ISSN : 0974 - 7443 Volume 8 Issue 2

CHEMICAL TECHNOLOGY

An Indian Journal

Full Paper

CTAIJ 8(2) 2013 [41-45]

Process simulation optimization of caprolactam polymerization

ChaXiu Guo[1]*, ShuLan Liu[1], Liang Liu[2]

[1]School of Chemical and Energy Engineering, Zhengzhou University, 450001 Zhengzhou, (CHINA)

[2]Sixth Design Institute Machinery Industry, 450001 Zhengzhou, (CHINA)

E-mail : guochaxiu@zzu.edu.cn; lsl3785290@163.com; liuliang7615@yahoo.com.cn

ABSTRACT

The process for the hydrolytic polymerization of caprolactam (CL) is analyzed by Aspen Plus software. Under the condition of 34t/d output, the influences of main parameters, such as feed flux, polymerization temperature of polymer tower, on the results of polymerization are presented. Results show that the increase of back section temperature of the tower should be avoided. Front section temperature should be lower when the daily output is lower, which can reduce the energy-consuming and the cooling load of back section of tower, and a higher front section temperature and a lower back section temperature are needed when molecular weight is no less than 20000, to ensure that extractable substance lower than 8.3%.

KEYWORDS

Optimization;
Caprolactam;
Polymerization;
Aspen Plus;
Simulation

INTRODUCTION

Capron is one of the most important chemical materials on the industrial scale due to the large utilization of the polymer in textile fibers. The industrial process for obtaining Capron from CL is mainly based on the hydrolytic polymerization of this molecule. The simulation on hydrolytic polymerization of caprolactam mainly was focused on the establishment and test of the mathematical model in domestic and overseas[1-2]. However, using aspen plus software[3] to simulate the whole process of polymerization was seldom reported. The purpose of the paper is to simulate and understand the influence of the operating parameters on the polymerization by using Aspen Plus software, in order to optimize the operation conditions and reduce the change of produce conditions to the quality of product.

SIMULATION MODEL

The hydrolytic reactions and addition polymerization reaction of caprolactam are heat-absorption reaction. The increase of temperature and pressure can improve reaction speed, but a large amount of CL vapor would produce and escape together with the steam if the temperature is too high. The process of polycondensation is a dehydration exothermic reaction, and the decrease of temperature and pressure could benefit the reaction, but have a bad effect on the reaction speed, and are not good for the produce of high molecular weight, so it is necessary to find a suitable temperature scheme for reactions by simulation. Based on the actual structure of the polymer tower for caprolactam shown in Figure 1, we determine the schematic of polymerization system of caprolactam used in simulation, as presented in Figure 2. In the first reactor (CSTR1), caprolactam and water are heated from 80°C to 245°C-260°C and carried out open loop reaction and polycondensation reaction, then the reactants in the second reactor (CSTR2) are heated up to the highest temperature of 270°C to continue further polymerization. At the bottom of the polymer tower, the reactants in the piston flow reactor (PLUG) are cooled to obtain larger molecular weight and lower content of ring dimerization components. Gas and liquid phase are separated by R1FLASH and R2FLASH. The distillation column is adopted for separation of gas phase caprolactam and water. In simulation, temperature is assumed as constant at different section and called as: temperature of CSTR1 and CSTR2, inlet temperature of PLUG-0, temperature at 45 % length of PLUG-0.45, and outlet temperature of PLUG-1. In polymer plus model, the simulation of caprolactam has been verified by the actual case[4], here the simulation is carried out under the design condition of 34t/d output, which the property method is polynrtl[5] and different reactor temperatures at three sections are considered, to analyze their influence on the rate of conversion, molecular weight of polymer, content of extractable substance and ring dimerization components.

