CHEMICAL ENGINEERING TRANSACTIONS
VOL. 88, 2021
A publication of AIDIC
The Italian Association of Chemical Engineering
Online at www.cetjournal.it
Guest Editors: Petar S. Varbanov, Yee Van Fan, Jiří J. Klemeš
Copyright © 2021, AIDIC Servizi S.r.l.
ISBN 978-88-95608-86-0; **ISSN** 2283-9216
DOI: 10.3303/CET2188079

Framework for Embedding Process Simulator in GAMS via Kriging Surrogate Model Applied to C3MR Natural Gas Liquefaction Optimization

Lucas F. Santos[a,*], Caliane B. B. Costa[a], José A. Caballero[b], Mauro A. S. S. Ravagnani[a]

[a] Chemical Engineering Department, State University of Maringá, Marigá, Brazil
[b] Chemical Engineering Department, University of Alicante, Alicante, Spain
lfs.francisco@gmail.com; pg54347@uem.br

Rigorous black-box simulations are useful to describe complex systems. However, it cannot be directly integrated into mathematical programming models in some algebraic modeling environments because of the lack of symbolic formulation. In the present paper, a framework is proposed to embed the Aspen HYSYS process simulator in GAMS using kriging surrogate models to replace the simulator-dependent, black-box objective, and constraints functions. The approach is applied to the energy-efficient C3MR natural gas liquefaction process simulation optimization using multi-start nonlinear programming and the local solver CONOPT in GAMS. Results were compared with two other meta-heuristic approaches, Particle Swarm Optimization (PSO) and Genetic Algorithm (GA), and with the literature. In a small simulation evaluation budget of 20 times the number of decision variables, the proposed optimization approach resulted in 0.2538 kW of compression work per kg of natural gas and surpassed those of the PSO and GA and the previous literature from 2.45 to 15.3 %.

1. Introduction

1.1 Natural gas liquefaction process

Natural gas is a cleaner fossil fuel compared to oil and coal, for example, that has gained popularity in the past decades to overcome the growing global energy demand. To be transported and commercialized safely and efficiently, the natural gas has to be liquefied to reduce its specific volume and flammability. This liquefaction is an energy-intensive cryogenic refrigeration process that cools the natural gas to about -160 °C so it is in the liquid state at near atmospheric pressure (Khan et al., 2017). Among different configurations of refrigeration cycles, the propane-precooled mixed refrigerant (C3MR) is highlighted by both researchers and practitioners as an efficient alternative, and it is the most used liquefaction technology in LNG plants worldwide. The C3MR process consists of two refrigeration cycles operating in series as illustrated in Figure 1. The first cycle operates with pure propane that provides heat sinks at different temperature levels to pre-refrigerate the natural gas and the mixed refrigerant, which is used in the second cycle to liquefy the natural gas stream.

1.2 Black-box optimization problem

Despite its current high efficiency, optimization techniques have been used extensively to enhance further the energetic efficiency of these processes in the design or operation level (Austbø et al., 2014). One difficulty of optimizing these processes is modeling them. It involves considering rigorous thermodynamic calculations at ambient and cryogenic conditions, for nonideal solutions that change phase in a multi-stream heat exchanger (MSHE). For that computation task, sequential-modular chemical process simulators are very useful because they have implemented state-of-the-art thermodynamic libraries as well as numerical methods to converge these iterative calculations.

Paper Received: 25 April 2021; Revised: 7 July 2021; Accepted: 12 October 2021
Please cite this article as: Santos L.F., Costa C.B.B., Caballero J.A., Ravagnani M.A.S.S., 2021, Framework for Embedding Process Simulator in GAMS via Kriging Surrogate Model Applied to C3MR Natural Gas Liquefaction Optimization, Chemical Engineering Transactions, 88, 475-480 DOI:10.3303/CET2188079

