inlet Temperature (ºC)	30	30	30
Propane (C3)	1.8	2.0	Flowrate (kgmole)	60000	82090	117100
n-Butane (n-C4)	0.1	-				
Nitrogen (N_2)	2.9	8.0				

Table 2: Cycle Parameters

Cycle	Parameter	Value
Precooling	ΔT_{min} all Heat Exchangers(HX) (ºC)	1
	ΔP_{Tube} all HXs (bar)	0.5
	ΔP_{Shell} all HXs (bar)	0.1
Liquefaction	$\Delta P_{Hot\ side}$ all HXs (bar)	5
	$\Delta P_{Cold\ side}$ all HXs (bar)	0.5
Other Parameters	$\Delta P_{Condenser}$ (bar)	0.1
	LNG Temperature (ºC)	-162

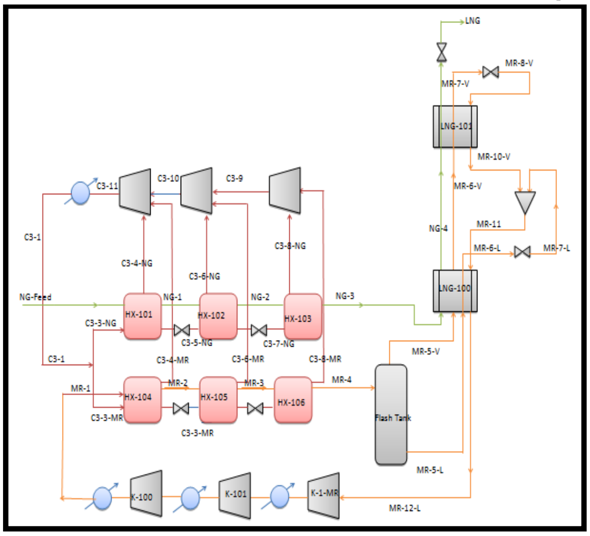
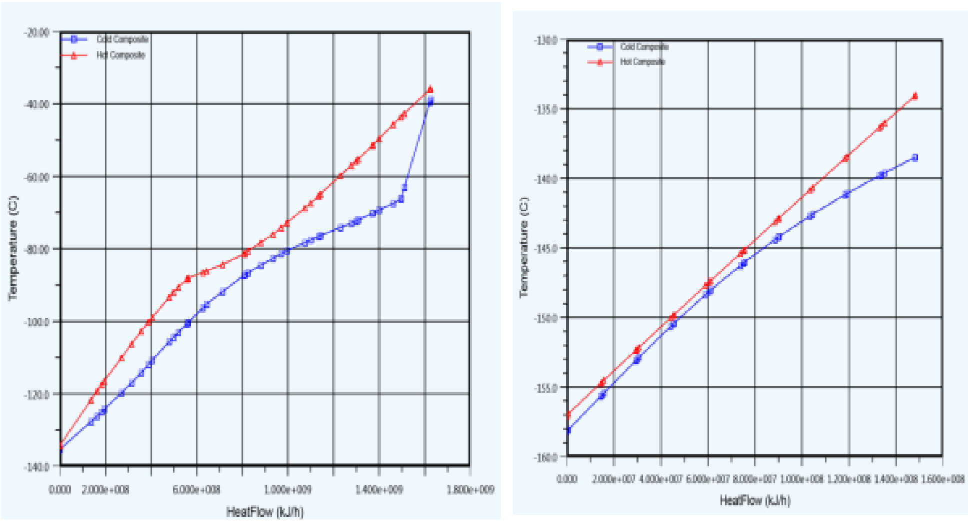


Figure 3: Process flow sheet of propane precooled mixed refrigerant cycle

Figure 3 indicates that a splitter is used in the process flowsheet of the YTool to separate the propane stream into two streams to provide cooling to the NG-feed and MR while other splits were carried out by flash tanks succeeding each heat exchanger. The propane vapor phases are sent via mixers to the compressors for recompression and recycle while the liquid propane passes onto the next phase of the precooling cycle. Shell and tube heat exchangers were used to model the kettle-type heat exchangers (or evaporators) used in the real process [4, 5]. Also, a weighted counter-current design model was used for all six heat exchangers in the pre-cooling cycle with a minimum temperature difference of $1^{O}C$. Two LNG-Type heat exchangers, representing the hot and cold parts, were used to model the MCHE. The YTool LNG heat exchanger is a multi-pass type that allows multiple streams with hot and cold sides [8]. To avoid liquid entering the compressors, the last two heat exchangers of the pre-cooling cycle and the bottom part of the MCHE were designed to superheat the propane (C3) and the MR streams respectively. Joule-Thomson effect was used to flash the sub-cooled NG at $-157^{o}C$ to LNG at $-162^{o}C$. Three compressors were used to raise the pressure of the C3 to initial conditions after which it was cooled to $30^{o}C$. Similarly, three compressors were used to raise the pressure of MR with inter-cooling. This is done to reduce compressor workload [5]. Figure 4 illustrates the hot and cold composite curves for the MCHE's warm and cold bundles.