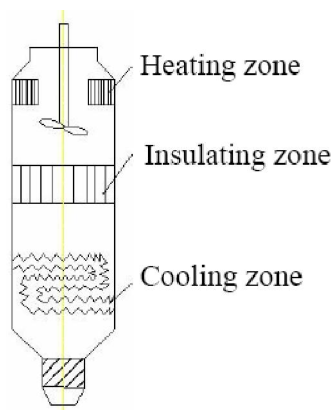

Figure 1 : Structure of the polymer tower

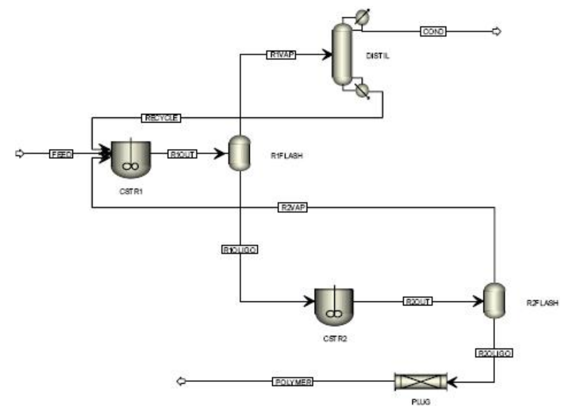

Figure 2 : Schematic of polymerization for simulation

RESULTS OF SIMULATION

Influence of the temperature of CSTR1

Keep the temperature of CSTR2, PLUG-0, PLUG-0.45, PLUG-1 as 260°C, 255°C, 245°C, 240°C, respectively, and design temperature of CSTR1 changes in a reasonable range. The effect of temperature of CSTR1 on molecular weight (MWN) and extractable substance value (EV %) are given in Figure 3a and Figure 3b, where simu8 to simu11 represents the temperature of CSTR1 is 260°C, 250°C, 240°C, 230°C, respectively. As can be seen in Figure 2a and Figure 2b, MWN and EV both increase with the decrease of the top temperature of polymer tower. So it needs to take care to choose proper temperature at top tower to ensure the quality of the product.

Influence of the temperatures of CSTR1 and CSTR2.

Keep the temperature of PLUG unchanged, but design temperatures of CSTR1 and CSTR2 are changed from 230°C to 250°C, 240°C to 250°C. The simulation results are presented in Figure 4a and Figure 4b., where temperatures of CSTR1 and CSTR2 in curve lines12 to 16 are 250°C and 250°C, 240°C and 250°C, 230°C and 250°C, 240°C and 240°C, 230°C and 240!, respectively. From curve lines13 and 15, curve lines14 and 16, it's clearly that MWN decreases obviously, but EV changes little, with the increase of temperature of CSTR2. So it benefits actual produce to have a higher temperature at the middle section of polymer tower.

