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# Recent Developments in the Assessment of Thermal Risks of Chemical Processes

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**Abstract:**

**In the past two decades, the assessment of thermal risks linked to the practice of chemical reactions on an industrial scale has made great progress. Nowadays chemists understand these risks and are able to assess them. Nevertheless, incidents still occur which indicate that some weaknesses still exist, especially in risk management systems. Recent developments aim at providing production staff with improved tools for the assessment of these risks and also for training purposes. Furthermore, for some special situations, more specific and more accurate experimental techniques and estimation methods are required. In the present paper, some recent developments realized in our safety research laboratories are reviewed.**

## Introduction

Thermal process safety is often considered to be a mature field, meaning that no great improvements are expected from research in the future. The methods to measure the relevant properties of materials and to assess thermal risks were developed in the early 1970s. Today we understand the nature of runaway incidents, and we know how to prevent them. The fact that such incidents still occur proves, however, that this knowledge, although available, is not always applied properly in chemical production. This is due to the complexity of the phenomena and also to the great diversity of the different tasks production managers have to deal with. The assessment of thermal risks involves very specialized knowledge which may not be accessible to everybody. Therefore, research and development in thermal process safety should provide tools which can be used by professionals in chemical production and development having only an average background in methods of physical chemistry, without compromising the quality of the assessment.

To be efficient in maintaining a high level of process safety, it is essential to make these tools available to individuals bearing responsibility for process safety in chemical production and process development units and to train them in their proper use. Recent developments in the science of computer-aided instruction allow to provide such tools.

Another aspect of the assessment of thermal risks opens a promising area for new developments: In their experimental techniques and especially in the interpretations of measurements, most safety laboratories often use short-cuts to keep their procedures simple and practicable. The consequence of the use of short-cuts is, however, that greater safety margins are required to compensate for the uncertainties of the approximations made. This may result in abandoning a process judged to be too risky which could have been accepted if more accurate methods had been used. This opens a further field for research and development in improving the interpretation techniques and allowing one to make more adequate recommendations for safety in chemical production.

The actual research fields of our laboratory are summarized in Table 1.

The five examples mentioned in Table 1 will be reviewed in this paper.

## 1. Assessment Tools: The Failure Scenario

The main risk linked to the performance of exothermic reactions on an industrial scale is the loss of control of the reaction, which may lead to a temperature increase resulting in a pressure increase or in triggering a secondary decomposition reaction. To avoid or to control such an event, it is necessary to understand how a reaction can "switch" from its normal course to a runaway reaction. A very powerful tool for this task is the runaway scenario. The scenario developed in our company some years ago[1] helps one to ask the right questions and to measure the data actually required for risk assessment. The strength of this tool lies in the systematics introduced by a set of questions related to the severity and to the probability of a runaway. Starting from the process temperature, after a cooling failure, the heat of reaction increases the temperature up to a level called the maximum temperature of the synthesis reaction (MTSR). At this level, a secondary reaction may be active, which leads to a further temperature increase. A reaction can be considered to be active if the temperature increase is fast, meaning the runaway would take place in a short time. This temperature can be characterized by the time to maximum rate under adiabatic conditions (TMRad). The TMRad is a function of the temperature: the higher the temperature, the faster the reaction and the shorter the TMRad. If the time to maximum rate is longer than 24 h, we can consider that the decomposition will not be triggered. In terms of our scenario, this means that, if the temperature level reached after the cooling failure (MTSR) is below the temperature where TMRad = 24 h, we can consider the decomposition reaction to be uncritical.

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*Table 1*

| objective of research | research fields | application fields and results |
|---|---|---|
| to make the methodology for the assessment of thermal risks easily available | knowledge-based computer programs<br>computer-assisted tutorials<br>calculation programs<br>hypertext providing help on concepts and data estimation | systematic use by production and development chemists and engineers<br>examples:<br>assessment tools<br>thermal safety tutorial<br>thermal safety assistant |
| to achieve more realistic safety margins<br>to achieve increased productivity | improvement of experimental techniques and of techniques for the interpretation of data | safe operation of processes previously considered critical<br>improved confidence of professionals in production and development in the results of risk assessment<br>examples:<br>evaporative cooling<br>autocatalytic decomposition |

