Matlab Chemical Engineering Assignment Sample

Introduction

Matlab is very essential software for chemical engineering. Moreover, with the help of advanced technology, this Matlab software can replace manual chemical calculation. Moreover, chemical calculation data are very reliable and effective in this Matlab software. Different types of chemical calculation can be solved with the help of this Matlab software. There are various types of application in chemical engineering. These applications are ranging from process control, process calculation, and numerical manipulation to process simulation and modelling and the last one is optimization. Moreover, different types of factors used in chemical engineering. These factors are math, physical science, and life science.

Main Body

A. Calculations

Taking Rate constant to be × m^3/kmol/min

- In case of normal operation, kmol/m $C_{B0>3}$

Operating Temperature Rate>-4 m^3/kmol/min

Mass>AV ,

Energy Balance: (r_A) V>UA(TT_c)

For this case>VkC_{A0}(1x) (C_{B0}2$C_{A0}x$)
C_{A0}

For Normal Operation, 0.9724 kmol/m^3 .>3.

???2x?

Without the use of numbers, we can show that *t*>

At 45 mins,
about 7%

Heat generation As the operation that has been conducted is isothermal, the rate constant i.e. *k* will be a constant for the current phase. The rate of the reaction will be maximum at the beginning as the concentration of A and B was maximum at that time. Therefore,

Maximum rate of heat>

Maximum Possible heat removal rate

Hence, with the control of feedback, it was easy to maintain the temperature of bath.

In phase two, the operation becomes adiabatic.

The equations that are needed to be solved are
>

() V>UA(TT_c)

i.e.

Integrating numerically, the conversion is to be 0.085 and the temperature is to be 188.7ºC. 0.0020 kmol/min is the maximum rate. The maximum heat generated at this stage is 3861 kcal/min which is quite less than the Maximum heat removal capacity (5869 kcal/min)

In the third stage if the coolant was supplied fully, then the mathematical integration shows that the bath will definitely cool down.

Thus, with the feedback loop, it is seen that it is easy to operate at 188.7 ? for the rest of the time. This type of operations running for 23hrs gives 94.5% conversion. If it would have been operated isothermally in the 2nd and the 3rd stage then the last conversion would have 87.2%

B. Investigation of two scenarios

Input has new values but in the second stage if the coolant supply is cut.

The starting concentration is 1.7668 and 6.4466 kmol/m^3 for A and B respectively.

Highest heat removal is equal, 5378 kcal/min, Max heat generated is 4091 kcal/min. At this point the first stage is okay.

Ratio of>

When the first stage comes to an end. The conversion is 0.033608 and the concentration of A and B are 1.7074 and 6.3278 kmol/m^3 respectively.

The second stage was running isothermally, found out that the highest generation of heat at the end is 3836 kcal/min, which was below the highest heat removal capacity (5378 kcal/min). The conversion is 0.0407.

The third stage was running isothermally gives about 59 % conversion after 23 hours.

C. Runaway reactions.

The starting concentration is 1.7668 and 6.4466 kmol/m^3 for A and B respectively. Rate Max is 0.0014

Highest heat removal is the same 5378 kcal/min, generation of maximum was 4091 kcal/min. The initial stage is ok.

Ratio of>

At the first stage ends, conversion is around 0.033608 and the concentration of A and B are 1.7074 and 6.3278 kmol/m^3respectively.

As the second stage completes, conversions is 0.043 and that temperature is 195º

K is 0.0002044 m^3/kmol/min. Max rate is 0.0022 kmol/min

The highest heat generated at the current stage is 6570 kcal/min, this is actually a lot more than the possible heat removal rate (6095 kcal/min)

The temperature raised in less than 0.5º C at the beginning, so it will be difficult to have a look at the problem in this stage.

Therefore, for input of regular, 10 mins cutting of the coolant (45mins to 55min) is not a big complication. Isothermal operation is not a problem for larger input. The problem lies with larger input and cutting of the coolant together.

D. Counter Measures

Accidents in the chemical industries are very rare and are very dangerous. It causes loss of life and income of their family. Changes can be a boon as well as a curse, so safety should be the first immediate concern when dealing with changes (mainly in chemicals) The main reason for someone to blame is the chemical engineer himself. He is the person responsible for carving out a more safe process and a system that can, in turn, protect the lives and health of the people working the plant (Bae*et al.*2017, p. 123).

Here, in this case, the measures that should have been taken are as follows:

- 9.004kmol of ONCB was charged for the reactor which is three times the normal, which is 3.17kmol. Proper measuring should have been taken by the operators and must have proper approval from the Chemical engineer in charge of the plant. SOP's should be followed strictly within the industry and chalking out one is very necessary.
- Proper tested and simulated designs should be used before carrying out the reaction. Moreover, new make for the rupture disc should have considered instead of repairing over and over for years. Here the plant management had removed an insulation layer that could be responsible for overcharging with ONCB. The materials had started leaking between the relief device and the rupture disk which increased the pressure and released from the gap developed. The relief system had doubled the pressure in the reactor even before the rupture disc would even open. The ruptured disc was designed in a way that if it had to burst it would have burst it in 48 bar which is corresponding to 48 bars and in fact, it did not. If the temperature was around 320° C this would have disastrous (Shi*et al.*2018, p. 915). If proper designs could have been designed then this could have been avoided.
- Heat exchange has been failed for 10 mins so proper supervision and constant monitoring were needed at the time of the reaction. The operators had neglected the pinhole leak that

the ruptured disc and the relief device has created due to high usage over the years. Here rather than maintenance and having a new disc was more viable.

In order to avoid the poor usage or handling as well as emergency responses to the accidents that occur, proper labelling should be done for chemicals. It should follow proper standardization. Putting up a label is easy to understand and more importantly, SOP's should be released within the industry with proper approval and tested methods. Identification of threats and hazards is very important (Longley, 2019, p. 10). As soon as the threat is identified, an immediate remedy should be provided. The engineers of bioprocess commonly use criteria for design to minimize the cost or maximize the gains. Moreover, more the barriers put on the potential threats and failures, it will definitely have an increase in the cost of the department. Most common reasons for chemical explosions in the industries due to the pileup of very reactive chemicals in the area of reaction.

Conclusion

This study mainly concludes on the application of Matlab in chemical engineering and ortho nitro chlorobenzene. The Matlab software is an important software in the chemical engineering field. With the help of advanced technology, this Matlab software can replace manual chemical calculation. Ranging from process control, process calculation, numerical manipulation to process simulation and modelling and the last one is optimization these are various type of chemical calculation that can be solved in the Matlab software. In this context, we get physical properties of ortho nitro chemical benzene. Moreover, we get the effect of ammonia concentration and the effect of sulphide concentration.

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