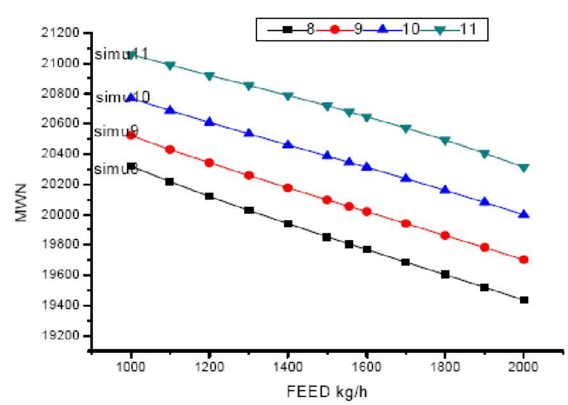

Figure 3a : Effect of temperature on MWN

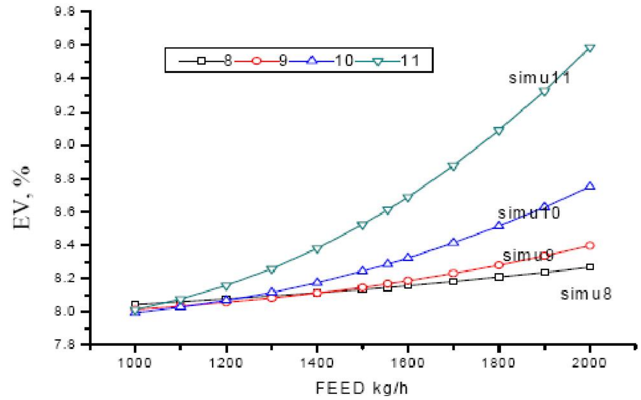

Figure 3b : Effect of temperature on EV

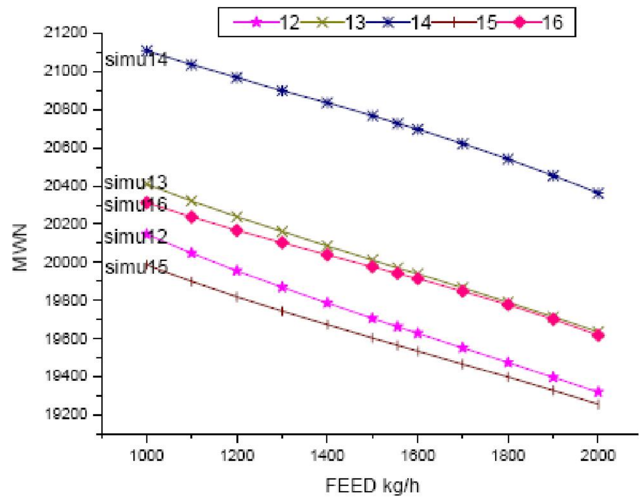

Figure 4a : Effect of temperature on MWN

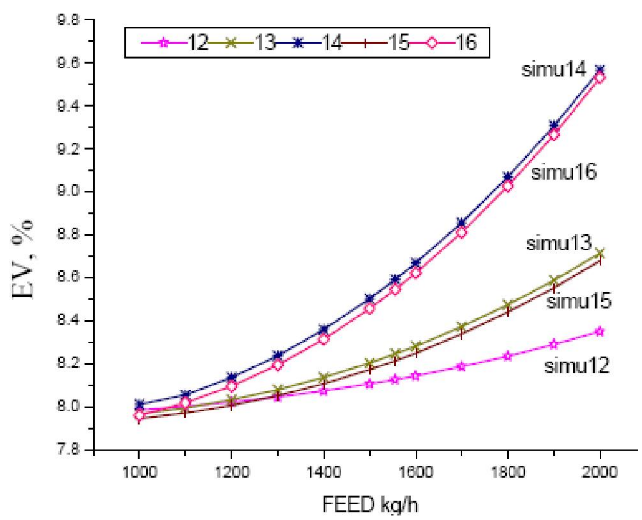

Figure 4b : Effect of temperature on EV

Influence of the temperature of PLUG-0

Figure 5a, 5b show that when the temperature of PLUG-0 from 245°C (curve line18) to 250°C (curve line17), MWN and EV are almost unchanged. Therefore, from point of view on energy saving and quality of product, lower temperature at Plug-0 is better.

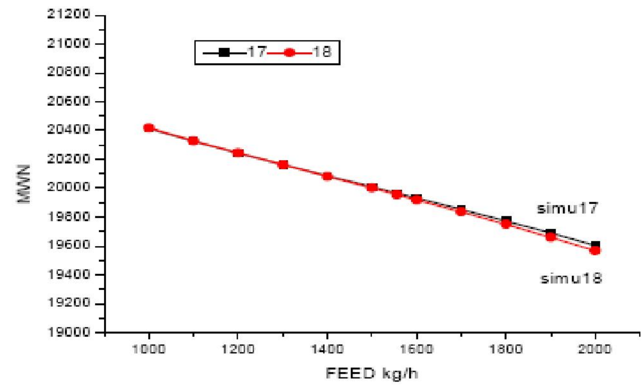

Figure 5a : Effect of PLUG-0 on MWN

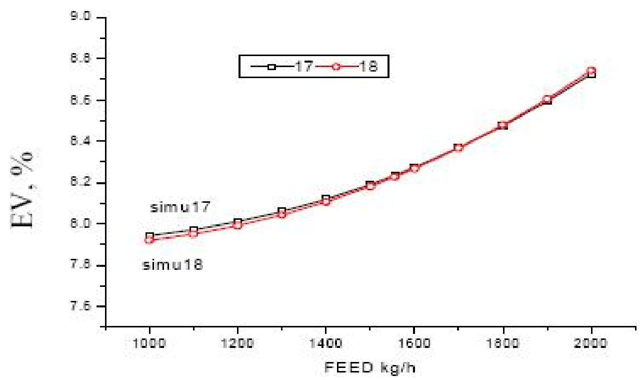

Figure 5b : Effect of PLUG-0 on EV

Influence of the temperature of PLUG-0.45

Figure 6a and Figure 6b show that MWN decreases when the temperature of PLUG-0.45 changes from 240°C (curve line19) to 235°C (curve line20). EV decreases with decrease of the temperature of PLUG-0.45 at lower feed flow but it is almost unchanged when the feed flow is bigger than 1600kg/h. It can be inferred that making a higher temperature of PLUG-0.45 is good for producing higher MWN, but without increase of EV at bigger feed flow.

