

Optimal Start-up Strategies for a Conventional Distillation Column using Simulated Annealing

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The start-up process for a distillation column presents a challenging control problem in the chemical industry. To address this problem, reducing wasting time and duty consumption during the transient period are crucial issues. In this study, the separation of the dichloromethane, chloroform, and carbon tetrachloride system ($\text{CH}_2\text{Cl}_2 + \text{CHCl}_3 + \text{CCl}_4$) was investigated as a start-up example. The single column was used to obtain 83.1% CHCl_3 and 99% CCl_4 . The distillation start-up steps were divided into the following four parts for investigation: feed control, bottom product discharge time, total reflux switch time, and medium temperature heating operation method of the reboiler duty. The feeding time depended on the sump level for safety, and the bottom product was discharged until reaching purity near the specification to avoid producing excess undesired products. Switch total reflux policies were presented using the minimum temperature difference or waiting until the top composition CHCl_3 reached 50 wt%. Furthermore, the simulated annealing (SA) algorithm was applied to determine the optimal heating step. The objective function (j) and a set of variables during optimization (d) were subsequently designed, and a flow chart for the SA approach was developed and connected to Aspen Plus Dynamic software. Following the SA calculation, the modified cases with optimal heating steps exhibited better behavior than did the example case. These rules enabled the complicated evaluation process to be simplified for designing a start-up strategy.

1. Introduction

Distillation start-up involves the complicated transfer of mass and heat, as well as a wide range of operating conditions; therefore, it is difficult to achieve in the field of chemical engineering. Because the process is unproductive during start-up, shortening the start-up period is recommended to reduce the off-specification products and energy costs. The earliest start-up simulation was conducted by Ruiz et al. (1988), who classified start-up performance into three stages: the discontinuous stage (which occurs at the onset of start-up and is mainly concerned with the on-off valves for the filling column), the semicontinuous stage (where optimization of the control strategy begins), and the continuous stage (where the nominal value is set and desired to reach a steady state). Accordingly, different operational strategies have been developed to correspond to the different steps. However, according to various product requirements and operating conditions, the dynamic behaviors involved in distillation start-up affect the time of start-up period. Kruse et al. (1996) investigated the total reflux removal strategy for start-up and product changeover, where the optimal switching time from reflux flow 0 to steady state was determined by the minimum temperature difference (MT-function). This strategy requires substantially less time than the conventional method. Subsequently, Woinaroschy (2008) presented time optimal control on the start-up distillation column of ideal and azeotrope mixtures. Woinaroschy (2009) extended the study to nonideal mixtures.

The distillation start-up operation includes a manual mode, feedback control, and nonlinear behaviors. Therefore, the optimal control strategy is crucial for designing a start-up operation. In this study, the simulated annealing (SA) approach is applied to determine the optimal solution. SA was first proposed by Metropolis et al. (1953) based on the arrangement of liquid molecules that tend to gradually steady under cooling conditions; the system energy eventually achieves the lowest possible value. Subsequently, Kirkpatrick et al. (1983) employed SA for optimization and SA began to be applied extensively. More recently, Li et al. (2000) investigated product

purity switchover, where the reflux flow rate and duty are optimized through SA. The researchers found that the optimal strategy considerably reduced the switchover time. No standard operation criteria for distillation start-up have been defined in previous studies. Therefore, this study focused on the start-up process for distillation columns. The column start-up example developed by Aspen Plus Dynamics software was employed as the base case for investigating the optimal start-up strategy. The aim of this case was to separate the CCl_4 , CHCl_3 , and CH_2Cl_2 in the mixture; subsequently, SA was applied to design the operational method of the reboiler duty. This study was divided into the following four parts: feed control, bottom product discharge time, total reflux switch time, and the heating medium temperature operational method of the reboiler duty. A detailed description of the start-up example is provided in the following section.

2. Start-up example: Distillation of the $\text{CH}_2\text{Cl}_2 + \text{CHCl}_3 + \text{CCl}_4$ system

In this study, the start-up example for distillation (ColumnStartup) developed by Aspen Plus Dynamics was adopted as the base case. The process is described as follows.

