Optimal Operation Mode Switching of Dividing Wall Distillation Based on Model-Predictive Control

Hao Pan[1,2], Haibin Yu[1], Mingzhe Yuan[1]

1. Shenyang Institute of Automation, Chinese Academy of Sciences, Shenyang 110016
E-mail: panhao@sia.cn

2. University of Chinese Academy of Sciences，Beijing 100039, China

Abstract: Dividing wall distillation(DWC) column is becoming a new standard of separating and purifying multivariate mixed liquid, because of DWC represents that forced operation will play a role in separation technology, which have high energy efficiency and compact structure. DWC is composed of a lot of equipments of diversified configurations, so it is complicated to operate process and requirements for specific or advanced control system technology. When operation objectives of DWC need to be online conversion, operation will be not smooth, etc.. In order to solve these problems, we used two-layer control structure. The bottom layer was basic control layer(PID) and model-predictive control(MPC), and the top layer was predictive functional control(PFC) or fast model-predictive control(FMPC) which can realize operation optimizing function. The main objective is to achieve a smooth transition between the optimal mode switching and to ensure optimum goal can be realized. By implementation of proposed operating strategy in a four-component mixture Kaible column, the simulation results showed that this new method was feasible and concise.

Key Words: Dividing Wall Distillation, Model-Predictive Control, Process Control, Optimal Operation, Fractionating Column

1 INTRODUCTION

The productive part of the a chemical industry can be seen as consisting of four parts by a chemical reaction, separation, heat exchanger networks, public utilities, wherein the distillation operation was studied at most in separation section, and this trend will continue in future. The one reason was the importance of the distillation operation itself, according to statistics distillation column were used more than 40000 in the United States and to undertake task more than 95% of completing the separation and purification. The other reason was that distillation was a highly energy intensive process and distillation columns alone in the US consumed 3% of the total energy consumption in the country and 40% of energy consumption in process industry.[1] The reason of such a large energy consumption was that the mixed liquid evaporated and heated at the bottom of rectification column, meanwhile vaporized mixed gas was required a certain amount of energy to congeal in the top of the rectification column, condensing operation required lower temperature, although the efficiency was low, but rectification column was still the most effective method to separate the different volatility of liquid mixing. The conventional distillation column was composed of the tower, reboiler and condenser. To separate n-ary mixed liquid completely needed n-1 towers of sequence configuration at least. For example, to separate ternary system ABC, can be isolated from component A and component BC on the first column, and then separated into component B and component C. Note that this operation led to component B was vaporized first and condensed later but not separated in first column, only able to achieve the separation in the evaporator of the second column; similarly, component C may also be condensed twice, it was the main reason of low efficiency of traditional multi-distillation operation, also has been an important starting point of operational research to improve the energy efficiency of distillation. Petlyuk noted that these inefficiencies thermodynamic mixing effect occurred in the feed, the bottom and the top, and proposed that the way of thermal coupling configurations of internal column and/or inter-column can reduce the number of the reboilers and condensers. The past 20 years, the thermal coupling distillation technology from the tower design, process configuration, operation control and other aspects have been sustained attention of academic and industry, the early formulation of thermally coupled distillation gradually integrated into the dividing wall distillation column (DWC) frameworks, such as ternary separation DWC tower was Petlyuk column and quaternary separation DWC was Kaibel tower. DWC was to increase a partitioning wall in a tower body from the view of structural, because of this wall can be designed and installed in the upper, middle or lower part of column, there were possibility of increasing two walls or more walls and a huge potential variety of combinations. Therefore, intensive operations of distillation became a hot spot of research and development at present.[2-5] Theoretical calculations and industrial applications has shown that DWC can improve energy efficiency by 10%-40% than conventional distillation

