Energy Efficient Global optimization of Reactive Dividing Wall Distillation Column

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An optimization problem to minimize energy requirements in the synthesis of bio-additive ethyl tertiary butyl ether (ETBE) via reactive dividing wall distillation column (RDWC) is considered. The contribution of the article is to solve a real-world optimization problem by addressing two challenges: 1) finding optimal process conditions in few numbers of simulations and 2) handling mixed-integer variables. An efficient global optimization algorithm is used to find optimal process conditions and adapted to handle both integer and continuous variables. ETBE is produced by the reaction of ethanol and isobutene in RDWC and has proven its niche in reducing the energy requirements for reaction-separation processes. However, the overall economics of the process is governed by the energy requirements. Therefore, it is crucial to find the optimal process conditions for achieving a cost-effective process. Reboiler duty of RDWC, considered as a measure of the energy requirements to be minimized by using the algorithm. Seven variables (four integers and three continuous) are used in the optimization process to minimize the reboiler duty. A very low value of reboiler duty is obtained after doing the optimization, which not only provides an insight when using RDWC but also shows the potential of the algorithm used.

Keywords: ETBE; RDWC; Bayesian optimization; Machine learning; Evolutionary computation; Gaussian processes; Genetic algorithm.

Introduction

In the chemical process industries which involved a reaction mechanism, the process constitutes of a reactor followed by separation units to get pure products. These separation units in case of liquid systems are mostly distillation columns, which require a lot of energy. A number of process intensification (PI) ideas have come up in the past to get products of high purity with least possible energy requirements. Dividing wall columns have been an interesting PI alternative in terms of energy saving in liquid-liquid separations [32,33, 34]. *Reactive dividing wall distillation column* (RDWC) has caught up the interest of research community in Chemical Engineering amongst all ideas. It is a case of high degree of process intensification, as it provides high purity of one reboiler, a dividing wall which splits reactive zone and the separation in a single shell distillation

setup. Design, modelling and simulation of these units have been reported in several studies[1]–[3].

This work is focused on obtaining optimal process conditions to achieve a cost-effective process when using RDWC for the synthesis of ethyl tertiary butyl ether (ETBE). ASPEN plus simulation tool is used for doing simulations. The computation time for one simulation on a computer with Intel i5-4310U, 2 GhZ processor, 4GB RAM is one to two minutes. As mentioned, maintaining the energy requirements when using RDWC is crucial because of economic reasons. Therefore, an expert in the domain needs to find the cost-effective process conditions. To the best of our knowledge, no work exists in the literature, which minimizes the energy requirements for the synthesis of ETBE via RDWC. Therefore, *the contribution of the article is to find optimal process conditions when using RDWC to produce ETBE by minimizing the energy requirements*. Reboiler duty is used as a measure of the energy requirements because reboiler mainly consumes energy in the system for the generation of the vapors. Two challenges are addressed in this work: 1) to find optimal process conditions in few numbers of simulations and 2) to handle mixed-integer variables.

The first challenge is addressed by using a widely used Efficient Global Optimization (EGO) [4] algorithm. The algorithm has been widely used in surrogate-assisted optimization [5]. The algorithm uses Kriging model[5] and finds promising samples to be evaluated with the simulator. However, the algorithm has the potential to find optimal process conditions in few numbers of simulations, it can handle only continuous variables. In this work, seven decisions (or design) variables influence the production. Out of these seven variables, four variables (number of stages, location of liquid and vapor stream, and side draw stage) are integers and three variables (liquid flow rate, vapor split flow rate and the reflux ratio) are continuous (or real). Therefore, the EGO algorithm is adapted to handle both kinds of variables integer as well as continuous.[1]

Ethyl tertiary butyl ether belongs to the renewable class of bio-fuel additives [6] and has certain advantages over other fuel additives. For instance, the blend of ETBE and gasoline gives less amount of emissions of volatile organic compounds, carbon monoxide and nitrogen oxide emissions. The maximum blending level specification for ETBE is 22%

[1] The source code in MATLAB is available from authors

in E10 gasoline and 17.24% (by mass) in E5. As compared to its competitive alternatives such as methyl tertiary butyl ether and ethanol, ETBE has low volatility and blending Reid vapor pressure. Therefore, ETBE can also be used during summertime. Moreover, the anti-hydrophilic nature of ETBE makes it less soluble in water and thus, it is less likely to penetrate and pollute the ground and underground water supplies [7]–[9]. The rest of the article is organized as follows: a brief introduction of the production of ETBE is provided in Section 2 followed by a brief description of RDWC and optimization problem formulation in Section 3. In Section 4, EGO algorithm is summarized with the strategy to handle mixed-integer variables. The results and discussion are detailed in Section 5 followed by conclusion in Section 6.