2.1 Process flowsheet and control scheme

The mixture of CH_2Cl_2 (40 wt%), CHCl_3 (54 wt%), and CCl_4 (6 wt%) was separated by a single column, and the nonrandom two-liquid (NRTL) thermodynamic model constructed in Aspen Plus Dynamics was used to calculate the vapor liquid equilibrium. The boiling points of all of the components in the atmosphere are shown in Table 1. The CHCl_3 purity of the top product must be more than 83.1 wt%, and the CCl_4 purity of the bottom product must be 99 wt%. The process flowsheet is presented in Figure 1. The feed flow rate was set at 10,000 kg/h with a temperature and pressure of 20 °C and 6 bar. In this process, the distillation column contained 20 stages and the feed location of the mixture was fed into the tenth stage. The heating medium temperature was used in the reboiler, and its nominal operating value was 140 °C. In the dynamic start-up simulation, out of flow is added above the column to purge nitrogen. Figure 1 shows that the following five controllers were placed in the control scheme: the feed flow rate (FC); reflux drum level (LC_D); reboiler sump level (LC_B); first stage pressure (PC), controlled by cooling the water to a sustained 2 bar; and temperature of the 16th stage (TC), controlled by heating the medium temperature to a sustained 102.75 °C. The ratio of reflux flow to distillate flow was set as 5.

Table 1: Boiling point of the $\text{CH}_2\text{Cl}_2 + \text{CHCl}_3 + \text{CCl}_4$ system

Component	B.P(at 1atm)
CH_2Cl_2	312.81 K
CHCl_3	334.25 K
CCl_4	349.88 K

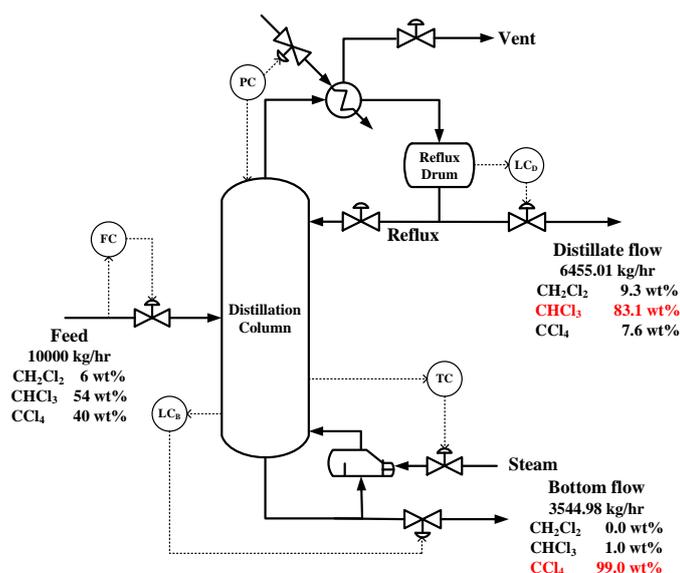


Figure 1: Concept design of the distillation of the $\text{CH}_2\text{Cl}_2 + \text{CHCl}_3 + \text{CCl}_4$ system.

2.2 Operation procedure of base case

The process was started from a cold empty state with all controllers in manual mode. The feed flow rate was set at 10,000 kg/h until the sump level reached 2 m (80%). At this time, the pressure was switched to automatic mode to begin to purge N₂. The heat flow temperature increased from 60 °C to 80 °C, and then to 100 °C with an interval of 0.1 h between each change. Subsequently, the column ran under total reflux with the reflux flow set at 30,000 kg/h. After 0.05 h, the heat flow continued to increase, eventually reaching 120 °C. The N₂ purge valve was then closed and the LC_D was switched to automatic mode. The mixture was then fed again until the sump level reached 2 m (80%) and the heat flow increased from 130 °C to 135 °C in 0.15 h. When the sump level reached 0.5 m (20%), LC_B was switched to automatic mode, and the mixture started to feed continuously. Additionally, the reflux flow and heat flow temperature were set as nominal values. Finally, when the TC achieved its nominal value, it was also switched to automatic mode and the set point of every controller was assigned a nominal operating value; these results are shown in Figure 2.