(a) *(b)*

Figure 4: Temperature profiles showing the cold and hot composite curves for the Bottom (a) and Top (b) parts of the MCHE.

In Figure 3, the NG-feed designated as NG-1, NG-2 and NG-3 represent the flow stream of natural gas at different levels in the cycle. C3-X-NG represents the flow rate of propane in the pre-cooling section that pre-cools the natural gas stream (where X denotes the level at the cycle). C3-X-MR represents the flow rate of propane in the precooling section that pre-cools the mixed refrigerant stream (where X, again, denotes the level at the cycle). HX-101, HX-102, etc., represents the heat exchangers at different levels in the cycle, K-1-C3, K-2-C3, K-3-C3, and K-100. The K-101 and K-1-MR represent the propane and mixed refrigerant compressors, respectively. LNG 100 and LNG 101 represent the main cryogenic heat exchanger in the liquefaction section. MR-X-V and MR-X-L represent the vapor and liquid composition of the mixed refrigerant at different states, X, in the liquefaction cycle.

2.3. Optimization in YTool

The main objective of the optimization presented herein is to minimize the power consumption of compressors [7]. The YTool optimizer is employed for this optimization due to its perceived simplicity and robustness when compared to the XTool. The flow sheet was divided into two parts: pre-cooling and liquefaction sections in an attempt to independently optimize the pre-cooling section and the MCHE section [1]. According to [11], if the utilities and pumping work are ignored, which are as a rule negligible compared to the refrigerant compression, the optimization problem can be formulated as follows:

$$J = \sum W.P_w - F_{LNG} \times P_{LNG} \quad (1)$$

Where W is the energy consumption of the compressors, F_{LNG} is the production rate and P_{LNG} is the price. If we assume a fixed production rate, equation (1) reduces to,

$$J = \sum W.P_w \quad (2)$$

For the pre-cooling section, we seek to minimize the power consumed by the three propane compressors, thus,

$$J = W_{K\text{-}1\text{-}C3} + W_{K\text{-}2\text{-}C3} + W_{K\text{-}3\text{-}C3} \quad (3)$$

Similarly, for the liquefaction section, we seek to minimize the mixed refrigerant compressor work,

$$J = W_{K\text{-}3\text{-}MR} \quad (4)$$

We specified eight variables [11] for the optimization of the pre-cooling section, including: (1) Flow rate of the two propane streams C3-2-NG and C3-3-MR i.e. $F_{C3\text{-}2\text{-}NG}$ and $F_{C3\text{-}2\text{-}MR}$; (2) Temperature of streams C3-1 and MR-1; (3) Four pressure levels in the propane loop specified in the streams C3-3-NG, C3-7-NG, C3-11-NG, and C3-18. Six variables are specified in the liquefaction section including: (1) flow rate of the mixed refrigerant stream MR-4-2; (2) pressure of streams MR-4-2 and MR-9-V (high and low pressures); and (3) composition of mixed refrigerant (i.e. mole fraction of ethane, propane and nitrogen). Summarily, we have, for the pre-cooling and liquefaction processes,

$$\boldsymbol{U_{Precooling}} = \{F_{C3\text{-}2\text{-}NG}, F_{C3\text{-}2\text{-}MR}, T_{C3\text{-}1}, T_{MR\text{-}1}, P_{C3\text{-}3\text{-}NG}, P_{C3\text{-}7\text{-}NG}, P_{C3\text{-}11\text{-}NG}, P_{C3\text{-}18}\} \quad (5)$$

and,

$$\boldsymbol{U_{Liquefaction}} = \{F_{MR\text{-}4\text{-}2}, P_{MR\text{-}4\text{-}2}, P_{MR\text{-}9\text{-}V}, x_{c2}, x_{c3}, x_{N2}\} \quad (6)$$

Equations (5) and (6) were solved subject to some constraints. For the precooling section, the following five constraints were set: (1) NG and the MR out of the precooling section (i.e streams NG-3 and MR-4) must be colder than -35°C; (2) $T_{NG\text{-}3} \leq -35^oC$ and $T_{MR\text{-}4} \leq -35^oC$; (3) C3 leaving the low pressure evaporation stage must be at least 2.5°C superheated; (4) $\Delta T > 2.5^oC$; (5) C3 leaving the condenser must be liquid only i.e. $T_{C3\text{-}18} \leq T_{bubble}$. Similarly, the following three constraints for the liquefaction section were set: (1) $T_{LNG} \leq -157^oC$; (2) $\Delta Tsup.MR \geq 2.5^oC$ (stream MR-13 to the compressor K-3-MR must be superheated); and (3) All internal temperature difference, $\Delta T > 0$

3. Results and Discussions

In Table 3, the baseline results for the YTool are listed for the most important alternatives. On specifying the constraints as stated above, as well as lower and upper bounds for each variable, and at default penalty values of the optimizer, the optimizer was successful in finding an optimal value for the objective function after twenty (20) iterations. The optimal values being the last values obtained before the optimizer failed. The baseline results are then compared with results obtained following optimization and Figure 5 shows a significant reduction in the amount of power consumed. Table 4, 5 and 6 compare the baseline versus optimization results in the respective pre-cooling and liquefaction sections.

