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Optimal design for dividing wall column using support vector machine and particle swarm optimization

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ABSTRACT

Dividing wall column (DWC) is a practical method to reduce energy cost and save capital cost in process intensification technologies for distillation columns. However, the optimization of DWC is a highly nonlinear and multivariable problem, which requires intensive research and investigation. The purpose of this paper is to study the optimal design for DWC using a combination of support vector machine (SVM) and particle swarm optimization (PSO). By generating a SVM model for optimization of DWC, the speed of calculation improves a lot. And SVM is based on rigorous mathematical theory, which overcomes the effect of human experience. PSO is applied to optimize the thermally coupled liquid and vapor flow rate and the stage numbers of different DWC sections. The proposed combination method achieves an encouraging result and proves to be a promising method for optimal design of DWC.

1. Introduction

Distillation is a widely used and significant separation technology in chemical industries. However, despite its simplicity and flexibility, distillation is still an energy- and capital-intensive process. Process intensification technologies are able to reduce energy cost and save capital cost (Kiss, 2014). Dividing wall column (DWC) has been successfully implemented in industry, which provides a promising trend for process intensification. It is a single shell, direct material coupling distillation column, as shown in Fig. 1, which demands much less energy, capital and space (Chu et al., 2011; Dejanovic et al., 2010; Staak et al., 2014; Yildirim et al., 2011). Compared with conventional configurations, the energy saving of DWCs is up to 30% (Emtir et al., 2001; Hernandez et al., 2003). Furthermore, DWCs can be applied to azeotropic, extractive, and reactive distillations, which lead to azeotropic dividing wall columns (ADWC) (Kiss and Suszwalak, 2012; Le et al., 2015; Sun et al., 2011; Wu et al., 2014), extractive dividing wall columns (EDWC) (Kiss and Ignat, 2012; Kiss and Suszwalak, 2012; Tavan et al., 2014; Xia et al., 2012) and reactive dividing wall columns (RDWC) (Delgado-Delgado et al., 2012; Ignat and Kiss, 2013; Kiss et al., 2009; Lee et al., 2012; Qian et al., 2015; Wang et al., 2014b).

The difficulties in the design of DWC are owing to its inner complex structures, and the optimal design of DWC is a highly nonlinear and multivariable problem. Therefore, the optimal design for DWC has been investigated by different researchers. Dunnebier and Pantelides (1999) studied the optimal design of DWC using detailed column models and mathematical optimization. Vazquez-Castillo et al. (2009) addressed the application of genetic algorithms to the optimization of intensified distillation systems for quaternary distillations. Bravo-Bravo et al. (2010) used a constrained stochastic multiobjective optimization technique to design an extractive dividing wall column. Gomez-Castro et al. (2011, 2008) considered a multi-objective genetic algorithm (GA) to design columns with dividing walls. Sangal et al. (2012) used Box–Behnken design (BBD) under response surface methodology (RSM)

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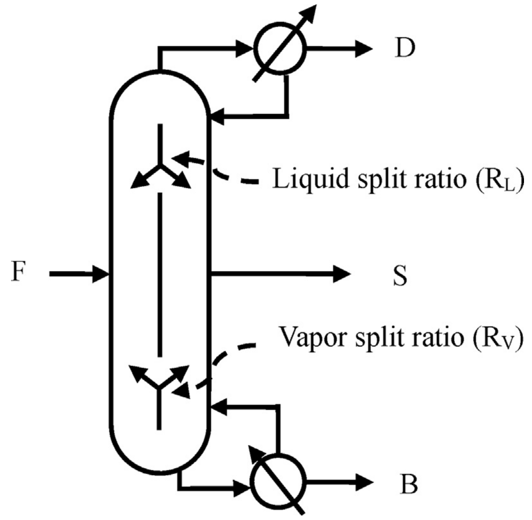

Fig. 1 – Dividing wall column.

