Surrogate-assisted modeling and optimization of a natural-gas liquefaction plant

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Abstract

In this study, surrogate-assisted modeling and optimization of the single mixed refrigerant process of natural-gas liquefaction is presented. The mixed refrigerant liquefaction process is highly nonlinear owing to the involved thermodynamics that increase the computational burden of any optimization algorithm. To address the computational-burden issue and obtain the results in a reasonable time for the complex single mixed refrigerant process, an approximate surrogate model was developed using a radial basis function combined with a thin-plate spline approach. Even with the reduced model, all the results obtained were comparable with those by rigorous first-principle models. This confirms that all the important characteristics of the model are correctly captured, and the surrogate models of the liquefaction plant are acceptable replacements of first-principle models, especially in computationally demanding situations.

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1. Introduction

Natural gas (NG) is the cleanest fossil-based source of energy. It emits 50% less CO₂ than coal during burning, and owing to its increasing abundance (shale gas, stranded, and hydrates) and cleaner emissions, it is widely considered the best bridge fuel away from coal and oil until zero-carbon-producing renewables can take over. NG is often found in remote locations, and bringing it to the world market requires NG liquefaction that is energy intensive and normally accounts for approximately 40–50% (Qyyum & Lee, 2018) of the total liquefied natural gas (LNG) value chain cost, depending on the plant site conditions (ambient temperature (Park, Won, & Shin, 2016) and relative humidity (Qyyum, Long, Minh, & Lee, 2018), Qyyum et al. (2018) and types of refrigeration cycle (Khan, Karimi, & Wood, 2017; Lim, Choi, & Moon, 2013). Several ways of liquefying NG evolved over time, and virtually all of them use a vapor/mixed refrigerant (MR) compression and expansion cycle to reject heat from the NG to ambient through air/water coolers (Finn, 2009; Mokhatab, Mak, Valappil, & Wood, 2013; Nogal, Kim, Perry, & Smith, 2008). Khan et al. (Khan et al., 2017) in their comprehensive review article presented a retrospective and future perspective of NG liquefaction technologies and stressed that MR-based single-MR (SMR) technology, because of its simple design, compactness, ease of operation, and small footprint, is suitable for small-scale onshore and offshore applications (Cao, Lu, Lin, & Gu, 2006; Khan et al., 2017; Khan & Lee, 2013). Thus, considering the ongoing interest in the SMR process, we attempted to optimize the operation of the SMR process by surrogate-assisted evolutionary optimization targeting compression energy minimization as the objective.

Enhanced operation through optimization has a great impact on the LNG process plant’s economics and ultimately contributes to low carbon emission (Lee, Smith, & Zhu, 2002; Nogal et al., 2008). During the liquefaction optimization, specifications such as the LNG temperature and heat exchanger approach temperature must be met. It is the interaction of these specifications and constraints, coupled with governing thermodynamics that makes the optimization problem even more challenging and computationally demanding. Despite the challenges, several successful attempts have been made toward SMR process optimization using deterministic (Khan, Chaniago, Getu, & Lee, 2014; Khan, Karimi, Bahadori, & Lee, 2015; Khan, Karimi, & Lee, 2016; Pham et al., 2016b), stochastic (Ali, Duong, Khan, Getu, & Lee, 2018; Ghorbani, Mafi, Shir Mohammadi, Hamedi, & Amidpour, 2014; Khan & Lee, 2013), evolutionary (Qyyum, Ali, Long, Khan, & Lee, 2018; Qyyum, Qadeer, & Lee, 2017), and knowledge-based approaches (Khan, Lee, Hasan, & Lee, 2014; Khan, Lee, Rangaiah, & Lee, 2013; Pham et al., 2016a; Pham, Long, Lee, & Lee, 2017). All claimed the superiority of their results in decreasing specific compressor power (compressor power required for liquefying the unit volume of NG). One remaining issue to be addressed that is associated with the optimization...
of complex processes, such as the SMR process, is the computational time involved, which can be hours or even days, as well as the time wasted in finding a good starting point for a deterministic approach and parameter tuning in the stochastic approach.