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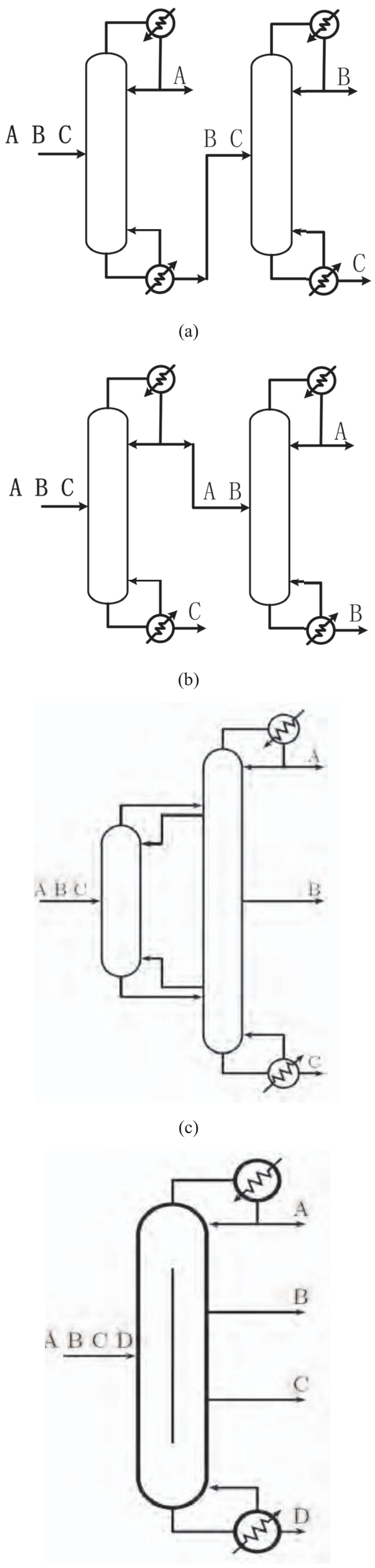
column, can also save additional capital investment and plot space taken up by the equipment.

Addition to the above advantages, DWC had several potential limits including both ends of column required a large temperature difference, corresponding to the need for high quality heat medium and the refrigerant mass, more walls number, and sometimes required a larger column diameter, and operation control more difficult, and so on. In fact, the concept of thermal coupling column first appeared in 1947, has been considered to poor controllability (tracking operation point changeing and the ability to resist interference), so it was not valued. In recent years, studies have shown that by implementing the appropriate control system architecture and advanced algorithms, DWC dynamic operating performance can be guaranteed.[6-9] Conventional distillation column control strategies include double-ended component control, single-side/double-side temperature control, single-side/ double-side temperature difference control and other implementation forms, and DWC control strategy can also design a similar control strategy. However, due to the components between the low boiling point and the high point were taken out from the middle of the tower, as well as additional control degree of freedom, such as reflux liquid and the distribution ratio of rise gas in both sides of the tower and so on, three or four-terminal control system architecture were proposed. Complicated configuration increased the difficulty of control design, but also provided a few opportunities to improve the separation efficiency based on a variety of advanced control technology. [10-14]

This paper proposed a control strategy base on basic control structure which increased an operation layer function for DWC, to achieve online best operating strategy of optimal operation target of different. The next sections were DWC mathematical modeling, determining of DWC optimum operating target mode, the method of the double layers structure model predictive control of PID basic control layer + fast model predictive control to achieve DWC optimization goal smooth transition, simulation experiments and evaluation.

2 DWC MODELING

Conventional rectification column, separation of ternary mixtures (Petlyuk), quaternary mixtures(Kaibel) dividing wall column structure were shown in Figure 1. Separation of ternary mixtures needed two conventional rectification columns to sequence configuration, two kind of configurations were shown in figure 1(a)-(b), the structure of Petyuk and Kaibel were shown in Figure 1(c) and 1(d) respectively.



(a)

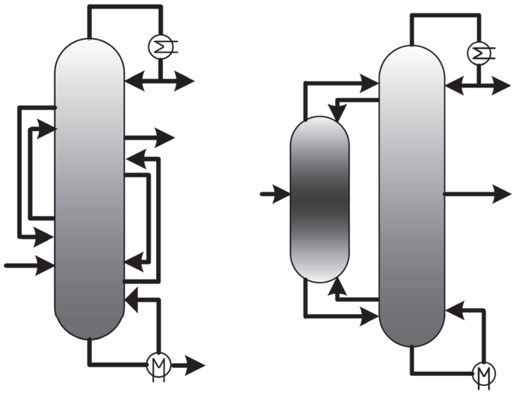
(b)