Table 2: Baseline results from the YTOOL Model

Parameter	Power Consumed (MW)			$T_{NG\text{-}3}$ °C	$T_{MR\text{-}4}$ °C
	$W_{K\text{-}1\text{-}C3}$	$W_{K\text{-}2\text{-}C3}$	$W_{K\text{-}3\text{-}C3}$		
Value	13.6	25.3	56.4	-36.04	-35.76
Total	95.3				

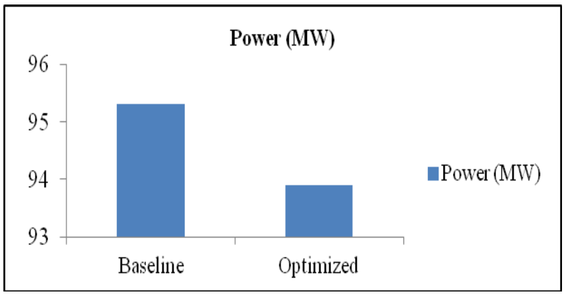


Figure 5: Optimized vs baseline results for power consumed using YTool Model

Table 3: Optimized vs baseline results for power consumed using YTool Model

Cycle Variables	$F_{C3-2-NG}$ kgmole/h	T_{C3-1} °C	T_{MR-1} °C	$P_{C3-3-NG}$ Kpa	$P_{C3-7-NG}$ Kpa	$P_{C3-11-NG}$ Kpa	P_{C3-18} Kpa	Power[1] MW
Baseline	13540	30	30	483.2	256.8	126.3	1091	95.3
Optimized	13429.5	28	28	484.0	260.0	128.7	1085	93.9

Table 4: Optimization results for constraints applied in the pre-cooling section

Constraints	T_{NG-3} °C	T_{MR-4} °C	ΔT_{C3} °C	ΔT_{MR} °C
Baseline	-36.04	-35.76	18.35	18.45
Optimized	-35.60	-36.04	4.807	2.713

Table 5: Optimization results for constraints applied in the liquefaction section

Cycle Variables	Power consumed (MW)
Baseline	233
Optimized	231

Lastly, a comparison is made with the results obtained by [8] based on an XTool Model, where a MATLAB function [15] is interfaced with the XTool Model. It can be seen from Figure 6 that there is a perfect agreement between the baseline results obtained by XTool/Matlab Function and that obtained in this work. However, the total power consumption for the XTool model shows a relatively higher heat consumption when compared to the YTool model, which indicates that the differences in calculated total power consumption are due to differences in robustness and assumptions in the respective models. It is also evident that the parameters in both models are different because different sources were probably used in the in-built files. The YTool equilibrium model with the updated parameters gives the lowest reduction in the amount of power consumed (see Figure 6).

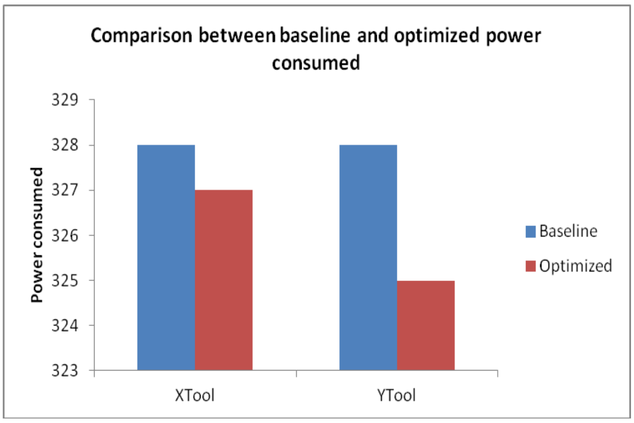


Figure 6: Comparison of Optimized Values with Base case for both YTool and XTool

4. Conclusion

An LNG production process configuration based on propane pre-cooled mixed refrigerant system have been simulated with the proprietary XTool (interfacing with a MATLAB function) and YTool Simulators. The XTool/Matlab function simulations calculated higher power consumption compared to the simulations based on YTool. The results from this work show that all the simulation models calculate the same trends in the reduction of total power consumption under a standard process. However, the results show that the YTool is a more robust tool as it captures the reduction in energy consumption of the LNG production process. In contrast, the XTool model does not offer the desired accuracy or robustness for optimization and detailed analysis of the process, hence the need to interface with a Matlab function. The problems encountered due to XTool design suggest that a simulator providing better robustness and a higher level of transparency towards the process equations, as demonstrated by the YToolmodel should be deployed. The YTool design is evidently the more suitable simulator for complicated LNG processes such as the C3-MR process. Optimization of the pre-cooling section was successful, as the optimized value of the objective function reduced by 1.5% from the baseline value while the optimization of the liquefaction section was also successful, with a 0.9% decrease in power consumption. The overall optimization of the C3-MR cycle using the YTool showed a 0.6% reduction in total power consumed when compared to the base case.

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