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Grid-search-and-box-search-assisted coordinate descent methodology for practical retrofit of the existing distillation columns to dividing wall columns

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ABSTRACT

A dividing-wall column (DWC) leading to savings in terms of substantial investment and operating costs, and a significant reduction in CO_2 emission constitutes an optimal solution for distillation process intensification. Recently, industrial applications of the DWC gradually increased although the need for an efficient, practical, and simple to implement optimization methodology persists. This study proposes a practical method that employs coordinate descent methodology, which is assisted by a grid search to avoid local optimal points and box searches to seek a more promising solution to optimize the retrofit of existing distillation columns to DWCs. The optimal DWC structure and operating conditions are determined in a practical and effective manner that is simple to implement and requires minimal simulation runs, which is suitable for industrial uses. The proposed method is examined in the optimal retrofit of a side stream column and a conventional two-column sequence that are widely used in the chemical process industry. The results show that the grid-search-and-box-search-assisted coordinate descent methodology combining mathematical programing techniques and statistical methods effectively avoids local optimal points but also corresponds to a more promising solution, and thus, it is competitive to coordinate descent methodology and response surface methodology that are popularly used in optimization processes in the chemical process industry. The retrofitted DWC systems lead to a substantial decrease in operating costs while effectively removing the bottleneck problem and mitigating CO_2 emission as well. Notably, operating costs are reduced to a maximum of 33.8% and 43.3% in retrofit of side stream columns and conventional two-column sequences, respectively. Both structural and operating variables are effectively and simultaneously optimized. It allows for the identification of interactions between design variables. Furthermore, the carbon dioxide emission is calculated and evaluated when retrofitting to the DWC.

1. Introduction

Distillation is an extremely common process in several chemical process industries such as oil and gas, petrochemical, chemical, biofuel, and biochemical industries. However, it leads to high operating costs and requires massive investment costs (Rong, 2011). Various process intensification techniques were proposed and applied to enhance distillation performance. These include a dividing wall column (DWC), as shown in Fig. 1, and this is one of the best proven configurations in distillation intensification (Halvorsen et al., 2013; Kiss, 2014; Long et al., 2016a). The main targets of most retrofit projects involve reduc-

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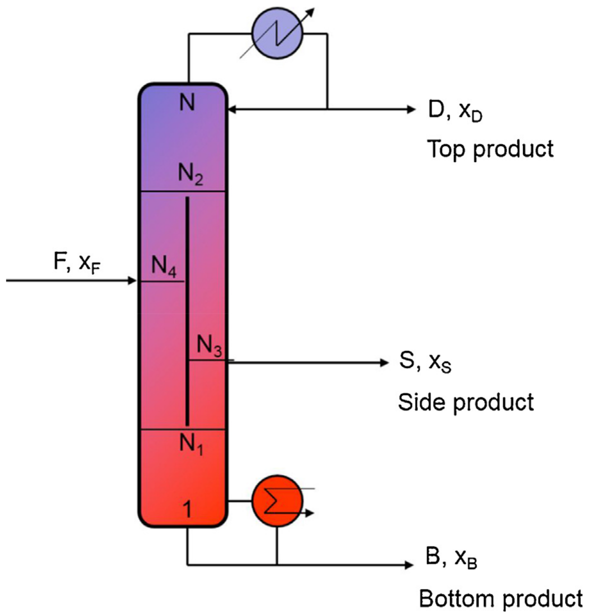

Fig. 1 – A simplified flow sheet illustrating the DWC.

ing energy requirement and/or increasing capacity, and thus a DWC is considered as a primarily attractive solution (Long and Lee, 2014).

The concept of a DWC involves azeotropic and extractive distillation as well as reactive distillation without any large modifications to the column internals (Olujic et al., 2003; Yildirim et al., 2011; Kiss, 2013; Long and Lee, 2014). Two important DWC devices correspond to an internal reflux splitter and a vapor splitter that are used to split liquid and vapor approaching from the column top and bottom, respectively, into sections divided by a wall (Lee et al., 2016). The energy performance of a DWC is deviated by slight fluctuations in the internal flows (Shin et al., 2013; Long and Lee, 2014; Lee et al., 2016). In most existing DWCs, only a liquid split is controlled during operation while it is not possible to arbitrarily adjust a vapor split once the column is fabricated (Lee et al., 2016). This leads to a few operability and controllability issues associated with the limitation of vapor split control during operation. Most recently, a novel active vapor distributor (AVD) was proposed to address the need for vapor split control during DWC design and operation (Kang et al., 2017). In the proposed AVD, vapor splitting was implemented by a modified chimney tray with a specially designed cap. The liquid level of the chimney tray on each end side of the dividing wall section was adjusted to control the vapor flow split. The proposed AVD efficiently adjusted the friction of the vapor flow path without any mechanical moving parts, and thus it realized a more reliable operation of a DWC. Thus, the DWC can constitute a standard column that is considered in separation and purification steps without any critical issues.

