Multi-objective optimization of natural gas liquefaction process simulation via kriging surrogate model

Lucas F. Santos,a,b Caliane B. B. Costa,a Jose A. Caballero,b Mauro A. S. S. Ravagnania

aDepartment of Chemical Engineering, State University of Maringa, Av. Colombo 5790, Maringá - 87020900, Brazil
lfs.francisco.95@gmail.com, pg54347@uem.br

Abstract
A multi-objective optimization framework is proposed to design single-mixed refrigerant natural gas liquefaction processes considering the conflicting goals of minimizing both power consumption and heat transfer area utilization. In the present approach, the black-box process simulation is embedded into a nonlinear programming (NLP) problem via kriging surrogate model. To deal with the conflicting objectives, the \( \varepsilon \)-constraint methodology is applied. The surrogate NLP problems with fixed \( \varepsilon \) are solved in GAMS using CONOPT to determine a non-dominated solution candidate of the original multi-objective problem. The Pareto Front achieved with the present framework dominates recent single-objective result from the literature. The non-dominated solutions have power consumption that ranges from 0.2800 to 0.4060 kW/(kg NG) and heat transfer area utilization multiplied by overall heat transfer coefficient varying from 0.0699 to 0.1852 kW/°C. A trade-off solution can be achieved by increasing 5.29 % of power consumption to save 31.8 % of heat transfer area.

Keywords: Multi-objective optimization, Kriging surrogate model, Natural gas liquefaction, Simulation optimization, Process simulation.

1. Introduction
The natural gas liquefaction process design presents a clear trade-off between energy consumption and equipment size (Khan et al., 2016). The concern of achieving high energy efficiency and diminished equipment size is further emphasized in offshore processes, where the plant site size is significantly restricted. These liquefaction processes consist of cryogenic refrigeration cycles to cool down the natural gas to about \(-160 \, ^{\circ}{\text{C}}\) to liquefy, store, transport, and commercialize it safely as liquefied natural gas (LNG). Optimization has been successfully used to determine refrigerant composition and thermodynamic cycle conditions in natural gas liquefaction processes to improve power consumption, exergy efficiency, or total annual cost (Austbø et al., 2014). Despite the vast literature on single-objective optimization, the evaluation of the natural gas liquefaction processes optimal trade-offs has been timidly addressed in the literature. Khan et al. (2016) investigated the optimization of the dual-mixed refrigerant LNG process under cold and warm ambient conditions. The authors used NSGA-II algorithm to trade-off between the minimization of specific compression energy and the area of heat exchangers in terms of overall heat transfer coefficient times the area (UA).
Ghorbani et al. (2016) used Genetic Algorithms (GA) for single and multiple objectives to optimize the propane-precooled mixed-refrigerant LNG process. The considered goals were to maximize exergy efficiency, minimize total product cost, and both objectives simultaneously. Song et al. (2017) optimized the nitrogen expansion LNG process with carbon dioxide expansion precooling. The authors used NSGA-II to increase the liquefaction rate from 0.77 to 0.81, while diminishing the energy consumption in 10.1% compared to a base case. Nguyen et al. (2018) compared the single-mixed refrigerant (SMR), single-expander, and dual-expander LNG processes with respect to the trade-off between power consumption and UA using a multi-objective GA. Mofid et al. (2019) optimized the parallel nitrogen expansion LNG process using a multi-objective particle swarm optimization algorithm in design and operation stages.

Previous works on multi-objective optimization of natural gas liquefaction processes relied on meta-heuristics, mainly GAs. However, recent papers have shown that surrogate-based approaches can be more efficient than meta-heuristics to these simulation optimization problems (Santos et al., 2021a), which can lead to further improvement to the LNG processes. The objective of the present paper is to propose a multi-objective optimization framework to the SMR natural gas liquefaction process design based on kriging surrogate models that replace the process-simulator-dependent, black-box objectives and constraints functions and introduce explicit algebraic formulation to the optimization problem. The \( \varepsilon \)-constraint method is used to handle the competing objectives. The surrogate optimization subproblems, which have explicit algebraic form, are embedded into a nonlinear programming (NLP) problem and solved with multi-start approach with CONOPT local solver in General Algebraic Modeling System (GAMS). The framework is applied to power consumption and heat transfer area as objectives. The Pareto Front determined by the present approach is compared with literature results.