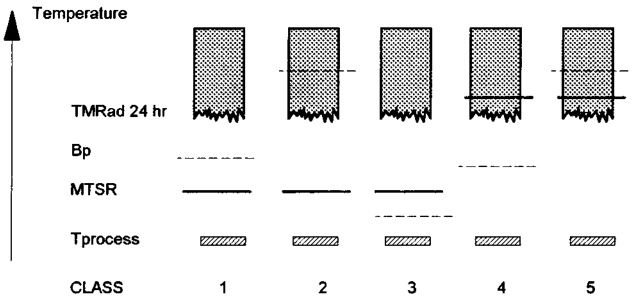

***Figure 1.*** **Assessment of the criticality of scenarios.**

Thus three temperature levels are used in the scenario: the process temperature, the maximum temperature which can be reached during the runaway of the synthesis reaction only (MTSR), and the temperature at which the decomposition reaction becomes critical (TMRad = 24 h). There is a further important temperature level: the temperature at which technical limits are reached. This may be the temperature at which the safety valve opens, the boiling point of the reaction mass, or the temperature limit of construction materials. In the following we consider the technical limit to be the boiling point. On the basis of these four temperature levels, five types of scenarios with increasing criticality can be defined[2] (Figure 1).

Scenarios 1 and 2 are not critical: the decomposition reaction cannot be triggered, and the boiling point is not reached. In scenario 3, the boiling point is reached but the decomposition reaction cannot be triggered. In scenario 4, the decomposition reaction could be triggered, but the boiling point is reached first. Scenario 5 is the most critical, since the decomposition reaction is triggered before the boiling point is reached.

This classification of the scenarios can be used to understand the phenomena which occur during runaway; then it is of great help to design the measures which allow one to regain control of the reaction.

## 2. Thermal Safety Tutorial

The basic knowledge required for the assessment of thermal risks is normally acquired in courses and seminars. For the personal training of professionals who are involved in risk assessment, a computer-aided tutorial, the Thermal Safety Tutorial, has been developed. The main purpose of the program is to lead to a better understanding of the analysis of the thermal risks of a chemical process or a unit operation by solving especially prepared case studies.

**Case Studies.** The first user version guides the user through the analysis of the thermal risks in four case studies: (1) addition reaction, (2) storage, (3) sulfonation, and (4) glycidylation.

**Structure of the Courseware.** Within a case study, the analysis of the thermal risks of chemical reactions is divided into four lessons.

*Lesson 1* is a step by step procedure which gives a preliminary evaluation of both the severity and the probability of an incident using simple techniques (screening).

*Lesson 2* expands the study using more data, if the conclusion of the previous screening is that the thermal risks of the process are high.

*Lesson 3* summarizes the results obtained in the previous lessons through the construction of a cooling failure scenario and the assessment of its criticality.

*Lesson 4* analyses the operating conditions required to maintain the process under thermal control as well as the measures that should be taken to prevent an incident from occurring.

**Thermal Safety Tutorial: Help File.** The computer-aided tutorial includes, in the standard format of a Windows help file, a glossary of relevant concepts of thermal safety analysis.

The help file can be accessed at any time while the program is running. It provides information about basic concepts of thermal safety analysis and measurement techniques.

This program has been used by more than 100 professionals and was found to be very useful as a complement to courses. In several sites it has been declared mandatory for production and development staff. This software package will be commercially available from the Expert Commission for Safety in the Swiss Chemical Industry.

## 3. Thermal Safety Assistant

A critical step in the course of risk analysis is to compile the basic thermal data necessary to build a failure scenario. The economy of the assessment requires one to ask only for

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(2) Stoessel, F. *Chem. Eng. Prog.* **1993**, *89*, (10), 68−75.

data really required. To help in this choice and also to assist the user in the evaluation of the data and of the thermal risks involved in a given process, a software package was developed.

This program provides guidance in data collection (thermochemical measurements in the laboratory; estimation and calculation of relevant parameters) and uses rules of inference ("if...then" rules) to assess the risks based on these results. Many attempts were made to formulate a decision tree as a help to apply this method. However, there is still no recognized procedure: many relationships between data and concepts are known only to the experts, and the complexity of the task makes it difficult to present them in a well-formulated, simple way. Here the benefits of the knowledge based programming technology can be of great help. Thus a computer program was developed for this task. Its main features are described hereafter.