(c)

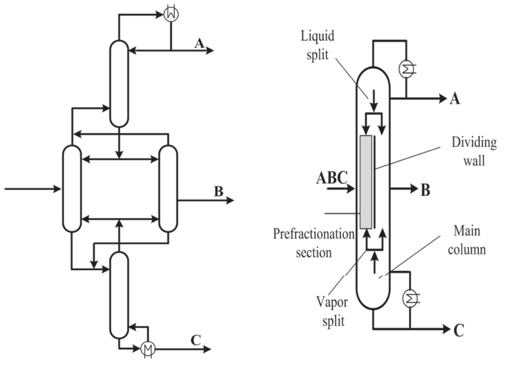
(d)

Fig.1. Schematic of conventional distillation columns and dividing wall distillation columns

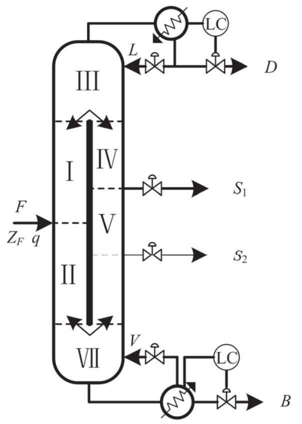
Modeling on has been very mature, and in commercial software such as Aspen Plus there were various forms of distillation column model to choose to choose, but modeling and simulation of DWC has not yet been packaged into a single module. The current main idea of DWC modeling was to decompose DWC into several different types equivalent combination of conventional rectification column module, it meant that each model of the column calculation used the conventional method, and each module joint did the special treatment to obtain a preliminary DWC model and refinement. For example of separation of ternary mixtures, the main existing DWC modeling methods were introduced as following. [10] (1) Pump-around model, the equivalent model was shown in Figure 2 (a), the main ideal was assumed that the liquid distribution ratio of both sides were accomplished by pump, gas flow was straight, and this method was simple to use. (2) Two columns sequential modeling method, the equivalent model was shown in Figure 2 (b), in fact, this type of modeling method was same as Petlyuk prototype tower, physical meaning was specific and easy to achieve. (3) Four columns sequential modeling method, and the equivalent model was shown in Figure 2 (c) , this model was composed of the upper rectifying section, the feed-side segment, an intermediate slipped out segment, bottom stripping section and other components, and these configurations were more truthfulness. The distribution ratio of fluid of both sides of wall, the number of wall in column can be considered separately, which increased the flexibility of design calculations, but significant increased the complexity. (4)Simultaneous equation modeling method, equivalent model was shown in Figure 2 (d), this method was suitable for modeling and simulation environment of the differential equation, such as Matlab/simulink, this method was in common use and general but needed for more expertise. In this paper, we used method (4), because the simulation calculation focused on the Kaibel columns, the equivalent column segments were 7, as shown in Figure 2 (e), and where the wall was divided into seven regions, region I and region II areas were pre-fractionation zones, the main column was divided into five zones.



(a) (b)



(c) (d)



(e)

Fig.2. Equivalent module schematic of modeling dividing wall distillation column

3 DWC OPTIMUM OPERATING

The main motivation to choose to use DWC was to reduce energy consumption. Compared with the traditional distillation columns, such compact integrated thermal coupling tower were proposed a number of new challenges for design and control. DWC design challenges mostly had a better solution currently, but still many issues in the operation and control needed to be explored, one of the problems was how to set the proper temperature profile to keep gas-liquid balance in each tray that is achieving a smooth operation of the tower; the other problem was under the premise of ensuring product purity how to achieve separation minimum energy consumption. The first problem was dynamic performance, the solution was mainly associated with the basic control system design. The second problem was static steady, but was closely related to DWC design, control, optimization and other aspects. In terms of design, "Borderline" design was energy efficient, but the dynamic performance needed to require some rigorous condition for control system, so DWC needed synchronous or interactive iteration design to achieve. In terms of control, DWC needed control system more flexible, link grade transition control and variable load regulation of air separation equipment in polymerization process. In terms of optimization, DWC was highly nonlinear, multivariable coupling, more constraints and other feathers which were difficult to control. Real-time optimization (RTO) layer depended errors between static model and dynamic model which was used by basic control layer, whatever the object implementation optimization strategies were challenging tasks under uncertain condition. Paper[15] defined optimum operating conditions of DWC by open-loop simulation calculation and in terms of four operation targets that were highest product (purity) income (Mode 1), minimum energy consumption (Mode 2), highest product income in case the price was difference (Mode 3), maximum yield (Mode 4), as well as design principle of self-optimization control system. Four operation modes were described as following.