2. Natural gas liquefaction process

The processes flow diagram of the SMR natural gas liquefaction is illustrated in Figure 1. This SMR process is based on Qyyum et al. (2020), who studied the potential energy-savings of using two stages of expansion to the PRICO process. This process is rigorously simulated in Aspen HYSYS V9 using Peng-Robinson equation of state and Lee Kesler for enthalpy and entropy calculations. The process specifications, constraints, and considerations are inspired in the work of Qyyum et al. (2020). The natural gas stream NG is considered to be at 5,500 kPa and 25.0°C, and its composition in mole fraction is 0.0022 of nitrogen, 0.9133 of methane, 0.0536 of ethane, 0.0214 of propane, 0.0046 of i-butane, 0.0047 of n-butane, 0.0001 of i-pentane, and 0.0001 of n-pentane. A basis of calculation of 1 kg/h for the natural gas mass flow rate is used. The considered decision variables in the present paper are mixed-refrigerant component mass flow rate of nitrogen \( m_{1,n} \), methane \( m_{1,c} \), ethane \( m_{2,c} \), propane \( m_{3,c} \), i-butane \( m_{i,c} \), and i-pentane \( m_{i,c} \), suction and discharge pressure \( P_{suc} \) and \( P_{dis} \), illustrated in Figure 1. The final pre-refrigeration temperature is considered to be -24.0°C. The pressure drop in the multi-stream heat exchangers (MSHEs) is 100 kPa for hot streams, 10 kPa for cold streams, and 50 kPa for water inter-stage coolers. The intermediate pressures are determined to guarantee a constant compression ratio in all four compressors, and the intermediate cooling temperature is 30°C. The temperature of all hot streams leaving the MSHEs is considered to be the same, i.e., -24.0°C for the first
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one and -157.2 °C for the second one to achieve the desired LNG condition of -160.0 °C, 110 kPa, and 3.7 % of vapor fraction.

The process design problem is formulated as a multi-objective optimization model, considering the minimization of specific power consumption and UA. The process constraint is that a minimum temperature approach of 3 °C must be assured throughout the MSHEs. To overcome the issue of this constraint not being smooth for kriging modelling (Santos, 2021b), Santos et al. (2021a) proposed to discretize the MSHEs in . The optimal process design can be formulated as the following multi-objective optimization problem

\[
\min_{x \in D} f(x) = \left[ \sum_{i \in PM} \frac{W_i(x)}{m_{NG}} : \sum_{ex \in HE} UA_{ex}(x) \right]
\]

s.t. \( g_\kappa(x) = 1 - \frac{\min_{k \in \Omega_\kappa} (T_{h_{\kappa,k}}(x) - T_{c_{\kappa,k}}(x))}{3} \leq 0, \kappa = 1, \ldots, (2K) \)

In Eq. (1) \( W_i(x) \) is the work consumption of the pressure manipulator unit \( i \) in the set of compressors and pumps \( PM \), and \( UA_{ex}(x) \) is the global heat transfer coefficient multiplied by the area of the heat exchanger \( ex \) in the set of all heat exchangers HE. \( T_{h_{\kappa,k}}(x) \) and \( T_{c_{\kappa,k}}(x) \) are the temperature of hot and cold composite curves in the \( \kappa \) section of the MSHEs, and \( \Omega_\kappa \) is the set of the \( k \) points from composite curves calculations that belongs to section \( \kappa \) (Santos et al., 2021a). \( D = [x^L, x^U] \) is a box constraint for the decision variables bounded by \( x^L \) and \( x^U \) as proposed in Qyyum et al. (2020), and \( m_{NG} \) is the mass flow rate of the natural gas stream.

3. Kriging-based multi-objective optimization

To solve the multi-objective simulation optimization problems as in Eq. (1), the proposed framework is presented in Algorithm 1. The computer code to compute \( f \) and \( g \) at given \( x \in D \) is a function written in MATLAB connected to the process simulator Aspen HYSYS. First, \( m_s \) samples of \( X \) is generated by a Latin Hypercube algorithm to maximize the minimum distance between points in the search space \( D \). The value of \( f \) and \( g \) are calculated in the simulation for each \( x \in X \). The initial data is defined as \( D_0 = [XY] \). Given \( D_0 \), \( m_s \), and \( D \), the single-objective optimization for each \( f_i \) objective is solved using the framework for constrained black-box optimization proposed in Santos et al. (2021a). In the case of Eq. (1), the objective function \( f_1 \) is the specific power consumption and \( f_2 \) is the overall UA. The above-mentioned approach consists of using the data in \( D_0 \) to fit kriging models for the objectives and constraints. These models are implemented in an NLP problem and solved in GAMS with multi-start local optimization with CONOPT local solver. The solution, which is promising a
minimizer candidate, is evaluated in the simulation and the values are appended to the data. This process is repeated until convergence or simulation evaluation budget \( m_f \). The values of \( f_1 \) at each single-objective solution, \( f_1(x_1^1) \) to \( f_1(x_1^2) \), bound the \( \varepsilon \) vector. The \( \varepsilon \)-constraint vector is defined as the equally distributed \( n_\varepsilon \)-vector from \( f_1(x_1^1) \) to \( f_1(x_1^2) \). The single-objective solutions are appended to the data, \( D_2 \). For the other entries of \( \varepsilon \), the \( \varepsilon \)-constrained single-objective optimization is solved using the same framework for constrained black-box optimization proposed in Santos et al. (2021a). Each optimization solution is appended to the data so that \( D_{he} = D_{he-1} \cup \{x_{he}^1, f(x_{he}^1), g(x_{he}^1)\} \). The last step of the proposed framework is to eliminate dominated and infeasible solutions from \( D_{he} \) to form the set of Pareto solution, \( P \), found by the algorithm.