In this study, a metamodel, also known as a “surrogate-based model,” of the SMR process was developed to reduce the computational effort during optimization. Surrogate modeling (SM) is an effective “model order reduction” approach to simplifying the complex process while capturing all the important features that reduce the computational time during optimization (Biegler, Lang, & Lin, 2014; Caballero & Grossmann, 2008; Choudhury et al., 2017; Oldani et al., 2015; Queipo et al., 2005; Wang & Shan, 2006). SM approaches, such as radial basis function (RBF), polynomial chaos, and kriging metamodels, are often generated from small datasets (Czoad, Sahinidis, & Miller, 2014). Both kriging and RBF use similar mathematical models and thus can give commonly good (or bad) results on the same data. The difference is mostly in tuning the shape factors for the best fit and the time required to do that. RBF does not provide a way to automatically tune the shape factors. Gaussian, multi-quadratic, and inverse multi-quadratic functions are required to specify a shape function value which must manually be experiment to find a good fit by viewing the plot and comparing cross-validation values. On the other hand, RBF linear, cubic, and thin plate spline functions do not require a shape factor value at all, therefore, these are the fastest options computationally. Xie et al. (Xie, Yu, & Wilmowski, 2011) compared traditional neural networks (NNs) and RBF based NNs and confirmed that RBF networks perform more robustly and tolerantly than traditional neural networks upon handling of noisy input data set. For a function approximation, RBF based NNs are especially commended for a surface with regular peaks and valleys for efficient (time of model construction and new predictions) and precise design (Xie et al., 2011). Zakharov et al. (Zakharov, Peach, Sitzmann, & Nicklaus, 2014) applied RBF to quantitative structure-activity relationships in which it was reported that the RBF interpolation gives more accurate prediction compared to RBF NNs. Further, Khairy et al. (Khairy Elsayed, d’Ippolito, & Lacor, 2012) investigated that RBF is faster than the kriging approach.

Nevertheless, not all approaches have the same accuracy for parameter estimation (Palmer & Realf, 2002). Recently, Choudhury et al. (Choudhury et al., 2017) formulated five surrogates for GTL diesel-conventional blend in order to improve the physiochemical properties of GTL based diesel. Dutta et al. (Dutta, Karimi, & Farooq, 2018) applied simulation-based optimization for the techno-economic analysis for LNG heating value reduction. Similarly, Bajaj et al. (Bajaj, lyer, Faruque, & Hasan, 2017) used a trust region based two-phase algorithm for black/grey-box optimization which works on the generation of the surrogate model and its optimization for general types of problems. Yu et al. (Yu, Wang, Zhuo, Wang, & Guo, 2016) presented a surrogate based chemical kinetic modeling for two different jet aviation fuels. In the present study, the SMR liquefaction process was modeled rigorously in a commercial process plant simulator, Aspen Hysys. Then, the date generated from the Aspen Hysys simulation model was regressed using the RBF methodology for the SMR surrogate model. The RBF approach featured a thin plate spline, and a smoothing kernel function was used through MATLAB to extract the data needed for metamodel generation, as shown in Fig 1. Correlation coefficients in the model and various errors for data validation were computed using leave-one-out cross-validation. Once the surrogate model of the SMR process was obtained, two different stochastic optimization algorithms, particle swarm optimization (PSO), and the genetic algorithm (GA) were applied. The results obtained were compared against published works, and the advantages and ease of the adopted method are discussed. In Section 2, the methodology used for the implementation of the metamodel is explained.

Section 3 describes the problem and its formulation for optimization purposes. The numerical results are explained through a composite curve in Section 4. Finally, Section 5 elucidates the main conclusions drawn from the research.