Mode 1, highest product (purity) income
Objective function,
$$\min_{u0} J = D(1-x_{a,D}) + S_1(1-x_{b,S_1}) + S_2(1-x_{c,S_2}) + B(1-x_{d,B})$$
Constrain condition, $F = F_0; V = V_{\max}$

Mode 2, minimum energy consumption
Objective function, $\min\limits_{u0} J = V$
Constrain condition,
$$F = F_0; x_{a,D} = x_{a,D\,\text{opt}} x_{b,S_1} = x_{b,S_1\,\text{opt}} x_{c,S_2} = x_{c,S_2\,\text{opt}} x_{d,B} = x_{d,B\,\text{opt}}$$

Mode 3, highest product income in case the price was difference
Objective function,
$$\min_{u0} J = -(w_D D x_{a,D} + w_{S_1} S_1 + w_{S2} S_2 x_{c,S_2} + B x_{d,B})$$
Constrain condition, $F = F_0; V = V_{\max}$

Mode 4, maximum yield
Objective function, $\min\limits_{u0} J = -F$
Constrain condition,
$$V = V_{\max}; x_{a,D} \geq x_{a,D\,\text{opt}} x_{b,S_1} \geq x_{b,S_1\,\text{opt}} x_{c,S_2} \geq x_{c,S_2\,\text{opt}} x_{d,B} \geq x_{d,B\,\text{opt}}$$

When DWC undertook the final product separation task, the market price volatility of energy and products will lead to operation targets changing, the operation mode needed to switch in time when the entire process during the continuous operating state. The process required the different operating objectives smooth handover, the existing research on the optimal operation of DWC focused on the design (such as the minimum number of theoretical trays, the minimum return flow, the minimum amount of evaporation, the minimum reboiler temperature and other estimate of parameters), the calculating the optimum parameters of each operating mode based on steady-state mechanism model, the combination of simulation evaluation of controllability and so on, there were no report about integrated research of operation and control. The next section will introduce two-layer control structure, the upper was fast model predictive control algorithm, and will study how to achieve online automatic optimal switching strategies between each mode to another.

4 USING TWO-LAYER CONTROL STRATEGY (PID+MPC) TO ACHIEVE OPTIMAL OPERATION

General industrial automatic control system was shown in Figure 3, one of which was operating function block which executed orders from plan/scheduling function layers, control function blocks were composed of feedback and feedforward algorithms, the algorithm can be classic PID or MPC or other advanced control strategies [16], the reference set points and associated logic blocks were from the operation function blocks. The movement time series of operation and control were on different time scales, the current way was control function automatically fast scale and manual low-scale operation function. When implementation double automatic control combined with these two function layer, as pointed out by the famous Swiss scholar Morari, integrated operation and control did not only represent an important development direction of automation system in future, but also needed to explore the impact of uncertainty and complexity disposal strategy and other scientific issues .[17]

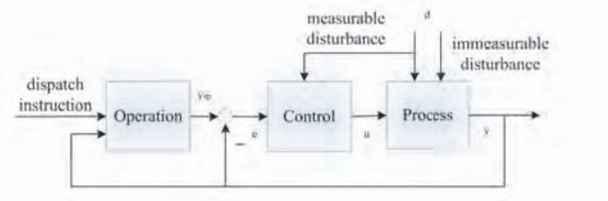


Fig.3. System of integrating operation and control functions immeasurable disturbance

Control layer design, PID algorithm

$$u(s) = K_p\left(1 + \frac{1}{T_I s} + \frac{T_D s}{1 + 0.1 T_D s}\right) e(s) \tag{1}$$