Ethyl tertiary butyl ether production

Conventionally, ETBE has been produced in a reactor from the reaction between isobutene and ethanol and the mixture is separated in a distillation column for the purification. At given temperature and pressure conditions the side reactions are neglected and the reaction kinetics for the reaction given in 2 are adopted from [10].

$$(CH_3)_2C = CH_2 + C_2H_5OH \leftrightarrow (CH_3)_3COC_2H_5 \qquad (1)$$

$$\mathrm{K_{ETBE}} = 10.387 + \frac{4060}{\mathrm{T}} + 2.89055 \ln \mathrm{T} + 0.0191544\,\mathrm{T} + 5.28586 \times 10^{-5}\mathrm{T}^2 + 5.32977 \times 10^{-8}\mathrm{T}^8$$

$$\mathrm{r_{ET\,BE}} = \frac{\mathrm{m_{cat}k_{rate}a_{EtOH}^2}(a_{iBut} - \frac{\mathrm{K_{ETBE}}}{\mathrm{a_{ETBE}a_{EtOH}}})}{(1+K_A\mathrm{a_{EtOH}})^3}$$

$$\ln \mathrm{K_A} = -1.0707 + \frac{1323.1}{\mathrm{T}}$$

$$\mathrm{k_{rate}} = 7.418 \times 10^{12} \exp(-\frac{60.4}{R\,T}) \qquad (2)$$

In equation (2), $\mathrm{r_{ETBE}}$ is the rate of reaction for the reversible reaction given in equation (1)based on the activities of the reactants and products. The $\mathrm{k_{rate}}$is the rate constant and $\mathrm{K_{ETBE}}$is the ETBE reaction equilibrium constant. The $\mathrm{a_{ETBE}}$, $a_{iBut}$and $\mathrm{a_{EtOH}}$are activity coefficients of ETBE, iButane and ethanol, respectively. $\mathrm{K_A}$ is ethanol adsorption equilibrium constant, R is the universal gas constant, T is the reaction temperature and

m_{cat} is the mass of catalyst. For more details about kinetics, see [11]. In last few years, RDWC columns have been used in application such as in transesterification of carbonates [12] and for the production of methyl acetate hydrolysis [13] because of their several advantages. In such columns, the reactions take place on one side of the wall and the products are separated on the other side of the wall. Therefore, the reactions and separation take place in a single unit.

The commercial production of ETBE started in 1992 by ARCO (Atlantic Richfield Company) and it was initially generated in a reactor via reaction of ethanol and isobutene, catalyzed by acidic ion exchange resin (Jensen and Datta1992). This liquid phase reaction for formation of ETBE from isobutene and ethanol has been reported in several studies [14]–[16].The isobutene feed to be used in this process has been reportedly obtained from catalytic cracker unit of refinery. Braskem international (Brazil) and Sojitz corporation (Japan) are already producing ETBE by reacting ethanol and isobutene.

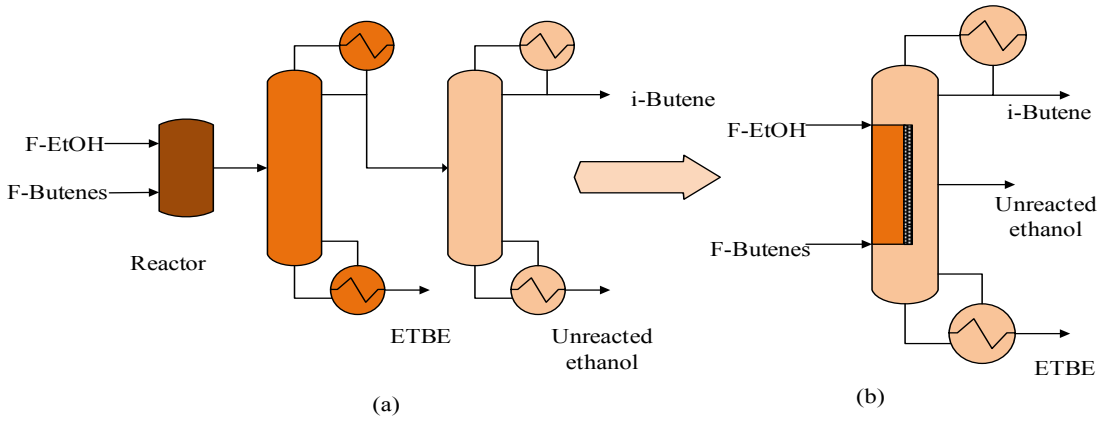

Figure 1: Transition from the traditional sequence to RDWC (a) conventional scheme which consists of reactor followed by two distillation columns (b) reactive dividing wall distillation column.

Table 1: Feed specifications for RDWC

Feed conditions	
Temperature Pressure	30°C 7 atm
Feed flow rates (kmol/hr)	
Ethanol feed Hydrocarbon feed	40 100
Composition of hydrocarbon feed (% mol.)	
Isobutene n-butene	40 60

The traditional method of production requires a lot of plant footprint as well as energy requirements as there are two reboilers which work in the separation process after the reactor [17]. The present work focuses on the reduction of energy requirements of the process by inculcating the reaction and separation process inside a single column (RDWC) as shown in Figure 1.

Reactive dividing wall distillation column for ETBE production.