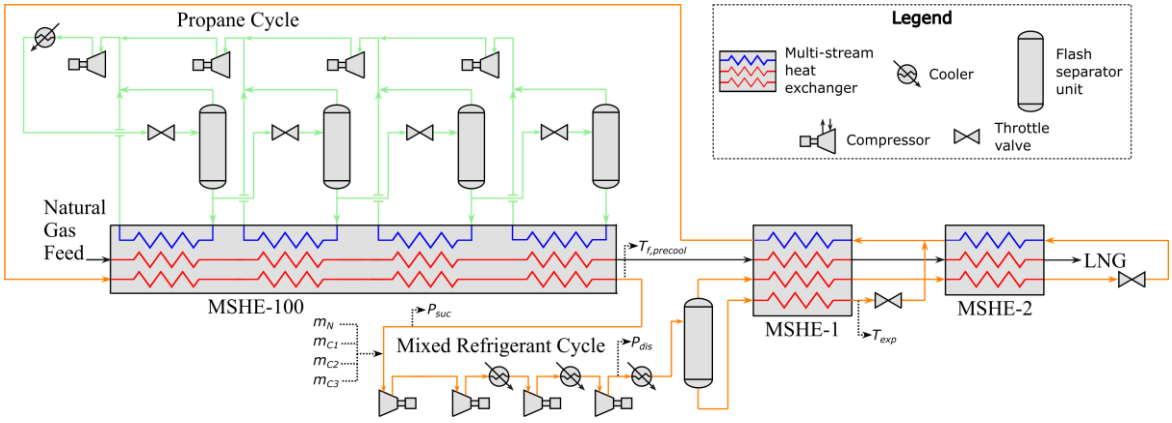

Figure 1: C3MR natural gas liquefaction process flow diagram.

Knowing that the models in these process simulators are in black-box fashion and that the optimization objective and constraints functions depend on the simulations, these black-box optimization problems are such that

$$\min_{\mathbf{x} \in D} \ f(\boldsymbol{x}) \qquad s.t. \ \ \boldsymbol{g}(\boldsymbol{x}) \leq 0, \tag{1}$$

in which f and $\boldsymbol{g}$ do not have symbolic formulation, but for a given $\boldsymbol{x} \in D \subseteq \mathbb{R}^n$, the values of $f(\boldsymbol{x})$ and $\boldsymbol{g}(\boldsymbol{x})$ are calculated in the simulation. For natural gas liquefaction processes, the objective function f is usually net compression power consumption, exergy destruction, heat exchanger area, or total cost. The constraints $\boldsymbol{g}$ are regarding the process operation, for example assuring a minimum temperature driving force in the heat exchangers, only vapor in the compressors, practical pressure ratios, minimum liquefaction ratio, and others.

1.3 Literature review on C3MR optimization

Some attempts to solve the problem in Eq(1) that is formulated to optimize the simulation of C3MR natural gas liquefaction process are now reviewed. Wang et al. (2011) investigated the energy consumption minimization of a C3MR natural gas liquefaction process based on rigorous process simulation in Aspen Plus, the sequential quadratic programming solver built in the simulator, and in-depth thermodynamic analysis. Hatcher et al. (2012) proposed a systematic analysis of optimization formulations for the C3MR natural gas liquefaction process that focused on identifying the most appropriate formulation considering four objective functions related to the operational aspects and four centered on design aspects using Aspen HYSYS for process simulation and its built-in BOX solver for optimization. Khan et al. (2015) considered the performance of a sequential coordinate randomization search method for optimizing single-mixed refrigerant and C3MR natural gas liquefaction processes using Aspen HYSYS for process simulations. Ghorbani et al. (2016) investigated the economic and exergetic optimization of C3MR natural gas liquefaction process using a GA employing single and multi-objective functions with Aspen HYSYS for process simulations. Mortazavi et al. (2016) analyzed the gradient-assisted robust optimization technique to design a refrigerant mixture for C3MR natural gas liquefaction cycles with an exaggerated variation in feed gas composition with Aspen HYSYS for process simulations. Qyyum et al. (2020) investigated a single-solution-based Vortex Search approach to find the optimal design variables corresponding to minimal energy consumption for C3MR using Aspen HYSYS for process simulations.

Differently from direct methods, another kind of optimization technique that can be applied to simulations is the surrogate-based (Caballero and Grossmann, 2008). Ali et al. (2018) used radial-basis functions as surrogates to model and optimize the single-mixed refrigerant natural gas liquefaction process employing GA and PSO to optimize the surrogate problem. Later, Santos et al. (2021a) developed a kriging-assisted framework with the probability of feasible improvement acquisition function optimization using PSO to guide the global search of the black-box problem for single-mixed refrigerant natural gas liquefaction design. Local search with the Nelder-Mead algorithm in the penalized simulation was also considered for local refinement (Santos et al., 2021b).

