Aspen plus Simulation and Analysis of Methanol Synthesis Process

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ABSTRACT: According to the actual situation of methanol production process, Aspen Plus software is used to build the methanol synthesis process flow model. The main and side reaction system is built in the model, which is realized by connecting the main and side reactors in series and setting the conversion rate of side reaction. Considering the model validation and process integrity, the methanol rectification system is connected in series on the basis of the methanol synthesis model, and the steady state simulation of the whole process is carried out. The methanol purity simulated is 99.74%, which shows that the model is reasonable. Through sensitivity analysis, the influence of feed flow change on the flow and purity of crude methanol and the influence of converter temperature change on the flow and purity of crude methanol were investigated. The relationship between the change of control parameters and the actual yield and equipment safety was preliminarily analyzed in order to provide reference and guidance for the development of methanol synthesis process.

1. INTRODUCTION

Methanol is not only a basic chemical product, but also an important chemical raw material. It has rich downstream products and also occupies an important position in the field of new energy1 . In recent years, methanol production enterprises have made continuous progress and development, applied new technologies to remove outdated production capacity, and the main role of the single alcohol unit has been enhanced. The whole industry is developing towards large-scale, efficient and clean 2. The core of improving methanol production technology is to promote the efficient operation of methanol synthesis reaction system3, which requires full consideration of the flexibility of reactor operation, catalyst efficiency, loading rate, service life, reaction heat recovery and utilization and other factors4. Most scholars choose Aspen Plus software for process simulation5, but most scholars seldom consider the generation of by-products due to the consideration of simulation process convergence. In this paper, with Aspen Plus software, two reactors are set up in series to simulate the main reaction part and a certain side reaction part in the methanol synthesis process, providing some technical support for methanol production.

2. PROCESS FLOW MODEL AND REACTION

Referring to the actual production of methanol plants, the methanol synthesis model in this paper is built by using the low-pressure method for reference. In this model, two reactors in series are selected to simulate the synthesis tower. Syngas and fresh air enter the reactor at the same time in a radial diffusion direction without back mixing, so RPlug horizontal plug flow reactor is selected as the main reactor R0101.B1. Assuming the reaction coefficient of the side reaction, the Rstoic stoichiometric reactor is selected for the side reactor R0101.B2. Considering the model validation and overall process integrity, the methanol synthesis system is followed by a crude methanol distillation system in series. The RadFrac module flow chart for the distillation system is as follows.

In the methanol synthesis system, the synthesis gas regulates the pressure through valve F0101, regulates the temperature through heater H0101, and finally enters reactor R0101 for methanol synthesis reaction. After being cooled by H0102, the reacted gas S0105 enters the gas-liquid separation tower V0101. One part of the separated gas passes through the condenser as the purge gas S0108 for venting treatment, and the other part returns to the mixer M0101 as the circulating gas, which is mixed with the fresh synthetic gas before recycling. The separated liquid crude methanol S0201 enters the distillation system.

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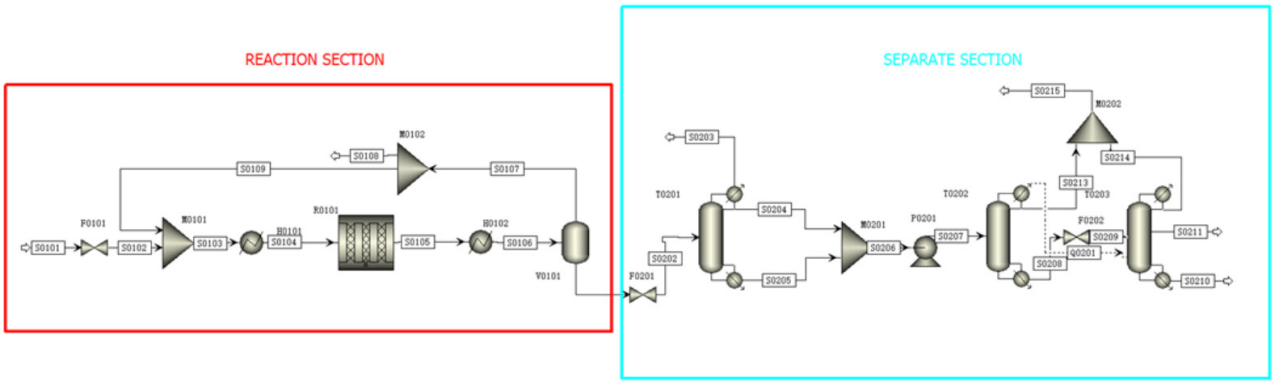

Figure 1. Methanol synthesis process flow chart.