Reactive dividing wall distillation column is a fully thermally coupled distillation column and can be represented as a Petlyuk column [18]. Simulation of RDWC is carried out using RADFRAC model in ASPEN plus [19], [20]. A post-fractionator arrangement is selected for representation of the RDWC [21]has been shown in Figure 2a and the flowsheet showing two RADFRAC columns has been shown in Figure 2b. Two RADFRAC columns have been used and connected through interconnecting streams as used by [20], these interconnecting streams have been shown in RDWC configuration of Figure 2b. Feed streams have been inserted at the top and bottom of the dividing wall section. The column shown in the Figure shows terms D, S and B; these are the purity of the distillate, side and the bottom product, respectively. Distillate contains mainly the non-reacted butenes, side stream contains unreacted ethanol and the bottom product comprises of ETBE.

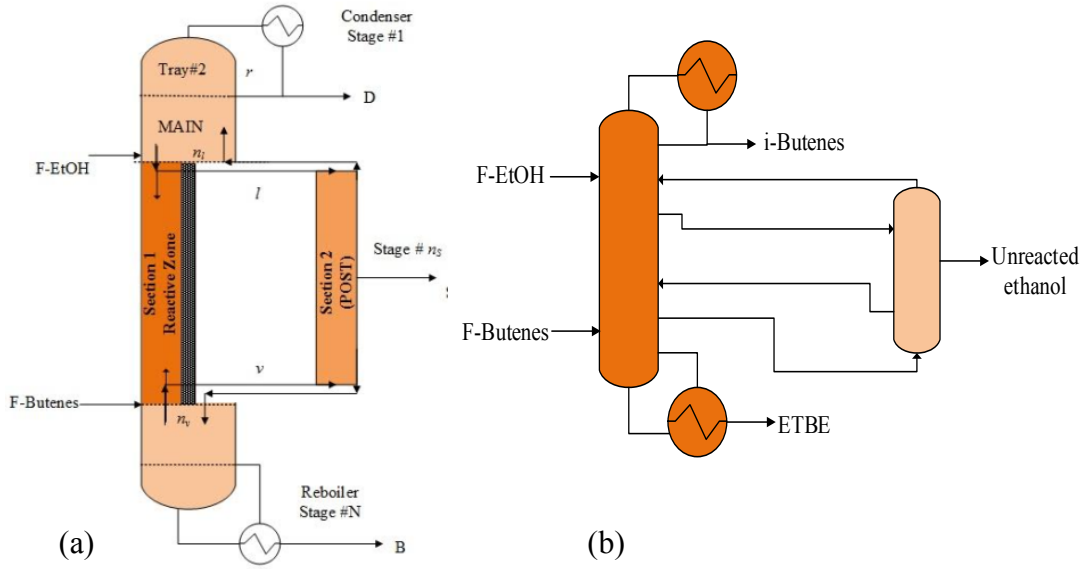

Figure 2a: Post fractionator arrangement to represent RDWC and (b) Two column arrangement of RADFRAC columns to simulate RDWC.

The reaction between isobutene and ethanol is assumed to be a liquid phase equilibrium reaction [11], [21]. The UNIFAC method [11, 35] is used for thermodynamic property calculations of the components present in the reaction system. It can adequately represent the non-ideality of the system, which is owed to the presence of azeotropes [18]. A minimum boiling azeotrope between ethanol and ETBE has been reported for the reaction system at the pressure 950 kPa [10]. The T-x-y diagram and residue curve map (RCM) plot of Figure 3 also demonstrates occurrence of ethanol-ETBE azeotrope. RCM of Figure 3 shows the distillation boundaries and the point where the direction of the curves changes, composition of azeotrope.

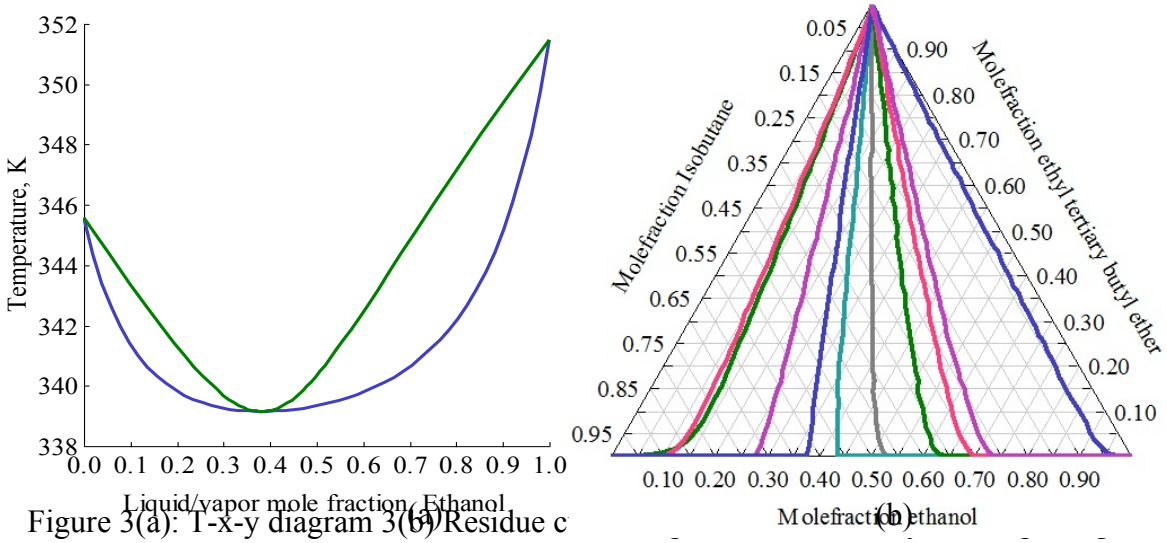

Figure 3(a): T-x-y diagram 3(b)Residue c

the presence of ethanol-ETBE minimum boiling azeotrope in the reactive system.