2. Methodology

2.1. Surrogate modeling through RBF

A surrogate is an engineering approximation of a higher-order model that is computationally expensive to use directly. There may be parametric (e.g., polynomial regression, Kriging) and non-parametric (e.g., projection pursuit regression, radial basis functions) approaches for constructing a surrogate model (Queipo et al., 2005). In a comparative study by Jin et al. (Jin, Chen, & Simpson, 2001) for polynomial regressions using various methods such as multivariable adaptive regression splines, RBF, and kriging approaches, RBF outperformed all in terms of accuracy, robustness, efficiency, transparency, and conceptual simplicity. The time involved in the model construction using RBF was in few minutes, whereas it was measured in hours for the kriging. RBF provides an excellent explicit function relationship in terms of transparency. Further, it is relatively straightforward and simple to implement, i.e., no user parameters are involved.

RBF uses a weighted sum of simple functions in an attempt to compete and try to mimic the complex functions. The method uses linear combinations of a radially symmetric function based on Euclidean distance to approximate complex response functions (D. S. Broomhead, 1988; Forrester & Keane, 2009). RBF is a real-valued function and depends on the distance from any reference point (p). It can be represented as follows:

$$\phi(x, p) = \phi(||x - p||)$$

(1)

Any function $\phi$ that satisfies the property in Eq. (1) is an RBF (Yoon, 2001). The type of RBF depends on the choice of $\phi$, which is important for the quality of the approximation and for the existence of the interpolants. Depending upon the Euclidian distance $A = \phi(r) = \phi(||x - x_j||)$, two infinitely smooth radial function kernels are Gaussian $A = e^{- \epsilon r^2}$, $\epsilon \geq 0$ and multi-quadratic: $A = \sqrt{1 + \epsilon r^2}$. As reported by Rocha (Rocha, 2009), the choice of RBF should be a part of optimization problem instead of an a priori choice. In the present study, a piecewise smooth thin plate spline (TPS) defined as $A = r^2 \ln(r)$ was used.

2.1.1. RBF function interpolation and approximation

There are three main stages in constructing a surrogate model: the first is to prepare the data used for metamodeling and choose the RBF function type, and the second is the parameter estimation and training. In the final stage, model testing is performed. For the function interpolation and approximation, n-dimensional Euclidean space $\mathbb{R}^n$ fitted with the Euclidean norm $|| \cdot ||$ is used. The n number of points for function approximation and their respective function value using $f: \mathbb{R}^n \rightarrow \mathbb{R}$ are $f(x_1), f(x_2), ..., f(x_m)$. Next, the approximations are then carried out for k component as: $f: f = (f_1, f_2,..., f_k)$. $f_i : \mathbb{R}^n \rightarrow \mathbb{R}, 1 \leq i \leq k$. Finally, the approximant can be created by the weighted sum of simple functions as follows:

$$\tilde{f}(x) = \sum_{j=1}^{n} \omega_j \phi(||x - x_j||), \ x \in \mathbb{R}^n$$

(2)

where $x_j$ are the data points, for known $f$ value, that lie in $\mathbb{R}^n$, and $x$ is a free variable to evaluate the approximant later. The $\phi$ is a univariate, normally continuous function $\phi: \mathbb{R}_+ \rightarrow \mathbb{R}$ or $[0,
\[ \mathbf{y} = \mathbf{\omega} \times \varphi. \]  

where \( \mathbf{\omega} \) is a vector of constant coefficients or scalar parameters. The function can be evaluated by enforcing \( f(x_t) = y_t \), which produces the system of linear equations represented below:

\[
\begin{align*}
\varphi &= \begin{pmatrix}
\phi(||x_1 - x_1||) & \phi(||x_1 - x_2||) & \cdots & \phi(||x_1 - x_n||) \\
\phi(||x_2 - x_1||) & \phi(||x_2 - x_2||) & \cdots & \phi(||x_2 - x_n||) \\
& \vdots \quad \vdots \quad \ddots \quad \vdots \\
\phi(||x_n - x_1||) & \phi(||x_n - x_2||) & \cdots & \phi(||x_n - x_n||)
\end{pmatrix} \mathbf{\omega} = \mathbf{y},
\end{align*}
\]

where \( \mathbf{\omega} = [y_1, y_2, \ldots, y_n]^T \).