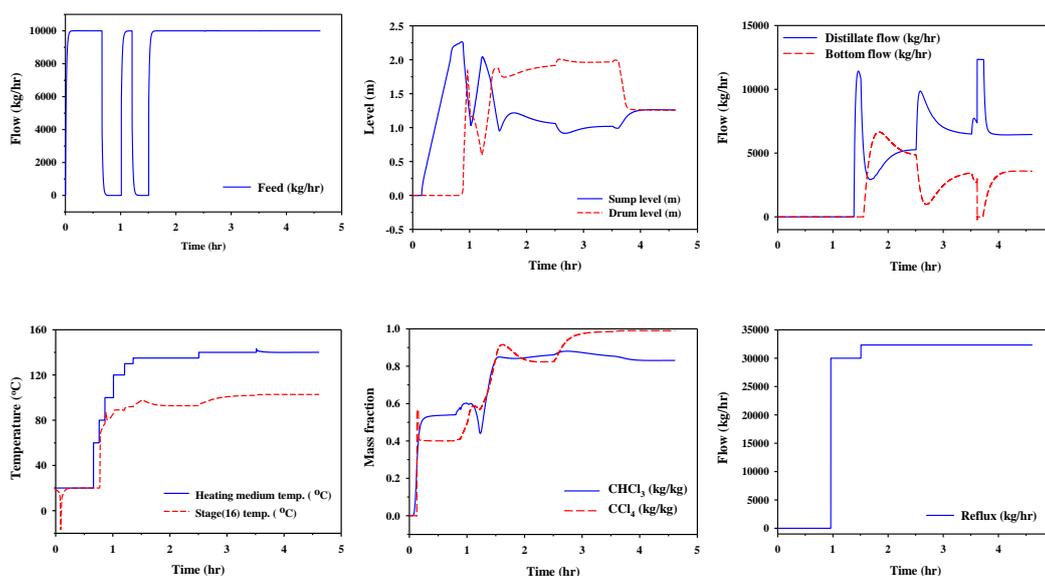


Figure 2: Start-up results of the base case.

Only one simple operation step was presented in the base case. The drum and sump levels represent a dramatic change in the start-up period. The dynamic results show that the purity of CHCl₃ and CCl₄ achieved steady states after approximately 4.61 h. The approximate amounts of off-specification product and reboiler duty during start-up were 23,316 kg and 28.1 GJ. Because the product discharge times at the top and bottom were earlier than the times that the products reached their specifications, a large amount of off-specification was produced.

3. Optimal start-up operation

In the Aspen Plus Dynamics example, some problems occurred during start-up. Therefore, in this paper, the optimal strategy is discussed according to the base case phenomenon. In this section, the start-up operation is divided into the following four parts: (1) operation of feed flow control; (2) bottom product discharge time; (3) the switch time from total reflux to nominal value; and (4) medium temperature heating operation.

3.1 Feed flow operation and bottom product discharge

Feed flow is assigned a nominal value when the sump level is below 75% of its height; by contrast, feed flow is closed when the sump level is over 90% of its height. Thus, the level can be prevented from becoming too high or too low. In the base case, the bottom product was discharged before the purity met its specification, enabling many off-specification products to be produced. Therefore, the time at which the bottom product starts to discharge was modified according to when the bottom product purity is close to meeting its specification.

3.2 Operation of switching reflux flow to a nominal value

Because the general operation of distillation start-up is under total reflux at the beginning of the process, the reflux flow is switched to a nominal operated value when the top product is close to meeting its specification. If the flow switches earlier, the start-up period can be shortened to reduce energy consumption; however, this also wastes part of the top product. This paper discusses two methods for reflux flow switch time. Case A applied the MT-function presented in Eq. (1), where $T_j(\tau)$ and T_j^{SP} are the current temperature of the j th stage and the corresponding nominal operating value, respectively. The reflux flow switch time selection result in case A is shown in Figure 3(a), and the switch point was 1.33 h. However, the purity of CHCl_3 under total reflux decreased after reaching approximately 50 wt% (Figure 3(b)). By contrast, to prevent the purity from decreasing, case B employed the 50 wt% of CHCl_3 as a switch point. Section 4 describes the differences between the cases.

$$MT = \sum_{j=1}^{NT} |T_j - T_j^{SP}| \tag{1}$$

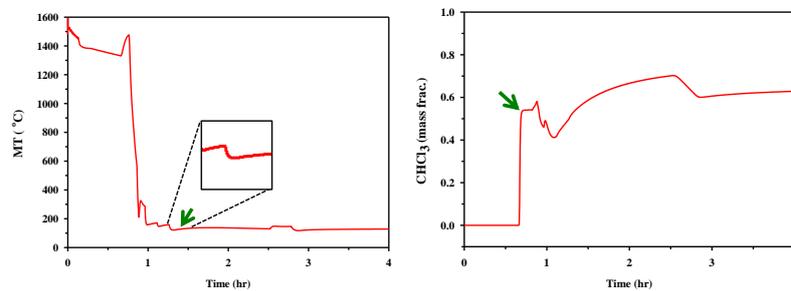


Figure 3: (a) MT-function under total reflux operation; (b) Concentration of CHCl_3 under total reflux operation.