Algorithm 1: Kriging-based multi-objective optimization framework

**Input:** Initial sample size \( m_0 \in \mathbb{N}_+ \), maximum number of samples \( m_f \in \mathbb{N}_+ \), box-constrained design space \( \mathcal{D} \subseteq \mathbb{R}^n \), the computer code to compute \( f \) and \( g \) at given \( x \in \mathcal{D} \), and the number of \( \varepsilon \)-constraint values \( n_\varepsilon \in \mathbb{N}_+ \).

1. Generate \( m_0 \) samples \( X \) with respective simulation output values \( Y = [f, g]^T \) and define \( D_0 = \{X, Y\} \).
2. Solve the single-objective optimization problem for each \( f_j \) using the framework proposed in Santos et al. (2021a) to determine \( x_j^1 \) and \( x_j^2 \), with \( D_0, m_f, \mathcal{D} \).
3. Define \( \varepsilon \) as the equally spaced \( n_\varepsilon \)-vector from \( f_1(x_1^1) \) to \( f_1(x_1^2) \).
4. Append to the data: \( D_1 = D_0 \cup \{x_1^1, f(x_1^1), g(x_1^1)\} \cup \{x_1^2, f(x_1^2), g(x_1^2)\} \).
5. Solve the \( \varepsilon \)-constrained single-objective optimization

\[
\min_{x \in \mathcal{D}} f_j(x)
\]

s.t. \( f_j(x) \leq \varepsilon_{he-1} \)
\( g(x) \leq 0 \),

using the framework proposed in Santos et al. (2021a) to determine \( x_j^1 \), with \( D_{he-1}, m_f, \mathcal{D} \).

6. Append the solution to the data: \( D_{he} = D_{he-1} \cup \{x_{he}^1, f(x_{he}^1), g(x_{he}^1)\} \).

7) Eliminate dominated and infeasible solutions from \( D_{he} \) to form \( P \), the set of Pareto solutions;

**Output:** Set of non-dominated solutions, \( P \).

4. Results

The proposed multi-objective, kriging-based optimization framework is applied to the design of SMR natural gas liquefaction processes considering power consumption and heat exchanger area utilization objectives. The considered parameters of the optimization approach are initial sample size \( m_0 = 10n \), function evaluation budget \( m_f = 20n \), number of decision variables \( n = 8 \), number of sections into which each MSHE is divided \( K = 10 \), and number of non-dominated solution \( n_\varepsilon = 18 \).

Figure 2 presents the Pareto Front determined by the non-dominated solutions of the present approach. It also includes the best result from the literature to this liquefaction process with the given specifications (Qyyum et al., 2020). This figure shows that the present approach was able to determine an energy-optimal solution that is better than the literature, with energy saving of 1.51%, from 0.2843 to 0.2800 kW/kg of natural gas. Also, given the present Pareto Front, the literature solution is a dominated one. It means that, for the same specific power consumption, the present approach would design a liquefaction process with reduced UA. The proposed Pareto Front ranges from 0.2800 to 0.4046 kW/(kg NG) for power consumption and 0.0699 to 0.1852 kW/°C for UA. The shape of this Pareto curve shows that the increase in heat exchanger area is more pronounced as the power consumption approaches low values. Based on this
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insight, one can choose non-dominated solutions that better balances high energy efficiency and heat exchanger area utilization as the solutions that presents the smallest $\ell^2$ and $\ell^1$ norm. These solutions are highlighted in Figure 2 in the blue square and magenta hexagram, respectively. The best trade-off based on the $\ell^2$ norm presents an increase in power consumption of 5.29 % and 31.80 % UA decrease compared to the energetically-optimum solution. The $\ell^1$ norm-based solution presents an increase in power consumption of 10.61 % and 44.65 % UA decrease compared to the energy-optimum solution.