for the optimization of the structural and operational parameters and evaluated the effects of these parameters and their interactions on the energy efficiency of a DWC. Safe et al. (2013) studied model reduction and optimization of a reactive dividing wall batch distillation column inspired by response surface methodology and differential evolution to achieve high purity for ethyl acetate and decreases the batch time. Wang et al. (2014a) explored the optimal design of reactive dividing wall column and azeotropic dividing wall column. Ge et al. (2014) studied a systematic optimization method based on combination of radial basis function neural network (RBFNN) and genetic algorithm (GA) for optimal design of DWC. Qian et al. (2015) investigated a particle swarm optimization (PSO) algorithm for optimal design of reactive dividing wall column (RDWC). Chemical process design is a multi-objective optimization problem which can be solved efficiently by calculating the Pareto frontier, a set of Pareto-optimal compromises. Burger et al. (2014) describes how multi-objective optimization and decision support techniques have been implemented in the process simulation software. Commercial flowsheet simulators suffer from limitations in problem formulation flexibility and numerical instabilities which potentially turn process simulation into a tedious task, so Hoffmann et al. (2016) embedded the process simulation into an optimization problem to find feasible design parameters using suitable nonlinear optimization algorithms. The very high complexity resulting from combination of green process engineering and rigorous model-based approaches poses great challenges for process design and design engineers, so Zitzewitz and Fieg (2016) presents an innovative methodology for the model-based process design with superimposed multi-objective optimization.

This paper studies the optimal design for a three-product dividing wall column using support vector machine (SVM). The optimal design of DWC is difficult to achieve because it is a highly nonlinear and multivariable problem. Simultaneous process simulation and optimization requires large amount of calculation. And the convergence problem is very difficult and time-consuming. The advantage of generating a SVM model for optimization of DWC is that the speed of calculation improves a lot. Also, SVM is able to avoid the effect of human experience, which plays an important role in neural network (NN), because SVM is based on statistical learning. Besides, SVM can provide more accurate model using less data. Furthermore, SVM ensures good spread ability and solves dimensional problems ingeniously. In machine learning, SVMs are learning models with associated learning algorithms which analyze data that used for classification and regression analysis. Support vector regression (SVR) is used in this paper. SVM nonlinear regression firstly makes input space become high-dimensional Hilbert space through nonlinear mapping $x \to \varphi(x)$, and then goes on to linear regression. And SVM solves the regression function in the high-dimensional space.

2. Process description

The separation of ethanol, *n*-propanol and *n*-butanol is used as a case study of optimization of the three-product DWC. The fresh feed is equimolar liquid and the feed flow rate is 1 kmol/h. The relative volatilities for ethanol (A), *n*-propanol (B) and *n*-butanol (C) are 4.46, 2.16 and 1, respectively.

The simulation of the case study uses the direct material coupling configuration, as shown in Fig. 2, which is thermodynamically equivalent to the three-product DWC as shown in Fig. 1. All steady state designs are simulated rigorously employing Aspen Plus. The distillation model is equilibrium stage. The thermodynamic model uses the NRTL liquid activity equation.

In Fig. 3, the V_{min} diagram (Halvorsen and Skogestad, 2003a,b) gives us the overall separation difficulty by showing minimum vapor flows in various sections required for sharp separation of equimolar A-B-C feed. The y-axis shows the normalized minimum boilup (V_B/F) and the x-axis shows the net product withdrawal (D/F) in a conventional two-product

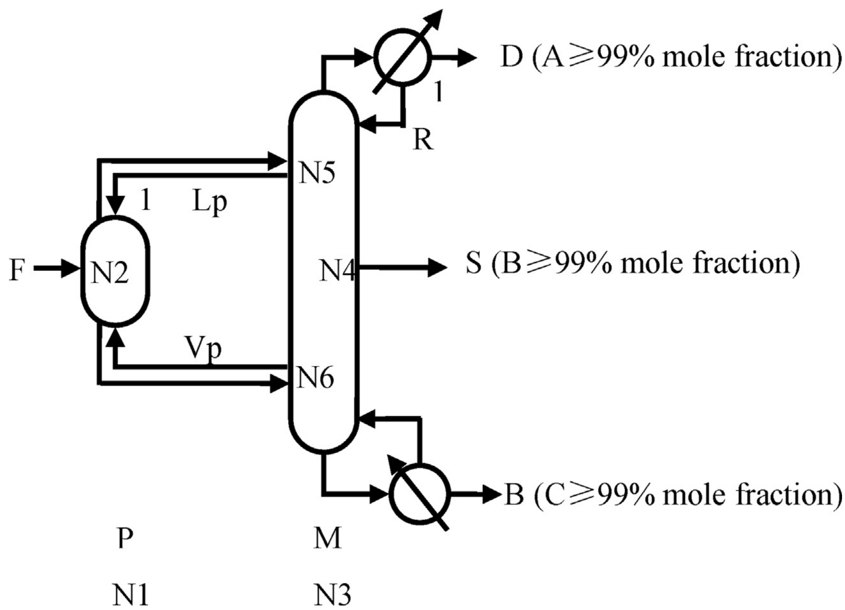

Fig. 2 – Prefractionator and main column configuration (Thermodynamically equivalent to Fig. 1).