The weights \( (\omega_i) \) can be estimated by solving Eq. (3), by using linear least squares (Mongillo, 2011). Choosing a suitable RBF kernel function is an important point of discussion, although many choices are available.

2.1.2. Basis functions

The choice of basis functions will determine which methods are suitable for solving Eq. (3). The interpolation matrix \( (\varphi) \) is symmetric positive definite. The interpolation matrix

\[
\mathbf{t}^T \mathbf{\varphi} \mathbf{t} > 0
\]

for every nonzero vector \( \mathbf{t} = [t_1, t_2, \ldots, t_n]^T \in \mathbb{R}^n \). Similarly, a symmetric kernel \( \varphi: \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R} \) is a positive definite if

\[
\sum_{i=1}^{m} \sum_{j=1}^{m} \varphi(x_i, x_j) t_i t_j > 0
\]

for any points \( x_1, x_2, \ldots, x_m \) in \( \mathbb{R}^n \) and every nonzero vector \( \mathbf{t} \in \mathbb{R}^m \). In an RBF interpolation with one basis function centered on each data site, Eq. (4) is a result of Eq. (5). Therefore, if \( K \) is a positive definite kernel, then the matrix \( \varphi \) defined in Eq. (3) is a positive definite matrix.

In this study, a relatively simple kernel TPS, alternatively known as a piecewise smooth RBF kernel, was adopted. In this approach, no shape parameter \( (\varepsilon) \), which has a significant impact on the accuracy of interpolation, is required to define, which therefore is the computationally fastest option. This is additionally beneficial because the nature of the LNG problem is unknown, and, hence, the value of the shape factor is difficult to choose. The corresponding TPS kernel function is defined as:

\[
A = \varphi(r) = r^2 \ln(r).
\]

2.2. Adaptive surrogate-assisted modeling and optimization

Using a surrogate model for optimization dramatically improves the computational efficiency. The significance of the strategy adopted and techniques used in this study, such as choosing the search algorithm, infill criteria, and adaptive sampling nature, are explained below briefly.

Evolutionary search algorithms such as GA and PSO are increasingly applied to solving complex real-world problems. These algorithms are attractive because they are good at passing on poor objective value regions quickly while simultaneously exploring several basins of attraction more aggressively; additionally, they help in assessing the surrogate model. In this work, the exploration ability of population-based global search is enhanced by the symmetric Latin hypercube design (SLHD) space-filling sampling technique, which offers a compromise between computing effort and design optimality (Ye, Li, & Sudjianto, 2000). SLHD is a special form of LHD and has good ‘built-in’ properties towards the optimal design. SLHD generates a symmetric Latin hypercube design with a goal to offer a compromise between computing effort and design optimality. The symmetry of SLHD provides some orthogonal properties. Specifically, Morris and Mitchell (Morris & Mitchell, 1995) first noticed that a large number of the optimal LHDs obtained are SLHDs and referred to them as ‘fold-over designs’. Intuitively, they claimed that the optimal designs are considered to have good space-filling properties. This claim was further verified by Ye et al. (Ye et al., 2000) by using a simulation study to compare random SLHD and LHDs with respect to both entropy and minimum inter-site distance criteria and later presented an algorithm for SLHD. After finding the basins of attraction, the exploitation step is performed with the sole focus to improve the accuracy in the optimum region. To provide optimization with a good model, an infill strategy is employed to enhance the general accuracy of the model by min-
imizing the mean square of error (MSE) in the optimum region. A minimum point response surface is used to select the next sample point. Later, the minimum point of the surrogate model is used as new evaluation.

