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The BLEVE Research of Reaction Runaway Based on the Aspen Plus-Fluent

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Abstract

A new scene analysis method of reactor thermal explosion accident based on process simulation and CFD method is proposed. The thermal runaway of batch reactor with methanol and acetic anhydride is simulated by Aspen Plus. The molecular weight and component concentration of steam after explosion overpressure are studied. The vapor cloud explosion is simulated by Fluent. The propagation law of vapor cloud explosion pressure wave and flame front is analyzed based on the simulation results.

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Keywords: reaction runaway, accident consequence, Aspen Plus, Fluent, BLEVE,VCE

Nomenclature

L_m	explosion limit of mixed gas
L_i	explosion limit of the ith component
Y_i	volume fraction of the ith component
G_k, G_b	turbulence kinetic energy generated by increasing laminar flow velocity
Y_m	compressible turbulent dissipation rate
σ_k , σ_ε	turbulent Prandtl constant
S_k, S_ε	custom source items

1. Introduction

The thermal runaway risk of reactor contains two aspects: the possibility of accidents and the severity of the sequence. Many researches focuses on the possibility of the accidents which depends on the inherent safety degree of reaction process and protective layer of the reactor[1-6]. Researches about the severity of the runaway accident are few. Because there are reactants and products in reactor at the same time. The mixture composition is in dynamic changes during the reaction process. The computation of explosion energy and consequences of dynamic components is very difficult. Process simulation software is helpful to analyze the severity of the sequence[7-8].

The vapor cloud explosion accident which is caused by reaction runaway can be seen as a special process of boiling liquid expanding vapor explosion (BLEVE) [9]. Because of the vapor pressure and the non-condensable gas under the high

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temperature, the reaction pressure will increase sharply with the increase of temperature. If the pressure increasing rate is higher than the discharge rate. The reactor will overpressure explosion. This physical explosion process can be viewed as an adiabatic flash process. The flashing model can be used to calculate the molar mass and material component of gas phase and liquid phase after physical explosion. Because the remaining components in the liquid phase are very close to the boiling point temperature and the reaction is very quickly at high temperature, the open reactor model is used to calculate the molar mass and material component of gas phase and liquid phase. Therefore, Aspen Plus is used to simulate the reaction runaway, adiabatic flash and open reactor model. CFD method is used to simulate the scenario of vapor cloud explosion[10].

2. Simulation study

2.1. reactant

The esterification reaction of methanol and acetic anhydride is selected in this research[11-12]:

$$(CH_3CO)_2O + CH_3OH \rightarrow CH_3COOCH_3 + CH_3COOH \quad (1)$$

The batch reactor volume is assumed as 5 m^3. Methanol mass is 1156 Kg. Acetic anhydride is 1844 Kg. The initial reaction temperature is 20 ℃.The worst conditions for the whole process correspond to either reactions under adiabatic conditions or cooling system failure event is studied in this research.

2.2. Aspen Plus simulation process

The BLEVE is simulated by Aspen Plus as shown in Fig.1. The RBATCH1 which is batch reactor run away and the overpressure explosion model is FLASH. The overpressure explosion process is adiabatic flash process. The VAPOR1 and LIQUID1 which generated by FLASH are gas-liquid two-phase which generated by explosion. The remaining LIQUID1 continue to reaction and the RBATCH2 which is batch reactor is selected. The reaction pressure is atmospheric pressure. Steam evaporation is VENT. The mixture of VENT and VAPOR2 create an explosive mixture in the air. It is important to pay attention during the simulation. VAPOR1 and VENT are characterized as flux in the software. The real quality of steam is the flux times the reaction time. The reaction time of RBATCH1 is different to the reaction time of RBATCH2. Therefore, the reaction time of VAPOR1 need a k magnification and then mix with VENT. K is the time ratio of FLASH and RBATCH2. The temperature of LIQUID2 will decrease due to the temperature of LIQUID2 is higher than the environment temperature. The remaining is difficult to volatile components. Therefore, the LIQUID2 don't need to calculate the evaporation.

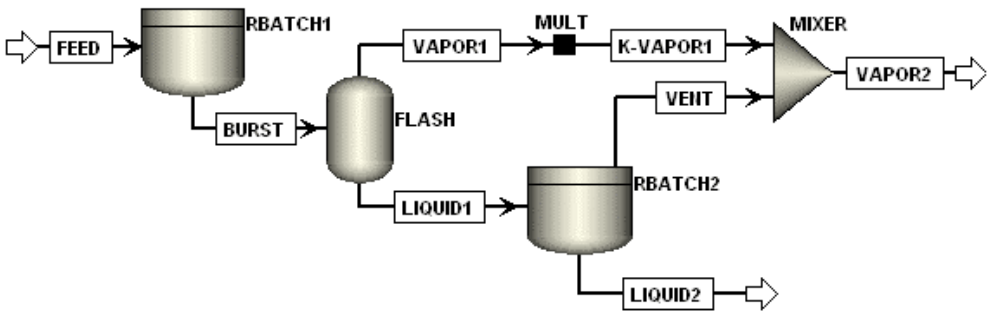

Fig.1 The BLEVE simulation process of reaction runaway

2.3. Aspen simulation results

There is gas phase association in the esterification reaction of methanol and acetic anhydride. So, property method is NRTL-HOC. The reaction order is one with the excess of methanol. The pre-exponential factor is 4.67×107 s^{-1} $kmol^{-1}$ m^3.

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