![Figure 2: Pareto Front and comparison with Qyuum et al. (2020).](image)

Table 1 presents the values of the decision variables and objective functions for the base case (Qyuum et al., 2020), energy-optimum, UA-optimum, $\ell^2$-norm trade-off, and $\ell^1$-norm trade-off solutions. The energy-optimum result presents a refrigerant composition that is reduced in propane and i-pentane in comparison with the literature result. The UA-optimum result shows that for reducing the heat exchangers area utilization high compression ratio and refrigerant with more contents of light-components are preferred. Differently from what one would expect, the trade-off solutions are complex and unique, i.e., not mere interpolations of the single-objective ones. Therefore, the use of multi-objective optimization approach is justified as a means to derive complex solutions that trades-off optimally between conflicting objectives to the process design. The computational time is dominated by simulation evaluation, which takes around 4.7 s. The mean elapsed time for the multi-objective optimization algorithm was 143 min. The advantage of the present approach over the well-established population-based meta-heuristics is the reduced budget of time-consuming simulation calculation, in the present case $10n \times n_2 = 1440$. The circumstances that the present approach would no longer be efficient is when the surrogate models do not capture the true functions behavior. That is often the case for high-dimensional problems or highly discontinuous functions.

5. Conclusions

This paper presented a multi-objective optimization framework to the SMR natural gas liquefaction process design problem, considering the trade-off between energy efficiency and heat exchanger area utilization. Kriging surrogate model, $\varepsilon$-constraint methodology, and gradient-based solver in GAMS are used in the proposed approach to determine candidates of non-dominated solutions of the original black-box optimization problem. The Pareto Front determined by the present approach shows that the recent literature result of energy-efficient SMR process is a dominated solution. The objective functions of non-dominated solutions range from 0.2800 and 0.4046 kW/(kg
NG) for power consumption and 0.0699 and 0.1852 kW/°C for UA. Two trade-off solutions were analyzed and the results showed that 5.29 % and 10.61 % increase in the power consumption can lead to 31.80 % and 44.65 % heat exchanger area decrease, respectively. The trade-off solutions are complex process configurations instead of interpolations of the single-objective optima, which justifies the use of multi-objective optimization approach to tackle competing objectives.

Table 1: Multi-objective optimization results for SMR natural gas liquefaction processes

<table>
<thead>
<tr>
<th>Optimization Results</th>
<th>Qyyum et al. (2020)</th>
<th>Energy-optimum</th>
<th>UA-optimum</th>
<th>$\mathcal{E}^2$-norm trade-off</th>
<th>$\mathcal{E}^1$-norm trade-off</th>
</tr>
</thead>
<tbody>
<tr>
<td>$m_N$[kg/h]</td>
<td>0.2210</td>
<td>0.2426</td>
<td>0.2620</td>
<td>0.1871</td>
<td>0.1500</td>
</tr>
<tr>
<td>$m_{C_1}$[kg/h]</td>
<td>0.4525</td>
<td>0.4344</td>
<td>0.5500</td>
<td>0.4132</td>
<td>0.4244</td>
</tr>
<tr>
<td>$m_{C_2}$[kg/h]</td>
<td>0.9420</td>
<td>0.9504</td>
<td>0.9976</td>
<td>0.8878</td>
<td>0.8090</td>
</tr>
<tr>
<td>$m_{C_3}$[kg/h]</td>
<td>0.9600</td>
<td>0.8000</td>
<td>0.8322</td>
<td>0.8001</td>
<td>0.8904</td>
</tr>
<tr>
<td>$m_{C_4}$[kg/h]</td>
<td>0.6525</td>
<td>0.6450</td>
<td>0.8000</td>
<td>0.6235</td>
<td>0.5775</td>
</tr>
<tr>
<td>$m_{C_5}$[kg/h]</td>
<td>0.8250</td>
<td>0.7108</td>
<td>0.6585</td>
<td>0.6838</td>
<td>0.6871</td>
</tr>
<tr>
<td>$P_{isu}$[kPa]</td>
<td>237.0</td>
<td>263.0</td>
<td>150.0</td>
<td>205.8</td>
<td>172.1</td>
</tr>
<tr>
<td>$P_{dis}$[kPa]</td>
<td>4080</td>
<td>5047</td>
<td>5500</td>
<td>5486</td>
<td>5500</td>
</tr>
<tr>
<td>Net work consumption</td>
<td>0.2840</td>
<td>0.2800</td>
<td>0.4064</td>
<td>0.2948</td>
<td>0.3097</td>
</tr>
<tr>
<td>[kW/(kg NG)]</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>UA [kW/°C]</td>
<td>0.1759</td>
<td>0.1852</td>
<td>0.0699</td>
<td>0.1263</td>
<td>0.1025</td>
</tr>
</tbody>
</table>

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References


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