Furthermore, an adaptive sampling strategy is added in which, initially, a certain number of points are sampled with some additional points that effectively increase the accuracy of the generated surrogate model. An adaptive sampling strategy quickly takes the experiment to the optimum function value (Wu & Hamada, 2011).

Fig. 2 shows an example to construct an adaptive surrogate model for optimization. An explanation of the overall strategy adopted in this work is explained below.

I. Initial parameter sets are generated using a Latin hypercube design-of-experiments method to run the simulation. The objective function values are then computed at all initial parameter/sample points to satisfy some space-filling criterion using lower and upper bounds of the parameter, as in Fig. 2(a).

II. RBF is featured with the thin plate spline kernel, and the SM is chosen for representing the response surface of the simulation model. Given the type of surrogate modeling, the surrogate model is built by fitting a statistical model to the performance measures of the simulation model at the sample points.

III. New sample points (red circles) for the parameters are generated using an adaptive sampling strategy to favor new sample points in the promising regions. Then, these new samples are used to update the existing response surface, as in Figs. 2(b) and 2(c).

IV. Finally, the convergence of the simulation is carried out based on an updated surface. The simulation model is run on current optimal values, and the recorded objective value is checked against previous best. With a better value of the new objective value, old values are replaced. Otherwise, new sets of adaptive samples are generated until the resulting response surface is acceptable, as in Fig. 2(d).

In this way, the fitness function identification changes during the exploration and exploitation steps for continuous optimization of the surrogate model. A flow diagram of the key stages involved in the surrogate-assisted modeling and optimization of the complex model is illustrated in Fig. 3.

3. Problem statement and formulation

Operations optimization of the LNG processing plant is an industrially important problem with the potential to improve process efficiency, leading to economic benefits. Most recently, Qyyum et al. (Qyyum et al., 2017) presented a comprehensive review of the design optimization of LNG processes, including SMR, DMR, C3MR, Cascade, and APX. They reviewed almost all optimization studies that have been presented corresponding to optimization of LNG plants with different deterministic/stochastic and heuristic algorithms (Qyyum et al., 2017). To date, no one study has focused on the computational efforts (required time) for the design optimization of LNG processes in order to reduce the overall energy requirements. In this context, the proposed surrogate-assisted modeling approach significantly reduces the computational time by reducing the model complexity and performs better on several selected metrics. Mousavi and Shourian (Mousavi & Shourian, 2010) reported the adaptive sequential space filling (ASSF) metamodeling method and the multi-objective adaptive recursive metamodeling optimization approach to improving water quantity planning
in lakes and reservoirs. They used PSO, a metaheuristic optimization algorithm, and concluded that ASSF can find a good candidate solution but not the global one, depending on the error criterion, by using significantly fewer simulations with the minimum computational burden. Wang et al. also recommended the use of adaptive surrogate modeling and optimization and found that minimum interpolating surface is the most effective sampling strategy, but they failed to provide an exact solution (Wang et al., 2014). The surrogate-assisted modeling approach is consistently giving better results for low- to medium-scale models, and it can assist greatly in optimization, as is apparent from the results presented in Section 4.

The efficacy of the discussed surrogate-assisted modeling approach (see Section 2) was tested on the SMR process of NG liquefaction by (Khan, Lee, & Lee, 2012) and shown in Fig. 4. A rigorous model of the SMR process was developed using Aspen Hysys, a commercial process plant simulator. The basis and feed conditions used for the simulator are summarized in Table 1. NG entered the LNG exchanger at ambient temperature and elevated pressure, as illustrated in Fig. 4, and exchanged latent and sensible heat with the refrigerant mixture evaporating over a range of boiling. After leaving the exchanger, the MR in a superheated state (stream-5) was restored to higher pressure and ambient temperature through a series of compression cooling assemblies. The compression energy requirement for restoring MR from suction to discharge pressure was the main energy consumption.