The stages are counted from top to bottom as can be seen in Figure 2a. The first stage is the condenser (stage 1) and reboiler is numbered *N* which is the last stage. Specifications for the two feed streams- F-EtOH (ethanol feed) and F-butenes (feed containing mixture of butenes) are given in Table I. The temperature and pressure conditions are chosen based on the maximum reaction conversion [22]. The feed stream is a mixture of isobutene 60 % (mol) and n-butenes 40 % (mol). The feed streams are placed at the top and the bottom of the column reaction zone due to the difference in boiling points of the components inside the feed streams. As mentioned, energy requirements of the column are very important for the process to be economical and environmentally viable. Therefore, in this study the reboiler duty (Q_b) is minimized by considering total number of stages (N), locations of liquid (n_l), vapor stream (n_v) and side draw stage (n_s), liquid split flow rate (l), vapor split flow rate (v), and reflux ratio (r) as the 3 design variables. In other words, the heat duty is considered as a function of seven design variables during the optimization process:

$$\mathrm{Q_b} = \mathrm{f}(N, \mathrm{n_l}, \mathrm{n_v}, \mathrm{n_s}, \mathrm{l}, \mathrm{v}, \mathrm{r}) \quad (3)$$

Table 2: Lower and upper bounds of the decision variables

	N	n_l	n_v	n_s	l	V	r
lower bound	22	4	16	2	7.50	29	0.5
upper bound	38	10	22	8	10	47	2.5

Moreover, the optimization of RDWC is itself a complex problem due to interaction of the variables amongst themselves. The variables N, n_l, n_v, n_s, l, v, and r; are interdependent and interact amongst themselves. The lower and upper bounds for the variables considered in this study have been given in Table 2. The limits of variables were chosen according to the material and energy balance of the RDWC based on several simulations prior to optimization. Out of these seven variables, the first four i.e. total number of stages and locations of liquid, vapor and side draw are integer variables and rest are continuous variables.

Efficient global optimization

Many industrial optimization problems use different kinds of simulations which are usually time consuming. Therefore, it is often desired to obtain a solution in few numbers of simulations. In the literature, surrogate or meta-model-assisted algorithms [23] have been applied to such kinds of problems. One of the widely used surrogate-assisted evolutionary algorithm is efficient global optimization (EGO) [4]. The algorithm uses Kriging model and has the potential of obtaining an optimal solution in few numbers of simulations. A flowchart representing the steps of the algorithm is shown in Figure 4. In the first step, the samples are generated e.g. by using some design of experiment (DOE) technique. These samples are then evaluated with the simulator (or

Aspen plus in this case). The values were manually transferred from Aspen plus to the optimization code in MATLAB no interface between the two has been established in the present work.

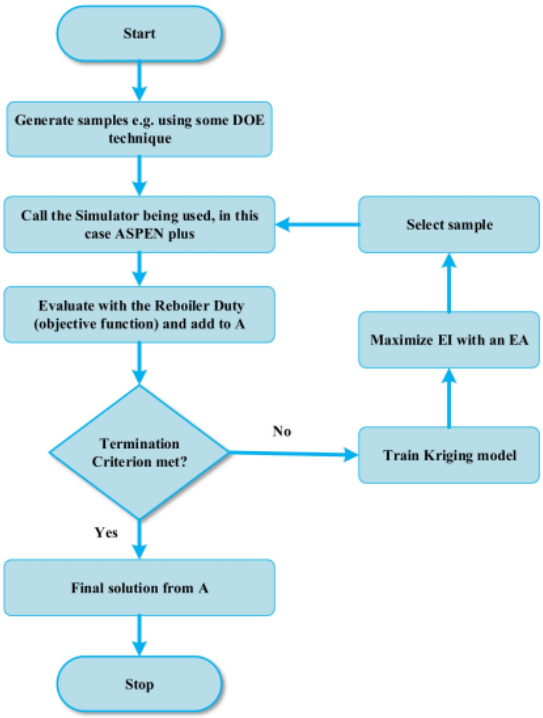

Figure 4: The steps in the EGO algorithm.