Despite the promising results of surrogate-based approaches to simulation optimization problems, they have not been used for the C3MR natural gas liquefaction process optimization. Also, none of the current literature on natural gas liquefaction process optimization used the full potential of surrogate-based methods, which is introducing simple algebraic formulation to the black-box functions for efficient gradient-based optimization. Instead, meta-heuristic methods have been used to the surrogate problem. Then, given the importance of the C3MR natural gas liquefaction process and the literature gap on surrogate-based optimization methods to black-

box problems applied to the C3MR process, the objective of the present paper is the application of a framework to embed black-box chemical process simulator to algebraic modeling language (conventional mathematical programming problem) via kriging surrogate model.

2. C3MR optimization

2.1 Process simulation

The C3MR natural gas liquefaction process illustrated in Figure 1 is simulated in the chemical process simulator Aspen HYSYS using Peng-Robinson equation of state and Lee-Kesler for enthalpy and entropy calculations. The thermodynamic package and the following process specifications and considerations are accordingly with the literature (Khan et al., 2015). The natural gas stream is considered to be at 5 MPa and 32 °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. Its mass flow rate is a basis of calculation of 1 kg h^{-1}. This material stream leaves the last MSHE at -149.5 °C, so that, when expanded to 120 kPa, it remains 92 % in the liquid phase at -158.6 °C.

The considered decision variables in the present paper are mixed-refrigerant component mass flow rate of nitrogen (m_N), methane (m_{C1}), ethane (m_{C2}), and propane (m_{C3}), suction and discharge pressure (P_{suc} and P_{dis}), expansion temperature (T_{exp}), and final pre-refrigeration temperature ($T_{f,precool}$), illustrated in Figure 1. The remaining degrees of freedom in the propane cycle are the temperature of the hot streams leaving the heat exchangers, and pressure drops. These temperatures are calculated so that the temperature decrease in each stage is the same $(T_{NG} - T_{f,precool})/4$. The pressure drop in the MSHE-1 is 25 kPa for hot streams and null for propane, and it is 25 kPa in the propane cooler. In the mixed-refrigerant cycle, the remaining degrees of freedom are intermediate pressures and temperatures, temperature of the hot streams leaving the MSHEs, and pressure drops. The intermediate pressures are determined to guarantee a constant compression ratio in all four compressors $(P_{dis}/P_{suc})^{1/4}$. The intermediate temperatures are 40 °C. The temperature of all hot streams leaving the multi-stream heat exchangers are considered to be the same, *i.e.* expansion temperature (T_{exp}) for the first one and -149.5 °C for the second one. The pressure drops in the MSHE-2 and MSHE-3 are 50 kPa for hot streams and 5 kPa for cold streams, and it is 25 kPa for the mixed-refrigerant coolers.

2.2 Process optimization

Given the process description, specifications, and considerations in Section 2.1, and considering that the main economic and environmental issue in natural gas liquefaction processes is the energy consumption for the compression system of the refrigeration cycles, the process optimization problem is as follows:

$$\begin{aligned} &\min_{\mathbf{x}\in D} \; f(\boldsymbol{x}) = \frac{\sum_{p\in PM} W_p(\boldsymbol{x})}{m_{NG}} \\ &s.t. \;\; \boldsymbol{g_l}(\boldsymbol{x}) = 1 - \frac{MITA_l(\boldsymbol{x})}{dTmin} \leq 0, \quad l = 1, \dots, n_{MSHE}, \end{aligned} \tag{2}$$

in which, for a given $\boldsymbol{x} = [m_N, m_{C1}, m_{C2}, m_{C3}, P_{suc}, P_{dis}, T_{exp}, T_{f,precool}]$, $W_p(\boldsymbol{x})$ is the compression power of the pressure manipulator $p \in PM$ the set of compressors and pumps, $MITA_l(\boldsymbol{x})$ is the minimum internal temperature approach or minimum temperature driving force along the l^{th} MSHE, $dTmin$ is the minimum value of $MITA$ allowed, considered to be 3 °C, D is a box constraint for decision variables $\boldsymbol{x}$ (defined in Section 4), and m_{NG} is the mass flow rate of the natural gas stream.

3. Optimization framework

The proposed framework is based on a previous work (Santos et al., 2021a), in which kriging models are used to replace the expansive-to-evaluate, noisy, black-box objective and constraints functions that depend on the chemical process simulation. The major difference now is that, instead of using acquisition function (*e.g.* probability of feasible improvement) optimization to lead the search for feasible optimum of the black-box problem, the surrogates are optimized directly in a standard nonlinear programming (NLP) problem.