3.1. Simulation basis and optimizing variables

Table 1 lists the feed conditions and other assumptions used in this study, which is taken from Khan et al. (Khan et al., 2012), used for simulating the SMR process in Aspen Hysys. The Peng Robinson equation of state was used for calculating the thermodynamic properties. Compression energy minimization was the optimization objective, because many researchers have suggested that the selected object can create the best fit between the hot and cold
composite curves (CCs), consequently leading the process toward reversible operation (Ali, Qyyum, Qadeer, & Lee, 2018; Hatcher, Khalilpour, & Abbas, 2012; Khan & Lee, 2013; Khan et al., 2012; Qyyum et al., 2018; Qyyum et al., 2018; Qyyum et al., 2018; Qyyum et al., 2017). The key decision variables affecting the overall operational performance in SMR process are the refrigerant compositions, MR degree of superheat, MR suction, and discharge pressures. The optimization problem was constrained by the minimum internal temperature approach (MITA) of 2–3°C in the cryogenic heat exchanger and the LNG product stream temperature of −150°C. The constraints were folded within the objective using the exterior penalty function (EPF) method. Optimization was carried out by varying the decision variables within the given bounds (Table 2) while keeping the amount of LNG flashed during atmospheric storage less than 10%.

3.2. Mathematical objective formulation and constraint handling

The following formulation of objective combined with decision variables and constraints was used in this study.

\[
\text{Minimize } f(X, p) = W_i \sum_{k=1}^{4} w_k
\]

subject to:

\[
h_i(X, p) = 0, \text{ equality constraints, } i = 1, \ldots, l,
\]

\[
g_i(X, p) \leq 0, \text{ inequality constraints, } i = 1, \ldots, l
\]

\[
X^l \leq X \leq X^u, \quad i = 1, 2, \ldots, n
\]

where \( X = [F_{NG}, F_{C_1}, F_{C_2}, F_{C_3}, F_{R}, T_{MR}] \) represents a vector of the key decision variable, \( W_i \) denotes the total power required in multistage compression, and \( p \) is the vector of process parameters (assumed as a fixed value).

Constraints: The EPF method was applied to fold both constraints into the single objective function (Venkataraman, 2001) so that the stochastic optimization engine can run.

\[
\text{Minimize } F(X, p, r_h, g_h) = f(X, p) + P(X, p, r_h, g_h)
\]

\[
X^l \leq X \leq X^u, \quad i = 1, 2, \ldots, n = 6
\]

Table 2

<table>
<thead>
<tr>
<th>Properties</th>
<th>Lower bound</th>
<th>Upper bound</th>
<th>Design constraints</th>
</tr>
</thead>
<tbody>
<tr>
<td>( F_{NG} ) mass flow (kg/h)</td>
<td>0.1506</td>
<td>0.3514</td>
<td>1. ( \Delta T_{\text{min}} \geq 3.0°C )</td>
</tr>
<tr>
<td>( F_{C_1} ) mass flow (kg/h)</td>
<td>0.3408</td>
<td>0.7952</td>
<td>2. The degree of superheat of MR ( \geq 36°C )</td>
</tr>
<tr>
<td>( F_{C_2} ) mass flow (kg/h)</td>
<td>0.3312</td>
<td>0.7728</td>
<td>3. ( T_{\text{LNG}} \leq -157.0°C ), LNG product temperature</td>
</tr>
<tr>
<td>Condenser pressure (bar)</td>
<td>1.7580</td>
<td>4.6880</td>
<td>4. Vapor fraction of LNG ( \leq 10.0% )</td>
</tr>
<tr>
<td>Temperature of MR after expansion (°C)</td>
<td>−162.0</td>
<td>−152.0</td>
<td></td>
</tr>
</tbody>
</table>
The penalty function is expressed as follows:

\[
P(X, p, r_h, r_g) = r_h \left[ \sum_{k=1}^{l} h_k(X, p) \right]^2 + r_g \left[ \sum_{l=1}^{m} \left( \max\{0, g_l(X, p)\} \right) \right]^2
\]

\[g_1 = \Delta T_{\text{min}} \geq 3^\circ C\]
\[g_2 = T_{\text{INC}} \leq -157^\circ C\]  
where \(f\) is the compression energy function and \(P(X, p, r_h, g_h)\) is the penalty function vector. The \(r_h\) and \(r_g\) are the penalty constants set as 0 for equality constraints \(h_k\) and 1 for inequality constraints.