The objective function values of these samples i.e. values of reboiler duty Q_b are calculated. The evaluated samples i.e. both the design variables and the corresponding objective function values are stored in an archive A. Solutions in A are then used to build Kriging model for the given objective function. In order to find the next sample point to be evaluated with the ASPEN plus, an infill or an updating criterion is maximized. The main motive of finding a sample by maximizing the criterion is to find a promising sample, which not only enhances the performance of the model but also improve the search efficiency of the algorithm. In EGO, a criterion called Expected Improvement (EI) is used, which balances between both convergence and diversity and can be expressed as:

$$\mathrm{EI} = \begin{cases} \left(y^* - \hat{y}(x)\right)\varphi\left(\frac{y^* - \hat{y}(x)}{\hat{s}(x)}\right) + \hat{s}(x)\phi\left(\frac{y^* - \hat{y}(x)}{\hat{s}(x)}\right) & \text{if } \hat{s}(x) > 0 \\ 0 & \text{otherwise,} \end{cases} \quad (4)$$

where, y^* is the minimum of the objective function value in A, $\hat{y}$ is the approximated value from Kriging model for an input x, $\hat{s}(x)$ is the uncertainty measure of the approximated value and ϕ and φ denote the cumulative distribution function and probability density function, respectively.

The criterion EI is usually a multimodal function and therefore, an evolutionary algorithm is used to maximize the criterion. In this study, genetic algorithm (GA) is used to find an optimum of the criterion at every iteration. The optimal sample obtained by maximizing EI is evaluated with the simulator and the objective function Q_b is calculated and combined with the already evaluated samples in A. This process is continued until a termination criterion is met which is usually the number of evaluations with the simulator. The solution corresponding to the minimum objective function values in A is used as the final solution. The algorithm has the potential to obtain an optimal solution in few numbers of simulations. However, it cannot handle different kinds of variables simultaneously. Therefore, the EGO algorithm was modified by proposing a methodology for handling mixed-integer variables in using the Kriging model.

Kriging (or Gaussian process regression) as a surrogate or meta-model has been widely used in the evolutionary community [24]. One of the main advantages of using the Kriging model is its ability to provide an uncertainty information in addition to the approximated values. Such uncertainty information can be further used in the optimization process to increase the performance of the model and the search efficiency in the algorithm used. Kriging approximates the objective function value of an individual x as:

$$y(x) = \mu(x) + \varepsilon(x); \quad (5)$$

where, $\varepsilon(x)$ is a Gaussian stationary process with the zero mean, variance σ^2 and covariance Ψ i.e. $\varepsilon(x) = N(0,\Psi)$. The mean is represented by μ and is usually assumed to be the form $\mu(x) = \sum_{j=1}^{i} \beta_j g_i(x) = g(x)^T \beta$ with l basis functions and coefficients β. In many cases, $\mu(x)$ is just taken as a constant value to avoid estimating the coefficients β.

For training a Kriging model, first a set of input samples is generated in the design space, which are evaluated with the expensive objective function evaluations. Let matrix $X = [\mathbf{x}^1, \ldots \mathbf{x}^{N_I}]^T$ represent the training data in the decision space with their corresponding objective vector, $\mathbf{y} = [y^1, \ldots y^{N_I}]^T$, where N_I represents the sample size, that is the size of the training data set. The covariance between two samples x^i and x^j is calculated as: $\mathrm{cov}[\varepsilon(\mathbf{x}^i), (\mathbf{x}^j)] = \sigma^2 R(\mathbf{x}^i, \mathbf{x}^j)$, (6)

where R is the correlation function or kernel. The Gaussian kernel $R(\mathbf{x}^i, \mathbf{x}^j) = \exp\left(-\theta\Delta(\mathbf{x}^i, \mathbf{x}^j)\right)$ is the most commonly used, where n is the number of design variables with, θ represent the hyper parameters and Δ is the distance measure between the samples. As mentioned previously, there are two kinds of variables, integers n_i and continuous n_c in the given problem. To deal with different kind of variables, an appropriate distance measure needs to be selected. The approach by Wilson and Martinez was used [25], where different distance measures are suggested to deal with different kind of variables. For integer variables, the Manhattan distance $\Delta_{\text{integer}} =$

$\sum_{t=1}^{t_c}\left|x_t^i - x_t^j\right|$ and for continuous variables, the Euclidean distance $\Delta_{\text{continuous}} = \sum_{t=1}^{t_c}(x_t^i - x_t^j)^2$ are used. To calculate the correlation function $\mathrm{R}(\mathbf{x}^{\mathrm{i}}, \mathbf{x}^{\mathrm{j}})$, these distances arecombined as:

$$\Delta = \sqrt{\Delta_{\text{continuous}} + \Delta_{\text{integer}}}, \tag{7}$$

In this way two different kinds of variables, integers and continuous are handled in using the Kriging model. The correlation is calculated for all input samples and a correlation matrix **R** is generated:

$$\mathbf{R} = \begin{bmatrix} \mathrm{R}(\mathrm{x}^1, \mathrm{x}^1) & \ldots & \mathrm{R}(\mathrm{x}^1, \mathrm{x}^{N_I}) \\ \ldots & \ldots & \ldots \\ \mathrm{R}(\mathrm{x}^{N_I}, \mathrm{x}^1) & \ldots & \mathrm{R}(\mathrm{x}^{N_I}, \mathrm{x}^{N_I}) \end{bmatrix} \tag{8}$$