Or MPC algorithm,

Objective function,
$$J = \sum_{k=0}^{N-1} \left(\left\| x_k - x_{k,ref} \right\|_Q^2 + \left\| u_k - u_{k,ref} \right\|_R^2 \right) + \left\| x_N - x_{N,ref} \right\|_P^2$$

Constrain condition,
$$\begin{aligned} u_{\min} \leq u_{k+i} \leq u_{\max}, &\quad i = 0,1,\ldots,N-1, \\ \Delta u_{\min} \leq \Delta u_{k+i} \leq \Delta u_{\max}, &\quad i = 1,2,\ldots,N-1, \\ y_{\min} \leq C x_{k+i} \leq y_{\max}, &\quad i = 0,1,\ldots,N. \end{aligned} \tag{2}$$

Operation layer design, PFC/FMPC algorithms

$$MV(k) = \frac{\textit{Predictive output increment-Free output increment}}{\textit{Unit forced output}}$$

We used predictive functional control (PFC) [18] to achieve fast-moving transition between optimum operating states. PFC algorithm based on discrete input-output model which was a common industrial application, for example, first order delay and pure lag model, convolution model (under damp) and so on. If the model had null points or open loop unstable poles or high order situations, the model can be decomposed into a combination of equivalent first order modules, because these low order models were easy to obtain, control algorithm design was simple and intuitive. Another advantage was that the interval time of operation function performance can be adaptively adjusted, that was in a one-time calculation of reference trajectory of entire future transition phase in the switching time, according to variable scale of the disturbances or loads to implement, such disposal methods was called the fast model predictive control (FMPC) in literature [19]. For FMPC, we assumed a linear process, and we can get the following theorem by linear superposition theorem.

Theorem 1 If a linear, time invariant multivariable process (without regard to the integration process) had an initial steady state operating point (u_0 , y_0), and control input was not changed in k time, so the steady-state value of process output $y_{ss,k}$ was only related to u_k and u_0 , whereas changing path of input was not effect on $y_{ss,k}$.

$$\begin{aligned} \boldsymbol{y}_{ss,k} &= \boldsymbol{y}_0 + \Delta \boldsymbol{y}_{ss,1} + \Delta \boldsymbol{y}_{ss,2} + \cdots \Delta \boldsymbol{y}_{ss,k} \\ &= \boldsymbol{y}_0 + \boldsymbol{G}\Delta \boldsymbol{u}(0) + \boldsymbol{G}\Delta \boldsymbol{u}(1) + \cdots \boldsymbol{G}\Delta \boldsymbol{u}(k) \\ &= \boldsymbol{y}_0 + \boldsymbol{G}\sum_{i=0}^{k} \Delta \boldsymbol{u}(i) \\ &= \boldsymbol{y}_0 + \boldsymbol{G}(\boldsymbol{u}_k - \boldsymbol{u}_0) \end{aligned}$$

The equation of control activity for first order delay plus pure lag model was written as below.

$$MV(k) = \frac{(y_{sp} - (y_p(k) + y_m(k) - y_m(k-nm)))l_h + y_m(k)b_{mh}}{K_m b_{mh}} \tag{3}$$

Where k was the current time, nm was pure lag, y was output, the subscript p and m was process output and model output respective, h was design parameter, l_h , b_{mh} and K_m were relevant parameters of model and design. When the current operation mode switching to another mode, calculation of increment of corresponding set point y_{sp} superimposed to set point of substratum control loop, and switching process close was under loop online state. For two order time delay and pure lag model and convolution model, the equations were shown in literature [8].