3.3 Medium temperature heating operation

In this study, the heating medium temperature must be increased to the nominal operated value, the optimal solution of which was determined using SA. The degrees of temperature change (0 °C, 10 °C, and 20 °C) and interval times (0, 0.1, and 0.2 h) were a set of variables during optimization (d). The error sum of the square between the dynamic value and nominal value for x_{D,CHCl_3} and x_{B,CCl_4} was defined as the objective function (j), and is presented in Eq. (2).

$$J = \int_0^{t_f} \{ [x_D(t) - x_D^{SP}]^2 + [x_B(t) - x_B^{SP}]^2 \} dt \tag{2}$$

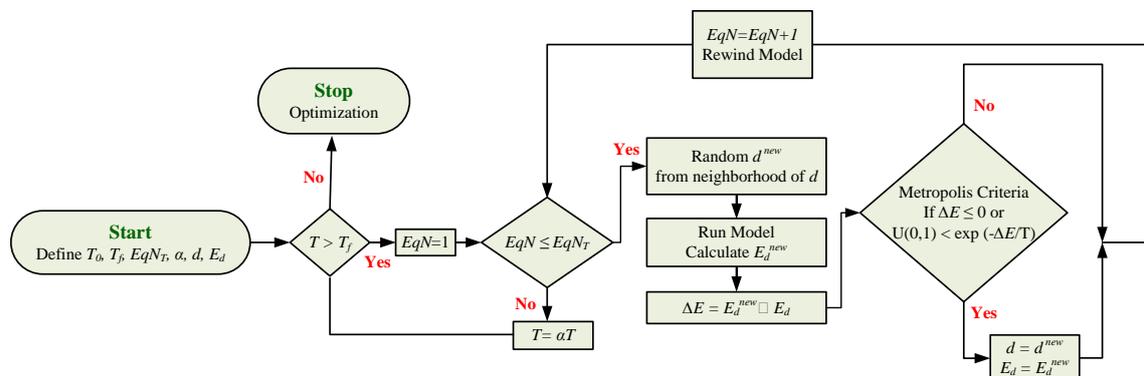


Figure 4: SA flowchart.

To determine the most suitable range within which to search for the optimal solution, several parameters were set, including the initial temperature (T₀), final temperature (T_f), criteria for thermodynamic equilibrium (EqNT),

and temperature decrement factor (α). Subsequently, the optimal evaluation configuration and optimal indicator were set, and the corresponding value of j (Figure 4) was computed according to the dynamic simulation with the given variables and initial d . Through the designed annealing schedule, the optimal solution was obtained.

4. Results and discussion

Figure 5 shows the simulation results of cases A and B. The response shows that the highest sump level was 1.8 m in both cases, which is lower than that in the start-up example. The modified feed flow operation can prevent dangerous scenarios from occurring, such as sump being full or dried up.