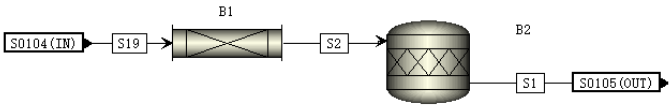

Figure 2. Reactor R0101 Model.

In the distillation system, the crude methanol S0201 enters the pre distillation tower T0201 after being depressurized to 0.1MPa through valve F0201. After condensation, part of the steam from the tower top is discharged as a non condensable substance S0203, and the other part is mixed with the methanol liquid from the tower bottom. After being pressurized to 1MPa through pump P0201, it enters the pressurized distillation tower T0202. After condensation, the steam from the tower top gets refined methanol S0213, After depressurization, the bottom liquid S0208 from the tower bottom enters the atmospheric distillation tower T0203 to continue distillation. The top steam after distillation passes through the condenser to obtain refined methanol S0214. The side line S0211 leaves fusel. The bottom liquid S0210 is treated as waste water.

In this paper, the low-pressure methanol synthesis method is adopted, and the copper based catalyst loading is set at 9000 kg, and void ratio of catalyst bed 0.4. The main reaction of methanol synthesis is as follows: $CO + 2H_2 = CH_3OH$; $CO_2 + 3H_2 = CH_3OH + H_2O$;$CO_2+H_2=CO+H_2O$.The side reactions of methanol synthesis are as follows:

$2CO + 4H_2 = C_2H_6O + H_2O$(Ethanol) (1)

$4CO + 8H_2 = C_4H_{10}O + 3H_2O$(Isobutanol) (2)

3. PROCESS CONDITIONS

The composition and flow rate of the feed gas are set as shown in Table 1, and the parameters of the converter are set as shown in Table 2. Assuming that side reactions occur during methanol synthesis, the CO conversion rate of side reaction (1) is set to 0.01, and the CO conversion rate of side reaction (2) to 0.02.

Aspen Plus software completes the steady-state simulation of methanol synthesis process, and obtains the phase molar flow and molar fraction of each stream, as shown in Table 3. The methanol purity in the end stream stream S0211 of the rectifying tower product has reached 99.99 %, meeting the requirements of industrial production, and the model is reasonable.

Table 1. Composition of Feed Gas.

components	CO	CO_2	H_2	N_2	CH_4
kmol/hr	3752.2	525.8	9465.8	412.1	56.8
mol%	26.4	3.7	66.6	2.9	0.4

Table 2. Basic parameter settings of reactor of synthesis tower.

parameter	R0101.B1	R0101.B2
Reactor	RPplug	RStoic
Reactor temperature	250℃	250℃
Effective phase state	Vapor phase	Vapor liquid two-phase

Table 3. Molar flow and molar fraction of components in different stream

stream	S0106		S0208		S0211	
omponents	Kmol/h	mol%	Kmol/h	mol%	Kmol/h	mol%
CO_2	19.88	0. 7	0.089	trace	19.88	trace
H_2O	261.24	9.7	261.23	10	261.24	trace
CH_4	32.426	1.2	0.001	trace	32.426	trace
H_2	2.70	0.1	trace	trace	2.70	trace
CH_4O	2348.3	88.0	2346.5	89.9	2348.3	99.9
CO	2.7393	0.1	trace	trace	2.7393	trace
N_2	0.5865	trace	trace	trace	0.5865	trace

4. SENSITIVITY ANALYSIS OF SIMULATION PROCESS

Aspen Plus sensitivity analysis was used to investigate the effect of feed flow change on the flow and purity of crude methanol, and the effect of temperature change in the synthesis tower on the flow and purity of crude methanol.

Figure 3 shows the influence of feed flow rate change of methanol synthesis tower on crude methanol flow rate and purity. When the feed flow rate changes within the range of – 10 % to 10 %, the flow rate and purity of crude methanol are disturbed slowly; However, when the feed flow variation deviation reaches 20 %, 30% and 40 %, the crude methanol flow and purity are disturbed to a greater extent. It can be seen that the methanol synthesis reaction can be effectively controlled by adjusting the feed flow, and it is advisable to control the fluctuation of the feed flow variation within 10 %. When the feed flow rate changes to – 40 %, that is, the feed flow rate is very small, the catalyst efficiency is high, the reaction is sufficient, the purity of crude methanol is 88.6 %, and it does not reach 95 %, and the conversion rate of side reaction set in the model does not exceed 0.03, which shows that the side reaction in the methanol synthesis process is inevitable. Moreover, with the continuous increase of feed flow, the methanol purity continues to decline. It is analyzed that the reason is that the catalyst efficiency is limited, the reaction is not sufficient, the methanol product rate decreases, and the by-products increase, leading to the reduction of methanol purity. In the future, the development of high yield and high efficiency catalysts for practical industrial production and application is still the development direction of the methanol industry.