The covariance matrix Ψ is then calculated as $\Psi = \sigma^2\mathbf{R}$. For a new input $\hat{\mathrm{x}}$, an approximated value $\hat{y}$ from (5) can be written as

$$\hat{\mathrm{y}}(\hat{\mathrm{x}}) = \mathrm{g}^{\mathrm{T}}(\hat{\mathrm{x}})\beta + \mathrm{r}^{\mathrm{T}}(\hat{\mathrm{x}})\mathrm{R}^{-1}(\mathrm{y} - \mathrm{F}\beta), \tag{9}$$

where, **F** is the matrix representation of the vectors $\mathbf{g}(\mathbf{x}^1), \ldots\ldots, \mathbf{g}(\mathbf{x}^{N_I})$and $r(\hat{x})$is the correlation vector of size N_I between the new input $\hat{\mathrm{x}}$ and the training data $\mathbf{x}^1, \ldots\ldots, \mathbf{x}^{N_I}$i.e.

$$r(\hat{\mathrm{x}}) = [\mathrm{R}(\hat{\mathrm{x}}, \mathbf{x}^1), \ldots\ldots, \mathrm{R}(\hat{\mathrm{x}}, \mathbf{x}^{N_I})]^T \tag{10}$$

To get an approximated value from formula (9), estimation of the hyper-parameters β, θ and σ^2 was done. Equation (9) has the generalized least square solution:

$$\beta = (\mathrm{F}^{\mathrm{T}}\mathrm{R}^{-1}\mathrm{F})^{-1}\mathrm{F}^{\mathrm{T}}\mathrm{R}^{-1}\mathrm{y} \tag{11}$$

And the estimated variance $\sigma^2$is given by:$\sigma^2 = \frac{1}{N_I}(\mathrm{y} - \mathrm{F}\beta)^{\mathrm{T}}\mathrm{R}^{-1}(\mathrm{y} - \mathrm{F}\beta)$ (12)

Values of θ can be obtained by maximizing the following likelihood function:

$$\psi(\theta) = -\frac{N_I}{2}(\ln\sigma^2 + \ln 2\pi) - \frac{1}{2}\ln\det(\mathrm{R}) - \frac{1}{2\sigma^2}(\mathrm{y} - \mathrm{F}\beta)^{\mathrm{T}}\mathrm{R}^{-1}(\mathrm{y} - \mathrm{F}\beta), \tag{13}$$

Where, *det* (**R**) is the determinant of the correlation matrix **R**. The uncertainty estimate or estimated mean is then calculated as:

$$\hat{\mathrm{s}}^2(\hat{\mathrm{x}}) = \sigma^2\left[1 - \left(\mathrm{g}(\hat{\mathrm{x}})^{\mathrm{T}}, \mathrm{r}(\hat{\mathrm{x}})^{\mathrm{T}}\begin{pmatrix}\mathbf{0} & \mathbf{F}^{\mathbf{T}} \\ \mathbf{F} & \mathbf{R}\end{pmatrix}\begin{pmatrix}\mathrm{g}(\hat{\mathrm{x}}) \\ \mathrm{r}(\hat{\mathrm{x}})\end{pmatrix}\right)\right]. \tag{14}$$

Results and discussion

This section provides the results by optimizing the reboiler duty Q_b by applying the EGO algorithm. In running the algorithm, some numerical settings need to be defined which are as follows:

1. Number of samples generated in the initial phase: 70.
2. Number of evaluations with the ASPEN plus (including the evaluations of samples generated with the Latin hypercube sampling): 100 Parameter values in using GA with the Kriging model.
3. Population size: 70.

4. Number of function evaluations in using the Kriging model: 10000.
5. Crossover probability: 0.9.
6. Mutation probability: 0.15.
7. Tournament selection size: 2.

The Latin hypercube sampling [26] was used in the design phase to generate the samples in the initial phase. In the literature, there have been several studies in selecting the parameters at different stages of the algorithm. For instance, number of samples in the initial phase [27], crossover [28], mutation [29]and population size [30]. In this article, the details about the sensitivity analysis of these parameters is not provided. Note that in the initial phase, 5 samples did not converge. Therefore, 65 samples were used to train the Kriging model.

The number of evaluations with the ASPEN plus was just kept to 100. In other words, only 35 evaluations were used with the EGO algorithm. It is noteworthy that all the evaluated samples were stored in the archive *A*, therefore, the maximum size of the archive *A* is also 100. In every iteration to maximize the EI criterion, the GA was used with the numerical settings mentioned above. Note that while using GA, the ASPEN plus was not called and only Kriging models were used to find the sample to be evaluated with the ASPEN plus.