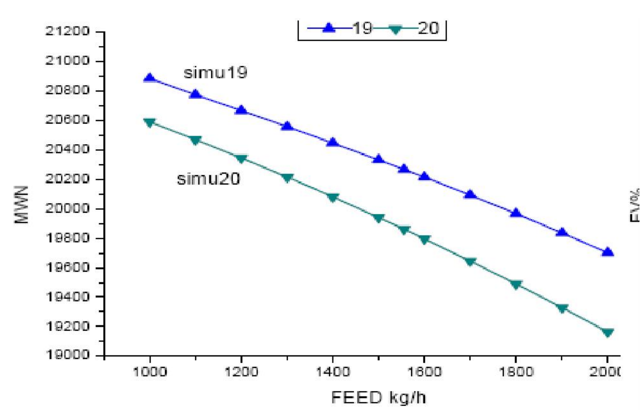

Figure 6a : Effect of PLUG-0.45 on MWN

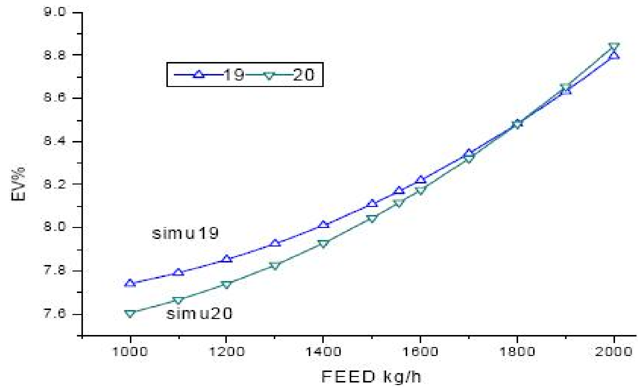

Figure 6b : Effect of PLUG-0.45 on EV

Influence of the temperature of PLUG-1

Simulation results are shown in Figure 7a and Figure 7b, where curve line21 means 245°C and 240°C; curve line22 means 245°C and 235°C, curve line23 means 250°C and 240°C; curve line24 means 250°C and 235°C for the CSTR1 and PLUG-1, respectively. MWN is larger when both the temperature of CSTR1 and PLUG-1 are lower, as can be seen from curve line22, but the temperature of PLUG-1has little effect on EV.