3.1 Kriging model

The kriging model is an interpolative data-driven model derived as the best linear unbiased predictor that has been used with promising success as surrogates of expansive-to-evaluate, noisy, and/or black-box functions in black-box optimization problems. A thorough derivation of kriging can be found in Lophaven et al. (2002), but here, for mathematical background, a simplified version of the kriging model with Gaussian process regression is presented. The kriging model $\hat{f}$ predicts the value of the true function f, given some data set, such that

$$\hat{f}(\boldsymbol{x}) = \hat{\beta} + \boldsymbol{r}(\boldsymbol{x})^T \boldsymbol{R}^{-1}(\boldsymbol{Y} - \boldsymbol{1}\hat{\beta}), \tag{3}$$

in which $\hat{\beta} = \frac{\boldsymbol{1}^T \boldsymbol{R}^{-1} \boldsymbol{Y}}{\boldsymbol{1}^T \boldsymbol{R}^{-1} \boldsymbol{1}}$, and $\boldsymbol{R}$ is correlation matrix at sampled data $\boldsymbol{X}$ considering the following correlation model:

$$\mathcal{R}(\boldsymbol{\theta}, \boldsymbol{x}^i, \boldsymbol{x}^j) = \exp\left[-\sum_{h=1}^{n} \boldsymbol{\theta}_h \left(\boldsymbol{x}_h^i - \boldsymbol{x}_h^j\right)^2\right]. \tag{4}$$

Also, $\boldsymbol{r}(\boldsymbol{x})$ is the vector of correlation between the untried point $\boldsymbol{x}$ and the data $\boldsymbol{X}$, $\boldsymbol{Y}$ are the values of the function being modeled at the sampled points, $\boldsymbol{1}$ is a column vector of m entries so that m is the number of sampled points, and $\boldsymbol{\theta}$ are the kriging parameters determined to maximize the likelihood of the model given the data.

3.2 Surrogate optimization problem

Considering the kriging model as in Eq(3) and Eq(4) that can be adjusted for f and $\boldsymbol{g}$, and after some algebra, the optimization problem in Eq(2) can be reformulated in algebraic formulation using the surrogate models such that

$$\begin{aligned} &\min_{\mathbf{x} \in D} \ \hat{f}(\boldsymbol{x}) = \hat{\beta} + \sum_{i=1}^{m} \boldsymbol{\alpha}_i \exp\left[-\sum_{h=1}^{n} \boldsymbol{\theta}_h \left(\boldsymbol{x}_h^i - \boldsymbol{x}_h^j\right)^2\right] \\ &s.t. \ \ \hat{\boldsymbol{g}}_{\boldsymbol{l}}(\boldsymbol{x}) = \widehat{\beta c}_l + \sum_{i=1}^{m} \boldsymbol{\alpha c}_i \exp\left[-\sum_{h=1}^{n} \boldsymbol{\theta c}_h \left(\boldsymbol{x}_h^i - \boldsymbol{x}_h^j\right)^2\right] \leq 0, \quad l = 1, \dots, n_{MSHE}, \end{aligned} \tag{5}$$

where $\boldsymbol{\alpha} = \boldsymbol{R}^{-1}(\boldsymbol{Y} - \boldsymbol{1}\hat{\beta})$ and $\boldsymbol{\alpha c} = \boldsymbol{R}^{-1}(\boldsymbol{G_l} - \boldsymbol{1}\hat{\beta})$, and $\boldsymbol{G_l}$ is the $\boldsymbol{g}_l$ value at the sampled points $\boldsymbol{X}$. For a given data set $\boldsymbol{X}$, $\boldsymbol{Y}$, and $\boldsymbol{G}$, and trained kriging models $\hat{f}$ and $\hat{\boldsymbol{g}}$, $\hat{\beta}$, $\widehat{\beta c}$, $\boldsymbol{\theta}$, $\boldsymbol{\theta c}$, $\boldsymbol{\alpha}$, and $\boldsymbol{\alpha c}$ are constant and, therefore, parameters in the surrogate optimization problem. Thus, the decision variables are only $\boldsymbol{x}$ in this standard NLP problem.

