Characterisation of pressure and temperature rise of run-away reactions using temperature-programmed measurements

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Abstract

In production buildings it is sometimes necessary to install an emergency relief system to protect reactors. Usually adiabatic measurements of the actual runaway are proposed to obtain the necessary data on temperature and pressure against time. This involves either containment of the whole apparatus and/or compensation of the resulting pressure rise. The latter is complicated and difficult to realize. Alternatively a small pressure resistant sample container can be used, which because of its heat capacity makes a cumbersome correction of the measured runaway curve necessary. To obtain the desired data for vent sizing an alternative method was therefore developed using isoperibolic calorimetry.

This method is based on temperature-programmed measurements and on the use of kinetic software. The thermal kinetics of the decomposition as well as the kinetics of the gas production are calculated. The combination of thermal and gas kinetics gives information on the temperature and pressure rise during a run-away. It also avoids the use of cumbersome adiabatic or pseudo-adiabatic experiments.

Using temperature-programmed measurements a relation describing the thermal conversion as a function of time or temperature is developed. It is therefore possible to predict a run-away of the reaction assuming adiabatic conditions.
Based on the same idea a relation describing the pressure signal, also recorded during the temperature-programmed measurements, as function of time or temperature can be found.
Combining these two relations it should now be possible to obtain the pressure profile during an adiabatic behaviour leading to the run-away and therefore to calculate a pressure relief system according to the equations described in the DIERS Workbook.