A number of DWCs were introduced in the retrofit of existing distillation columns (Kolbe and Wenzel, 2004; Spencer and Plana Ruiz, 2005; Slade et al., 2006; Parkinson, 2007; Premkumar and Rangaiah, 2009; Long et al., 2010; Long and Lee, 2011, 2013). Recently, a suitable candidate for the first industrial application of a fully thermally coupled four-product DWC was suggested (Jansen et al., 2016). The results from the fore-mentioned retrofit projects suggest that the employment of DWC was identified as a good solution with lower capital and operating costs when compared with other conventional methods given that it may achieve higher product purity. Conversely, a few practical difficulties occur in the execution of conceptual design, detailed design, and implementation steps. Specifically, DWC optimization is very important during retrofit projects because it significantly affects the final results of those projects and can constitute a challenge due to the large number of design variables and their interactions.

Various optimization methodologies of DWC were proposed. An external optimization routine based on an evolutionary algorithm that links with the Aspen Plus™ software was suggested (Wenzel and Rohm, 2003). Additionally, a constrained stochastic multiobjective optimization technique based on the use of genetic algorithms (GA) was proposed with the objectives of reducing the energy requirement and total annual cost (Bravo-Bravo et al., 2010). GA is like a black art and fine tuning of all the parameters often depend on trial and error searching. Furthermore, a sequential quadratic programming (SQP) method that was implemented in Aspen Plus™ was proposed (Kiss and Suszwalak, 2012). This methodology is only guaranteed to find a local solution. These methods are based on mathematical programing techniques while a response surface methodology (RSM) based on statistical methods to build an empirical polynomial model was developed to optimize the structure of DWCs (Long and Lee, 2012). RSM is quite powerful, however, a polynomial model is unlikely to be a reasonable approximation of the true functional relationship over the entire space of independent variables.

Coordinate decent methodology (CDM) solves optimization problems by sequentially performing approximate minimization along coordinate directions (Wright, 2015). It corresponds to an iterative method in which each iterate is obtained by setting most components of the variable vector x at their values from the current iteration and approximately minimizing the objective with respect to the remaining components. The main advantages of the CDM include the simplicity of each iteration, simple implementation, and high efficiency (Long et al., 2016b). This methodology is suitable for the optimization of a highly nonlinear and complex system. However, this methodology, like SQP, can get stuck in local optimum.

Thus, there is a need of a new optimization methodology, which should be not only simple, efficient, and practical but also can overcome some above problems related to mathematical and statistical approaches. That methodology should utilize the advantages of mathematical and statistical approaches, while eliminating their disadvantages by supporting each other. This study involved employing a simple, efficient, and practical methodology to optimize DWCs by using CDM that is assisted by grid search (GS) to avoid the local optimal points and box search (BS) to overlook a more promising solution for optimal retrofit of existing distillation columns to DWCs. This methodology was termed as a grid-search-and-box-search-assisted coordinate descent (GSBSCD) methodology. The proposed methodology that combines a mathematical programing technique and a statistical method was implemented in the MS Visual Basic application and connected to the Hysys model via the MS Excel platform. Excel worksheets and Excel Macro were employed to interface and calculate the objectives and to implement the optimization algorithm. Two case studies including the retrofit of a side stream column (SSC) and a two-column sequence, which are widely used in chemical process industry, were employed to validate its application.

2. Design and optimization methodology

2.1. *Design*

The initial design of a DWC structure and operating conditions is easily investigated by using a shortcut design procedure, which is constructed by using a conventional column configuration as shown in Fig. 2 (Long et al., 2010; Lee et al., 2016). Subsequently, as shown in Fig. 3, a rigorous simulation of a DWC based on a configuration including two columns with two recycle loops is implemented. The prefractionator column (*Pre*) without a reboiler and a condenser is modeled by using an absorber column. To solve the *Pre*, a recycled vapor stream and recycled liquid stream to the prefractionator are initially specified (Lee et al., 2016). It is necessary to supply five specifications while simulating the *Main* column because it includes five degrees of freedom. It should be noted that this procedure solves the *Pre* first and then the *Main* column. Another method includes first solving the *Main* column by specifying two inlet streams including *Vapor pre out* and *Liquid pre out* that are based on the shortcut design results. Next, the *Pre* is simulated with