3.3 Optimization algorithm

The present optimization algorithm includes three environments: programming workspace (MATLAB), process simulator (Aspen HYSYS), and algebraic modeling system (GAMS). The first step is connecting MATLAB and Aspen HYSYS via object linking and embedding technology using the MATLAB built-in function “actxserver” to create in its environment a component object model server of the HYSYS application with the process simulation variables and methods. Then, m_0 initial samples in D are generated employing the Latin Hypercube algorithm to maximize the minimum distance between points in the design space. For each sample point in $\boldsymbol{X}$, the rigorous simulation is performed to calculate $\boldsymbol{Y}$ and $\boldsymbol{G}$. Given the data sets $\boldsymbol{X}$, $\boldsymbol{Y}$, and $\boldsymbol{G}$, the kriging models are adjusted for f and $\boldsymbol{g}$ as in Eq(3) to maximize the likelihood of the model considering the available data with the MATLAB implementation of an interior-point method in the built-in function “fmincon” to determine the $\boldsymbol{\theta}$ and $\boldsymbol{\theta c}$ parameters of the kriging models. After adjusting the kriging models, the surrogate optimization problem is ready to be solved in GAMS. To do so, MATLAB communicates with GAMS to send the values of parameters $\hat{\beta}$, $\widehat{\beta c}$, $\boldsymbol{\theta}$, $\boldsymbol{\theta c}$, $\boldsymbol{\alpha}$, and $\boldsymbol{\alpha c}$ via GDX (GAMS Data eXchange) files, which provide an interface to read and write values of GAMS sets, parameters, variables, and equations. After sending the parameters' values, MATLAB calls the GAMS environment to solve the NLP problem using the MSNLP solver with CONOPT for NLP subproblems. Then, GAMS writes back to MATLAB a GDX file with the optimization results $(\boldsymbol{x}^*, \hat{f}^*, \hat{\boldsymbol{g}}^*)$ so it can calculate rigorously the value of f and $\boldsymbol{g}$ at $\boldsymbol{x}^*$ in the Aspen HYSYS simulation and append the new data to $\boldsymbol{X}$, $\boldsymbol{Y}$, and $\boldsymbol{G}$. The incumbent solution is updated if the current value of f improves previous solutions feasibly ($\boldsymbol{g} \leq 0$). This process is iterated until a limit of sampled points m_f is reached or if the surrogate optimization fails to provide a promising candidate of solving the original black-box optimization problem five times (probable convergence).

4. Results

The optimization framework presented in Section 3.3 is applied to the C3MR natural gas liquefaction optimization problem as in Eq(5) with initial sample size $m_0 = 10n$, where n is the number of decision variables that is equal to 8, and the budget of simulation evaluations is $m_f = 20n$. The design space D is given by $[0.33\boldsymbol{x_{base}}, 1.66\boldsymbol{x_{base}}]$, except the temperatures that are bounded heuristically, and the nitrogen mass flow rate, which lower bound of zero to consider no nitrogen in the mixture, as presented together with the heuristically determined base case $\boldsymbol{x_{base}}$ in Table 1. This table also presents the best result from running three times the present approach with the above-mentioned parameters as well as the results from running well-established meta-heuristics of global optimization, PSO, and GA. For a fair comparison, the main parameters of PSO and GA are chosen so that the simulation evaluation budget m_f is not violated; therefore, $2n$ particles or individuals and 10 iterations or generations. To further enhance the validity of the present results, they are compared to

two literature results from Khan et al. (2015) and Qyyum et al. (2020), who also investigated the C3MR liquefaction process optimization with the same process specifications, considerations, and constraints.