4. Results and discussion

4.1. Computational time through surrogate-assisted modeling

In this study, the surrogate-assisted modeling approach featuring TPS of RBF was used for SMR process model reduction. The reduced model was optimized with GA and PSO. Six decision variables were used in the surrogate model building and attempted to follow two potential constraints, i.e., the MITA and LNG end flash temperature as shown by Eq. (10). Furthermore, in the SM fifteen initial set of design simulations were used for initial model building. A total 300 maximum number of simulations were taken as a convergence criterion for both SM and optimization task.

For the sake of reliability, three solutions of the surrogate-assisted modeling approach were used for each optimizing algorithm. All the constraints (MITA, end flash gas (EFG) fraction and MR degree of superheat) were precisely satisfied during optimization, giving confidence in the optimized results. Table 3 represents the optimization results with and without using a surrogate-assisted model. The computational time required by a 3.3-GHz processor with 32-GB RAM for optimization without the surrogate-assisted model was 5.8717 h through GA and 1.066 h by PSO. When the same computer specifications were used for the surrogate-assisted model, the computational time required for optimization dropped to 6.749 min for GA and 4.059 min for the PSO algorithm. The difference in time required by GA and PSO with/without a surrogate-assisted model is not the topic of interest here, and readers are referred to other research for the details (Panda & Padhy, 2008; Souza Lima, Lapa, Pereira, da Cunha, & Alvim, 2011). In general, it was observed and suggested by several authors that PSO outperforms GA in terms of its computational time requirement (Hassan, Cohanim, de Weck, & Venter, 2005; Rajendra & Pratihar, 2011; Samsami, 2014).

4.2. Optimized LNG plant performance

4.2.1. Composite curve analysis

This work is focused on making the LNG process operations more energy efficient through optimization that can yield results in the acceptable computational time limit. For this, the surrogate-assisted modeling approach was applied to obtain the optimization results. The optimal results were physically explained by CC analysis, which provided a good way of visualizing the difference between the optimized and base case results. The gap between the cold and hot CCs represents the process irreversibility. Although some irreversibility in the process is inevitable through optimization, this irreversibility can be reduced by bringing the CCs closer. The closing down of CCs naturally minimizes the MITA value in the heat exchanger. However, the validity of the optimization results can only be ascertained by keeping the MITA higher than the agreed value of 3°C, although MITA values of 2–3°C (Hasan, Karimi,
Alfadala, & Grootjans, 2009; Pattison & Baldea, 2015; Qyyum et al., 2017) are also acceptable due to the discovery of new material, improvement in the design of the compact heat exchanger, and the manufacturing technique.

Fig. 5 shows the hot and cold CCs for the base case study. Fig. 5(a) indicates CCs on the scale of heat flow vs. temperature profiles. The result in Fig. 5(a) illustrates that the MITA is already satisfied at the heat exchanger cold end and that, along with the length of the heat exchanger, some extra refrigerant of the suboptimal composition is flowing that artificially inflates the CCs, indicating room for improvement. Fig. 5(b) explicitly shows the approach temperature between cold and hot CCs along the length of the exchanger and how it increases from 3°C to 25°C in the temperature range of −160°C to −75°C, and then decreases from 25°C to 15°C in the temperature range of −75°C to −50°C. Thereafter, it increases sharply to 68°C and then decreases linearly to 3.5°C in the temperature range of −50°C to 40°C. The components of MR boil at different temperatures and provide cooling in the heat exchanger at different temperatures, and they correspond to the decrease and increase in the approach temperature in the heat exchanger. Refrigeration is expensive at the coldest temperatures, and little closing of CCs in that temperature range translates into significant efficiency improvement. Little can be done for the approach temperature of 68°C in the temperature range of −50°C to 40°C, because the MR must exit the heat exchanger in a superheat state to avoid damaging the compressor blade at the suction head. Figs. 6 and 7 show the optimized results using the surrogate model for the GA and PSO algorithms, respectively. All the efforts of optimization are restricted in the temperature range of −160°C to −75°C, as illustrated in Figs. 6 and 7.