5 CASE STUDIES

Here, we considered to separate four equimolar liquid mixture which were composed of methanol, ethanol, propyl ethanol and butanol and used Kaibel column as shown in Figure 2 (e). There were seven available degree of freedom including feed rate(F), vapour boil up rate (V), liquid reflux rate (L), the two side stream rates (S_1 and S_2), the liquid split ratio (R_L) and the vapour split ratio (R_V). The distillate rate (D) and the bottoms product rate (B) were in all cases assumed to be used for inventory control of the condenser and reboiler respectively (usually referred to as the LV-configuration for binary columns). The literature [15] in terms of self optimization principle [20], structured four kind of corresponding control structure of operation mode. If disturbance did not led to active constraints changing, control structure which was gotten by optimization principle still kept set point stable and performance loss was allowed. In order to verify optimizing strategy mentioned the previous section, this paper used column model which composed of 64 trays, R_V was a constant, four basic control loops were composed of T10 tray temperature paired with R_L , T35 tray temperature paired with L , T45 tray temperature paired with S_1 and T57 tray temperature paired with S_2 , the control algorithms were PID. Optimizing operational tasks required following conditions. Firstly, based on the model to determine the four operating modes corresponding to the optimum operating point, the paper considered two control loops of the tower level and bottom level were carried out in the case of closed-loop simulation, so this result was more practical. Secondly, close-loop models of four control loops were needed to identify. Finally, based on the identified models to design controller, and used decentralized control structure and ignored interactions between the loops.

Simulation 1 switched mode directly each other and did not have optimizing control function layer. In 200 minutes, operation was switched from mode 1(corresponding set points of optimum temperature, T30=341.9, T17= 368.3, T59= 355.8, T49=379.6) to mode 3(corresponding set points of optimum temperature, T30=340.5, T17=361.3, T59= 357.9, T49=376.9). In 900 minutes, the operation was switched to mode 1. We can observe from Figure 4 that the component changed a lot when operation mode switching.

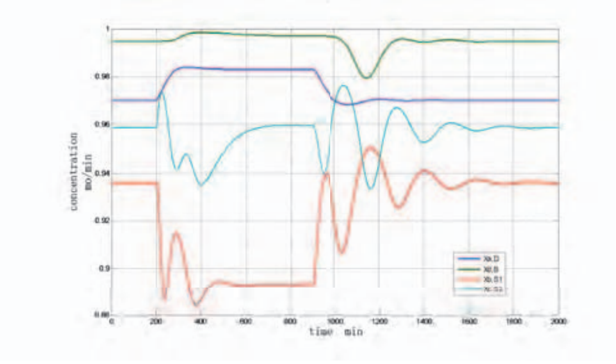


Fig.4. The curve of four components concentration when switching directly from mode 1 to mode 3

Simulation 2 had the same experimental conditions as simulation 1, except that the upper layer added optimize operating function which proposed in this paper in other word used fast model predictive control algorithm to achieve closed-loop operation. Seen from the figure 5, when four trays temperature switched to a new operating point by preinstalled track, corresponding to the molar concentration of the four components product were converted to the new operation mode. It can be seen that the fluctuation reduced significantly and optimal operating function played a positive role.

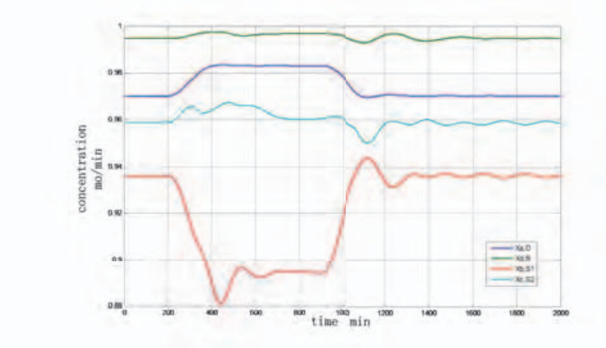


Fig.5. The curve of four components concentration of switching from mode 1 to mode 3 when increased operation function in upper layer

6 CONCLUSION

The dividing wall distillation column compared with conventional distillation, including column tower design, process configuration, operation control and other aspects were more complex. Although the dividing wall distillation column has been in industrial applications, but also need to solve many challenging issues to become the new standard of separation techniques. It represented the future development of strengthen process technology of chemical science and technology, equipment, process and operation and so on needed to consider together. Equipment and process computing design were generally based on a static model, and operational control will have to be carried out in a dynamic environment. The calculated process optimal operating objectives used to online closed-loop control to achieve, which was instead of direct manual switching operation. This paper used an integrated operation and control mode to achieve optimum process indicators, and the preliminary results indicated that this work was feasible in this new direction. Stability and disturbance constraints of such integrated systems need to be further explored.

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