The values of reboiler duty with the number of function evaluations (or number of simulations) is shown in Figure 5. As can be seen from the Figure 5, the EGO algorithm obtained a substantial improvement in minimizing the reboiler duty compared to the first 65 evaluations generated with the Latin hypercube sampling. The optimal value of the reboiler duty obtained was 135000 cal/sec or 564.57 kW and the corresponding design variable values were N=25, n_l = 4, n_v= 21, n_s= 5, l =7.63 kmol/hr, v = 46.98 kmol/hr and r= 0.5. The optimal value of the reboiler duty and the variables obtained for the bounds mentioned in Table 2 was 564.57 kW. Plots of the reboiler duty with all seven design variables is shown in Figure 6. As many of the variables values are on the boundary, we updated the bounds of the variables and continued the optimization. The updated bounds of the variables were {20,30}, {2,6}, {18,25}, {2,8}, {7,9}, {40,50} and {0.2,1.0} for N, n_l, n_v, n_s, l, V, and r respectively. With the revised bounds, the reboiler duty was reduced to 510.84kW, which is significantly lower than the previous optimization study. The revised optimal values of variables were: N = 26, n_l = 2, n_v = 21, n_s = 5, l = 7, v = 50 and r = 0.2.

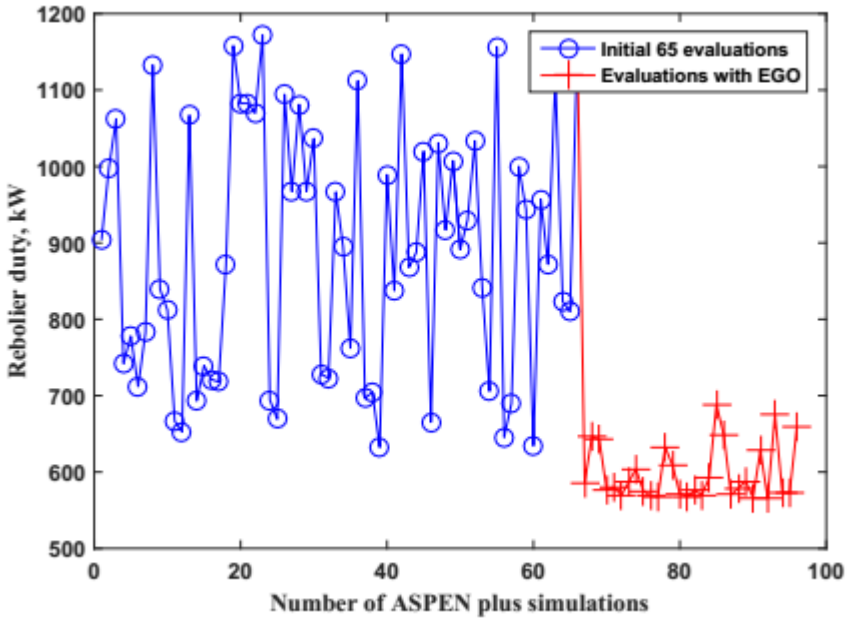

Figure 5: The reboiler duty Q_b with number of simulations.

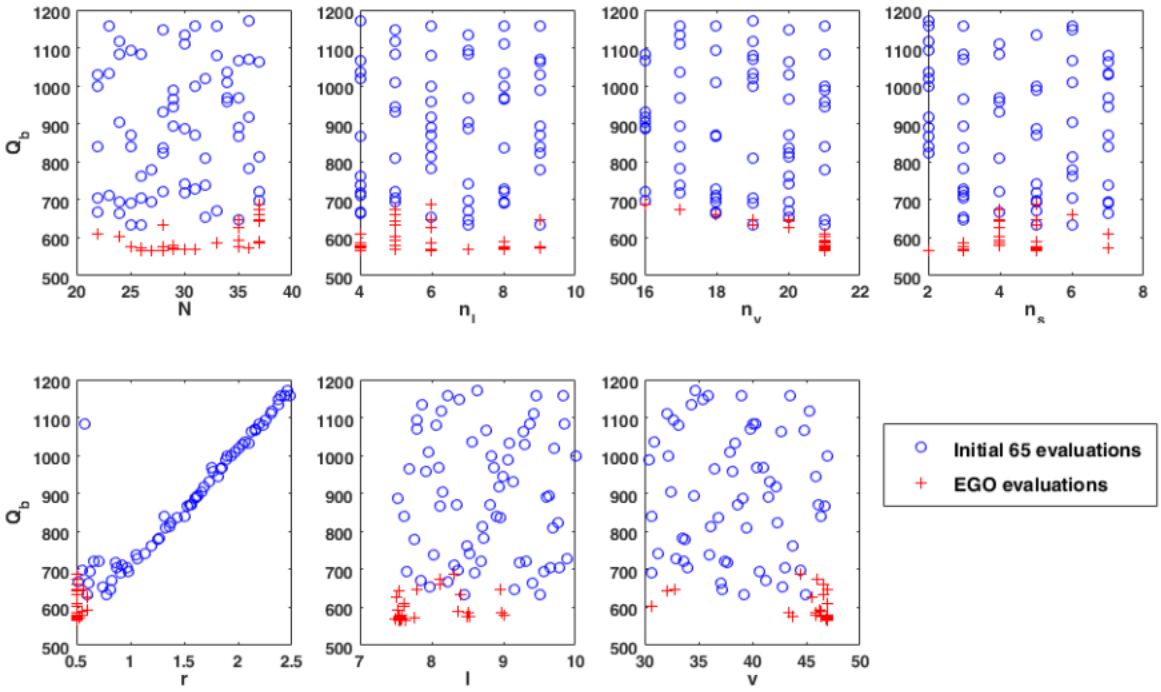

Figure 6: Reboiler duty with all seven design variables

As can be seen in Figure 6, the initial design samples are uniformly distributed for all seven design variables when using the Latin hypercube sampling. After using the EGO algorithm, solutions converged to a small region of the design space for all variables. It is also clearly indicated in Figure 6 that there is a very strong interdependence of the objective function, Q_b and design variables.