In comparison with Fig 5, significant improvement is visible in narrowing down of CCs all through the range of −160°C to −70°C. This improvement in the CCs is a clear indication of liquefaction efficiency improvement, which is also apparent from the numbers in Table 4.

Figs. 8(a) and 8(b) show the optimization results using GA and PSO for approach temperature vs. heat flow for the hot/cold composite curve. The approach temperature decreased by an order of magnitude in the optimized case, causing CCs to become close in the low-temperature range. Throughout the range of −160°C to −65°C, the PSO algorithm outperforms GA while the approach temperature remains 3°C.

4.2.2. Overall LNG plant optimal performance

A summary of optimization results along with the optimum decision variables is shown in Table 4. A maximum of 10% of the NG was specified to be converted to EFG after the subcooled LNG was flashed to atmospheric pressure. Table 5 shows the compression power used in every stage along the compression assembly. The compression ratio in each stage was calculated to be less than 2.5 (Lee, Tak, Lee, Ko, & Moon, 2015).

4.2.3. Validation of heat exchanger performance

The optimized performance of the cryogenic exchanger is shown in Table 6. The surrogate-assisted modeling was successful in finding the values of optimizing variables that ensure a close temperature approach between the hot and cold streams over the entire length of the heat exchanger, resulting in improved energy efficiency. The efficiency of the surrogate-assisted modeling can be
clearly seen through a comparison of the composite curves and exchanger performance.

The overall specific energy requirement using the proposed optimal values was found about 3.6% higher than the previously optimized SMR process by Khan et al. (2012), which is based on rigorous first-principle model, as shown in Table 7. Although the optimal performance obtained by the surrogate-assisted optimized SMR process was little lower than the previous optimized process by Khan et al. (2012), the optimality still seems to be reasonably close to the result based on a rigorous model. Note that the liquefaction rate directly affects the overall specific energy requirement and the required power increases as the liquefaction rate increases (Qyyum, Qadeer, Lee, & Lee, 2018). The lower optimal performance from the proposed study can be partly due to different liquefaction rates applied to both studies: a liquefaction rate of 95.3% was used in the proposed study, whereas 90% in the previous study by Khan et al. (2012).

5. Conclusions

The optimization of SMR process of NG liquefaction using surrogate-assisted modeling approach was presented. The results were obtained within an acceptable time frame nevertheless of applying computationally intensive stochastic optimization approaches. The optimal performance obtained using the surrogate-assisted modeling methodology was reasonably close to that from the rigorous model-based approach. This shows that the proposed surrogate-assisted modeling can capture all the important characteristics of the first-principle liquefaction plant model and can replace a rigorous model when the computational time is more important than exact results. The surrogate-assisted modeling provided the advantage of reducing the computational burden in op-
timization, which was two orders of magnitude lower than for any other reported approach. Therefore, further improvement in finding optimal conditions could be possible by applying more sophisticated and computationally intensive stochastic optimization algorithms. Surrogate-assisted modeling of liquefaction plants can be a good alternative in model predictive control, where the model solved multiple times in a short duration for predicting the trends.

**Declaration**

The authors declare no competing financial interest.

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**Supplementary materials**

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.compchemeng.2018.08.003.

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