Table 1: C3MR natural gas liquefaction optimization results

Decision variables	Base Case	Lower bound	Upper bound	Present approach	PSO	GA	Khan et al. (2015)	Qyyum et al. (2020)
m_N [10^2 kg h^{-1}]	20.00	0.000	33.20	1.482	13.12	20.42	9.000	8.000
m_{C1} [10^2 kg h^{-1}]	60.00	19.80	99.60	39.48	55.20	55.11	51.30	44.90
m_{C2} [10^2 kg h^{-1}]	100.0	33.00	166.0	82.05	103.3	117.1	83.00	84.30
m_{C3} [10^2 kg h^{-1}]	60.00	19.80	99.60	58.77	58.35	73.42	53.20	56.90
P_{suc} [kPa]	250.0	82.50	415.0	210.3	369.5	351.8	330.0	275.0
P_{dis} [10 kPa]	400.0	132.0	664.0	317.5	426.1	408.9	500.0	434.3
T_{exp} [°C]	-115.0	-135.0	-100.0	-126.4	-118.9	-118.2	-133.4	-130.6
$T_{f,precool}$ [°C]	-30.00	-37.00	-25.00	-37.00	-32.07	-33.41	-33.34	-33.34
				Other results				
Power consumption [kW (kg NG)$^{-1}$]	0.3270	-	-	0.2538	0.2732	0.2926	0.2629	0.2600
$MITA_1$	9.754	-	-	3.010	3.251	4.144	3.015	3.000
$MITA_2$	12.59	-	-	3.007	5.872	10.09	-	-
UA_1 [kJ (°C s)$^{-1}$]	103.8	-	-	236.8	200.1	194.2	203.1[a]	220.8[a]
UA_2 [kJ (°C s)$^{-1}$]	8.985	-	-	18.06	19.63	13.96	15.03[a]	11.90[a]
Q_1	1304	-	-	1051	1209	1266	1155[a]	1144[a]
Q_2	138.6	-	-	100.2	156.1	164.6	85.10[a]	84.80[a]

[a]These results were not originally reported by the authors, but simulated for the present work.

From the results in Table 1, it is possible to infer that the present optimization approach is efficient to solve the C3MR natural gas liquefaction optimization problem using few simulation evaluations considering the improvement of 22.4 % from the base case value and compared to well-established meta-heuristics of PSO by 7.64 and GA by 15.3 %. Also, the present results surpass the ones from the considered literature by 3.59 and 2.45 %, even though the other authors did not restrict the number of simulation runs.

From an engineering point of view, the results in Table 1 show a trade-off between power consumption and heat exchanger area (estimated from UA that is the heat exchanger area time the global heat transfer coefficient). In other words, the proposed C3MR configuration is very efficient energetically at the price of having bigger MSHEs. That kind of result is expected because high energy efficiency is achieved when the process generates as little entropy as possible. Following the calculation as in Santos et al. (2021a), the entropy generation of the results obtained by the present approach is 1.782, the PSO is 2.014, and the GA is 2.251 kJ °C^{-1} per kg of natural gas processed. And, knowing that the operation units that produce the most entropy are the MSHE-1 and MSHE-2 (12.1, 16.2, and 17.6 %, respectively), the energetically-favorable C3MR process has the hot and cold Composite Curves of these heat exchangers close together, *i.e.* small temperature driving force throughout the heat transfer. On the other hand, small temperature driving forces implicate bigger equipment to the heat transfer task. Figure 2 presents the almost perfect match between Composite Curves in the MSHEs of the optimized C3MR process.

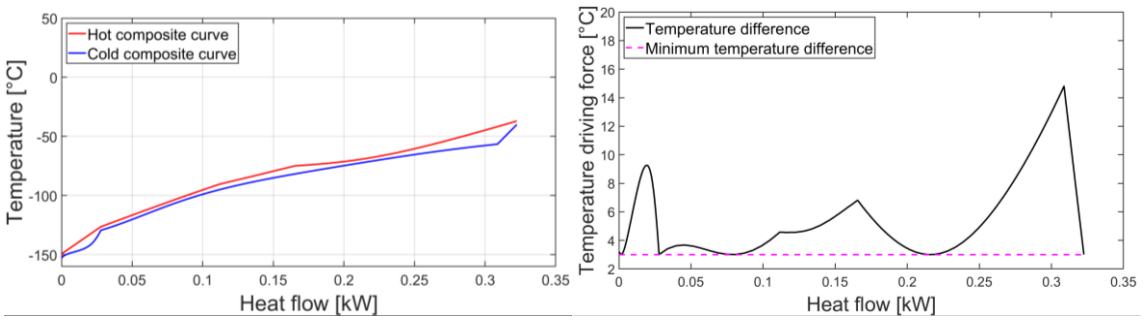

Figure 2: Temperature and driving force profiles in the MSHEs from optimized C3MR process.