Figure 4 shows the influence of temperature change in the synthesis tower on the flow and purity of crude methanol. The change of reaction temperature in the synthesis tower will directly affect the reaction in the tower. When the temperature of the converter changes within the range of – 10 % to 10 %, the flow rate of crude methanol increases slowly, and the purity of crude methanol increases from 87.06 % to 88.51 %, with a slow increase. Obviously, the increase of temperature promotes the methanol synthesis reaction to go forward and the output of crude methanol increases; When the temperature of the synthesis tower changes to 20 %, the flow rate of crude methanol decreases, and the purity increases to 88.82 %. It can be seen that the continuous increase of temperature will not promote the methanol synthesis reaction. When the temperature of the converter changes within the range of 25 % to 45 %, the purity of crude methanol decreases from 88.8% to 86.8 %, the flow rate of crude methanol decreases sharply, and the methanol synthesis reaction is limited while the side reaction is promoted. At the same time, too high reaction temperature of the synthesis tower will lead to overpressure of the synthesis tower, equipment damage, and increased fire and explosion risk. In order to ensure the safe and stable operation of the methanol synthesis system, it is recommended that the operating temperature of the synthesis tower be controlled within the range of – 10 % to 20 %, that is, 243.7 ℃ to 301 ℃. When the temperature of the converter changes within the range of - 50% to - 10%, the flow rate and purity of crude methanol increase sharply. It can be seen that the reaction does not reach the optimal temperature during this period, which will cause waste of production capacity in the production process. In the start-up phase, the converter should be preheated.

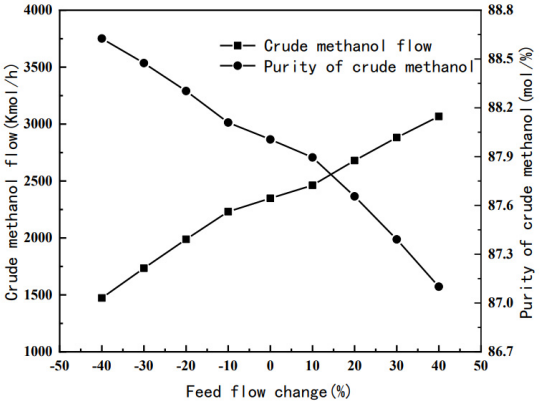

Figure 3 Influence of Feed Flow Change of Tower on Crude Methanol Flow and Purity

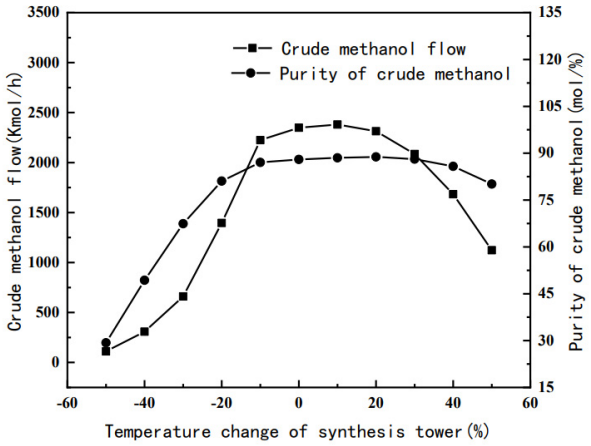

Figure 4 Influence of Temperature Change of Synthesis Synthesis Tower on Flow and Purity of Crude Methanol

5. CONCLUSIONS

(1) The whole methanol synthesis process is simulated by Aspen Plus software, and the parameters of each component of the unit under the set operating conditions can be obtained safely and efficiently; Extreme conditions can also be assumed to provide reference and guidance for the setting of the boundary line of the safety area and the quantitative analysis of the flow during production and operation.

(2) The methanol synthesis tower in this paper has successfully simulated some side reactions through the series connection of reactors. The model converges as a whole, providing reference and guidance for the design of other side reactions.

(3) Through Aspen Plus software simulation, the control of methanol synthesis reaction by regulating feed flow and converter temperature is quantitatively displayed. Considering the requirements of output, yield and safety, the variation deviation of feed flow should be controlled within the range of 10 %, and the variation of the operating temperature of the synthesis tower should be controlled within the range of – 10 % to 20 %.

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