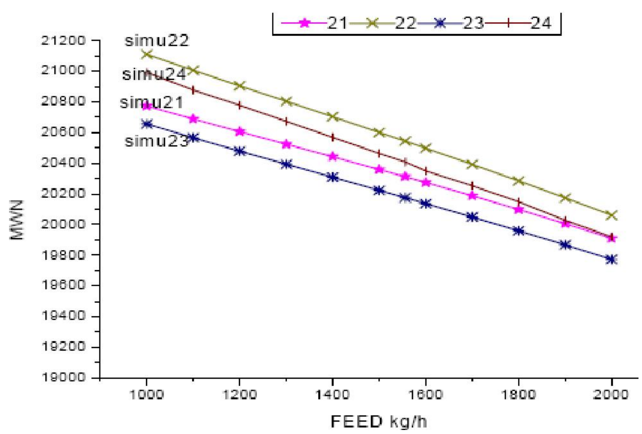

Figure 7a : Effect of PLUG-1 on MWN

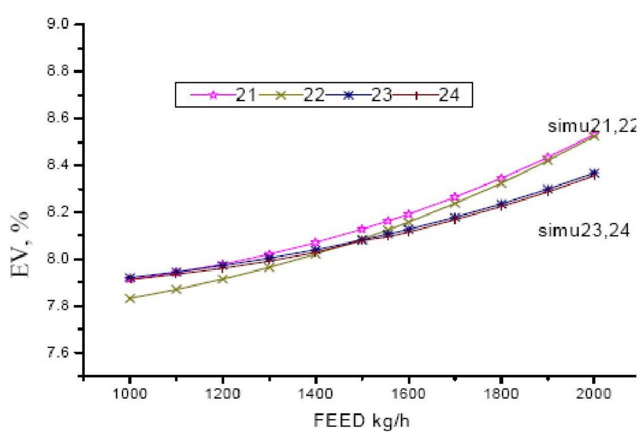

Figure 7b : Effect of PLUG-1 on EV

Influence of the temperature of CSTR1 and PLUG-1

The temperatures of CSTR2, PLUG-0, PLUG-0.5 are unchanged, simulation analysis of the influence of temperatures of CSTR1 and PLUG-1. We can notice that from Figure 8a and Figure 8b which curve line25 represents for 250°C and 245°C; curve line26 for 260°C and 240°C, curve line27 for 265°C and 230°C for the CSTR1 and PLUG-1, MWN increases and EV decreases with the temperature of CSTR1 rising from 250°C to 260°C. This condition is benefit for produc-

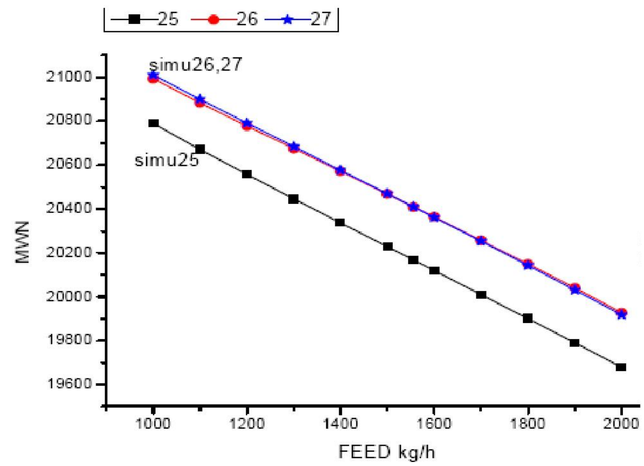

Figure 8a : Effect of temperature on MWN

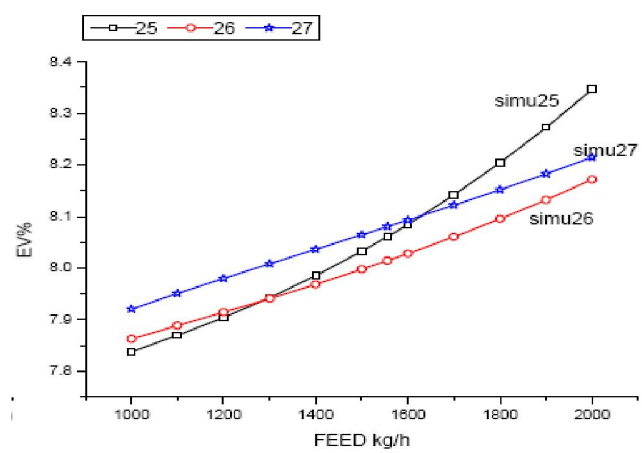

Figure 8b : Effect of temperature on EV

tion.

CONCLUSIONS

1) MWN reduces and EV increases with the increase of feed when temperatures of polymer tower are fixed.
2) The temperature of Plug has a large effect on pro-

duction, since MWN decreases and EV increases with temperature increase. In operating, this case should be avoided.

3) Front section temperature should be lower for a small daily output, as demonstrated in curve13, temperatures of CSTR1 and CSTR2 may be 240°C and 250°C, respectively. In this way, not only energy but also cooling load can be reduced. Meanwhile, the quality of production is also improved. On the other hand, increase front section temperature and reduce back section temperature if the daily output is increased to 40t. For example, operating condition could be obtained from curve27 for MWN higher than 20000 and EV lower than 8.3%.

ACKNOWLEDGEMENTS

This work was financially supported by National Natural Science Foundation of China (51176173).

REFERENCES

[1] J. J.Xie; Polymer Materials and Engineering. No.6 In Chinese, 13-17 **(2000)**.

[2] N.K.Kohli, R.Sareen, S.K.Gupta; J.Appl.Polym. Sci., **162**, 1219-1230 **(1996)**.

[3] Information on http :// www. aspentech. com.

[4] L.Liu; Master Dissertation, Zhengzhou University, **(2010)**.

[5] Aspen Technology, in: Aspen Plus Physical Property Methods and Models, Aspen Technology, 31-40 **(2000).**