The trade-off between energy consumption and MSHE area could be dealt with multi-objective optimization, which is beyond the scope of the present paper but should be considered in future work. Also, the proposed C3MR process presents some particularities compared to previous results. First, the light components flow rate in the mixed refrigerant (m_N and m_{C1}) is diminished, which makes the refrigerant heavier and requires less power for compression. The pressure levels of the proposed process are lower than the other results, which is not favorable for energy efficiency as the refrigerant volume is increased. However, it is an interesting result from operation point of view as the compressor suction and discharge pressures are milder. Finally, the final precooling temperature in the optimized result shows that using the propane precooling section to the limit (lower bound) favors the process energy efficiency.

5. Conclusions

This paper presented a framework to embed black-box chemical process simulators to algebraic modeling language via kriging surrogate model. It was applied to the C3MR natural gas liquefaction process optimization. The kriging surrogate models are adjusted to data generated by the simulator-dependent, black-box objective, and constraints functions from the optimization problem, which introduces a simple symbolic formulation to be used in standard mathematical programming in GAMS. This approach showed to be efficient as it converges in short simulation evaluation budget of 20 times the size of the problem to good results of 0.2538 kW per kg of natural gas, which surpassed the ones from PSO and GA in 7.64 and 15.3 % with the same evaluation budget and the results from the literature that optimized the same C3MR process from 2.45 to 3.59 %. For future work, the present framework can be tested to more complex natural gas liquefaction processes, and more difficult analyses, such as multi-objective optimization, robust design, and process synthesis.

Acknowledgements

The authors acknowledge the National Council for Scientific and Technological Development – CNPq (Brazil), processes 148184/2019-7, 440047/2019-6, 311807/2018-6, 428650/2018-0, and Coordination for the Improvement of Higher Education Personnel – CAPES (Brazil) for the financial support.

References

Ali W., Khan M.S., Qyyum M.A., Lee M., 2018, Surrogate-assisted modeling and optimization of a natural-gas liquefaction plant. Computers & Chemical Engineering, 118, 132–142.

Austbø B., Løvseth S. W., Gundersen T., 2014, Annotated bibliography—Use of optimization in LNG process design and operation, Computers & Chemical Engineering, 71, 391–414.

Caballero J.A., Grossmann I.E., 2008, An algorithm for the use of surrogate models in modular flowsheet optimization, AIChE Journal, 54, 2633–2650

Ghorbani B., Hamedi M.-H., Shirmohammadi R., Hamedi M., Mehrpooya M., 2016, Exergoeconomic analysis and multi-objective Pareto optimization of the C3MR liquefaction process, Sustainable Energy Technologies and Assessments, 17, 56–67.

Hatcher P., Khalilpour R., Abbas A., 2012, Optimisation of LNG mixed-refrigerant processes considering operation and design objectives, Computers and Chemical Engineering, 41, 123–133.

Khan M. S., Karimi I., Wood D. A., 2017, Retrospective and future perspective of natural gas liquefaction and optimization technologies contributing to efficient LNG supply: A review, Journal of Natural Gas Science and Engineering, 45, 165–188.

Khan M.S., Karimi I.A., Bahadori A., Lee M., 2015, Sequential coordinate random search for optimal operation of LNG (liquefied natural gas) plant, Energy, 89, 757–767.

Lophaven S.N., Nielsen H.B., Sondergaard J., 2002, DACE - A Matlab Kriging Toolbox.

Mortazavi A., Alabdulkarem A., Hwang Y, Radermacher, R., 2016, Development of a robust refrigerant mixture for liquefaction of highly uncertain natural gas compositions, Energy, 113, 1042–1050.

Qyyum M.A., Yasin M., Nawaz A., He T., Ali W., Haider J., Qadeer K., Nizami A.-S., Moustakas K., Lee M., 2020, Single-Solution-Based Vortex Search Strategy for Optimal Design of Offshore and Onshore Natural Gas Liquefaction Processes, Energies, 13, 1732.

Santos L.F., Costa C.B.B., Caballero J.A., Ravagnani M.A.S.S., 2021a, Kriging-assisted constrained optimization of single-mixed refrigerant natural gas liquefaction process, Chemical Engineering Science, 241, 116699.

Santos L.F., Costa C.B.B., Caballero J.A., Ravagnani M.A.S.S., 2021b, Design and optimization of energy-efficient single mixed refrigerant LNG liquefaction process, Brazilian Journal of Chemical Engineering.

Wang M., Zhang J., Xu Q., Li K., 2011, Thermodynamic-analysis-based energy consumption minimization for natural gas liquefaction, Industrial and Engineering Chemistry Research, 50, 12630–12640.