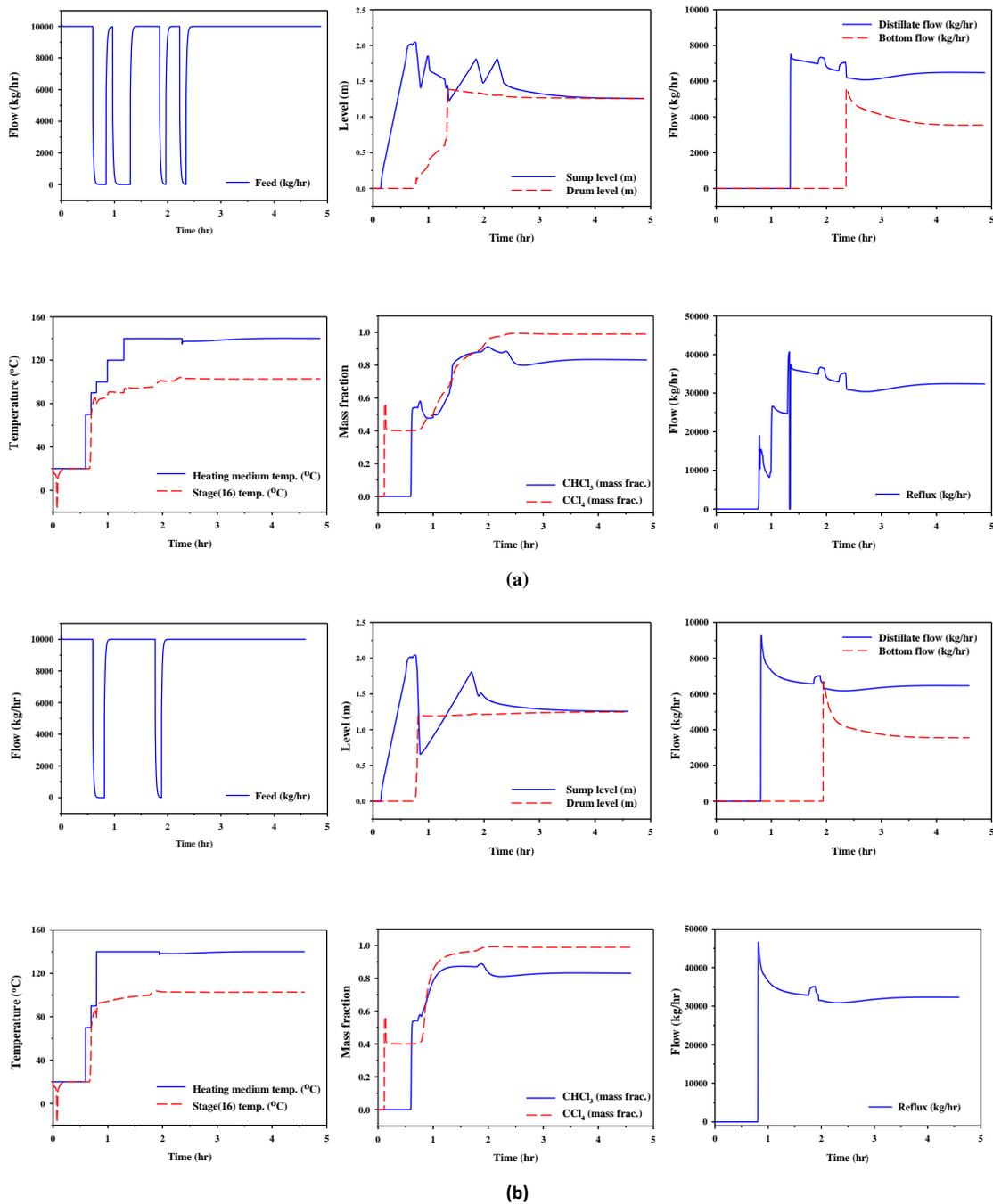


Figure 5: (a) Case A start-up result; (b) case B start-up result.

The bottom product of CCl_4 , which discharged after composition of CCl_4 reaching 99 wt% can reduce the product consumption during startup period. By switching the total reflux rate to the nominal operated value, the trend of CHCl_3 composition in the dynamic simulation in case B did not decrease as it did in case A (where the overhead composition of CHCl_3 dropped after reaching 50 wt%).

Through the optimization process based on the SA calculation, the optimal heating operation was obtained. Case A underwent heating from 70 °C to 90 °C to 100 °C to 120 °C to 140 °C within time intervals of 0.1, 0.1, 0.2, and 0.3 h, respectively. By contrast, case B underwent heating from 70 °C to 90 °C to 140 °C within time intervals of 0.1 and 0.1 h. The total start-up times in cases A and B were 4.882 h and 4.595. The off-specification products and reboiler duty are listed in Table 2. Although the total start-up time in case A was greater than that in the base case, product consumption and duty were reduced. Moreover, 39.8 % of the off-specification products and 8.5 % of the reboiler duty were reduced in case A, compared with 34.1 % and 16 % reductions in case B.

Table 2: Start-up period, off-specification products, and reboiler duty for base case, case A, and case B

Strategy	Base cases	Case A	Case B
Start-up period (hr)	4.614	4.882	4.595
Off-spec product (kg)	23316	14017	15357
Reboiler duty (GJ)	28.1	25.7	24.5

5. Conclusion

In this study, column distillation start-up was divided into four parts and the optimal strategies were investigated. Cases A and B represent two methods for determining the total reflux switch time to nominal reflux ration. Case B was able to reduce more reboiler duty than case A. With modified operations, both cases exhibit less off-specification products and reboiler duty than the base case. Furthermore, the simulation results reveal that applying SA to determine the optimal heat step can reduce reboiler duty significantly compared with the bases case. This optimal start-up strategy simplifies the complicated start-up operation and decreases the time required to determine the optimal heating method.

Acknowledgments

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