The algorithm explored for the number of stages by keeping the reboiler duty very low. The reboiler duty usually decreases with increase in number of stages. However, in this case, the optimal value for the number of stages obtained was 25. Therefore, a sensitivity analysis was done for the number of stages on the reboiler duty by keeping values of other variables fixed to their optimal values. The resulting plot is shown in Figure 6. The reboiler duty decreases with increase in number of stages. However, after 25 stages, there was a slight increase in the reboiler duty. This is due to interaction among variables during the optimization. In other words, instead of doing optimization by using one variable (e.g. number of stages), all variables were used simultaneously. Such behavior clearly shows the importance of doing optimization when many variables need to be optimized simultaneously.

It was observed that lowering the reflux ratio lowers the amount of heat requirements within the distillation column, thus reducing heat input to the column in the form of reboiler duty [31]. This is the reason; the EGO algorithm finds the solution with low reflux ratio. Results of similar nature were obtained for l, v, n_l and n_s. The lesser is the value of vapor split flowrate lesser is the heat requirement of the system, as it is the reboiler which takes up energy for vapor generation. The reboiler duty is not much affected by the variation of total number of stages of the distillation column, or by the location of the vapor and liquid split flowrates. The variation in values of these variables just affects the total cost of the column. From these results it may be inferred that in order to control the energy requirements main variables are reflux ratio and vapor flowrate. The reflux ratio can be controlled by varying the reflux rate and the vapor flow rate is adjusted by changing the boil-up rate of the reboiler which are easy to adjust.

These results provide an insight to the practitioners to achieve the minimum energy requirements. The optimization study reveals the effect of several variables on the reboiler duty. The final value of the reboiler duty 510.84 kW was found to be significantly lower than non-optimized evaluations.

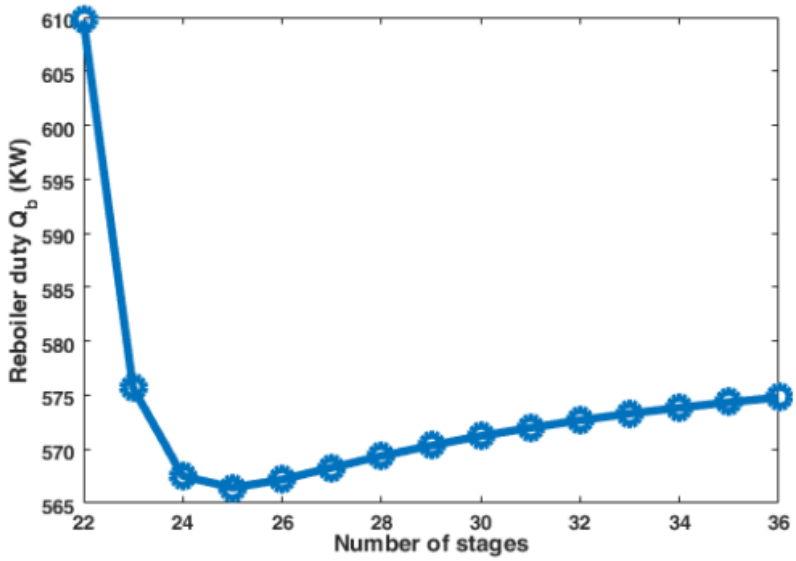

Figure 7: Sensitivity analysis of the number of stages by keeping values other variables to optimal values.

Conclusions

In this work, the main focus was on obtaining optimal process conditions in the synthesis of ETBE via RDWC by minimizing the reboiler duty. A great emphasis was given on obtaining solutions in few number of simulations by using the EGO algorithm. It was adapted to handle different kinds of variables i.e. continuous as well as integer variables, which is a challenge in itself. The algorithm by maximizing the expected improvement balances both convergence and diversity. The results after doing optimization had a very low value of the reboiler duty. This work can be further modified by making an interface between MATLAB and Aspen plus which would be taken up as future work. Moreover, considering costs as objective functions with appropriate variables and comparing the results with other algorithms are also topics for the future research.

Acknowledgements

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APPENDIX

Both capital and operating costs were calculated using the same parameter values obtained when minimizing the reboiler duty. The total cost by adding capital and operating costs with number of simulations is shown in the figure below. As can be seen, after building the models, the cost was very high. This is due to the reason that variables considered in minimizing reboiler duty are not appropriate in minimizing costs. Therefore, we consider making a different optimization problem with costs as objective functions with appropriate variables as a future work.