**Collection of Data.** The user is asked in a dialogue to enter the physicochemical data. The screen reproduces the data sheet of the risk analysis, associated with a context-sensitive help section which gives information about (a) the scientific or technical definition of the data, (b) the available experimental techniques and estimation procedures to obtain a value, and (c) a selection of significant values.

A comprehensive handbook on thermal risk assessment can be accessed just by pressing a key and clicking the highlighted topics of a Windows help file.

**Computation of Data.** To obtain calculated values from data already introduced in the form, (a) the computer assistant can obtain automatically the calculated value if all of the necessary data were already entered; (b) the computer assistant can check for data which are not already introduced and indicate what is missing; (c) the context-sensitive help section can give the calculation formula with the corresponding units and the scientific and technical meaning of the terms; and (d) auxiliary calculation programs can help to get the values which are required for the assessment.

**Appreciation of the Thermal Risks Based on the Existing Data and Calculated Parameters.** (a) The computer assistant may help by applying rules of inference to the existing data to draw conclusions regarding the risks linked to the process under study. (b) On the basis of the conclusion of the preceding inference rules, the program gives more comprehensive information and suggestions about the relevant measures to render the process safe.

This program has been tested at different levels. First, data from case studies representing typical industrial processes have been introduced to the program. The answers obtained are in good agreement with the expected safety assessment. In a second phase and during approximately 1 year, the results of a significant part of the safety studies of our laboratory have been compared with the advice given by the thermal safety assistant. Presently about 20 safety and process development specialists from different countries are testing the program. Their remarks and suggestions are evaluated, and improvements are incorporated into the program; so far, no errors in the safety assessment have been detected.

## 4. The Boiling Point: Hazard or Safeguard?

If the boiling point is reached during runaway (classes 3−5), a possible secondary effect of the evaporation of a solvent is the formation of an explosive vapor cloud, which in turn can lead to a severe room explosion if ignited. The amount of solvent evaporated can easily be calculated using the energies of the reaction and of the decomposition, but there was no method available to assess the effect of such a boiling with regard to the technical possibilities of the equipment: either (a) the temperature will be stabilized when the boiling point is reached and evaporative cooling will help to control the runaway or (b) the boiling rate will be too high and the result will be a pressure increase, with the consequences described above. Thus the boiling point can be a safeguard or a hazard. A systematic method for the assessment of the hazards linked to the boiling of a reaction mass was developed[3] to allow a quantitative prediction of the behavior of a reaction mass at the boiling point (Figure 2). Besides the determination of the heat release rate, which was treated in a previous paper,[4] and the design of the condenser, which is a classical engineering task, two further aspects must be taken into account: flooding of the vapor tube (when the condensate flows down in countercurrent with the rising vapor, flooding may occur) and swelling of the reaction mass (the apparent volume variation due to the presence of vapor bubbles in the reaction mass).

The results of this study are summarized here.

**Flooding of the Vapor Tube.** If the diameter of the vapor tube is insufficient for a given vapor release rate, the high vapor velocity results in a pressure increase in the reactor leading to a temperature increase and a further acceleration of the reaction. The consequence will be a thermal explosion until the rupture of weak parts of the equipment allows pressure relief.

In order to avoid this type of reaction course, it is important to know the maximum vapor velocity admissible in a given tube and consequently the maximum admissible heat release rate for the reaction. To predict whether flooding will occur in existing equipment, an empirical correlation was established experimentally. The experimental study was performed in the laboratory, in the pilot plant, and also on an industrial scale with various organic solvents and water, for tubes with an inside diameter between 6 and 141 mm. The maximum allowable heat release rate is obviously a function of the latent heat of evaporation and of the tube cross section. It can be calculated by

$$q_{\max}(W) = [4.52\Delta H_V + (3.37 \times 10^6)]s \qquad (1)$$

The vapor limit superficial velocity, $j_{G\max}$, at the surface of the film can be calculated from the maximum allowable heat release rate. It depends only on the physicochemical properties of the solvent:

$$j_{G\max} = \frac{4.52\Delta H_V + (3.37 \times 10^6)}{\Delta H_V \rho_G} \qquad (2)$$

with $j_{G\max}$ = vapor limit superficial velocity, m·s$^{-1}$; $\Delta H_V$ =

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(3) Wiss, J.; Killé, G.; Stoessel, F. *Chimia* **1993**, *47*, 417−423.
(4) Wiss, J.; Stoessel, F.; Killé, G. *Chimia* **1990**, *44*, 401−405.

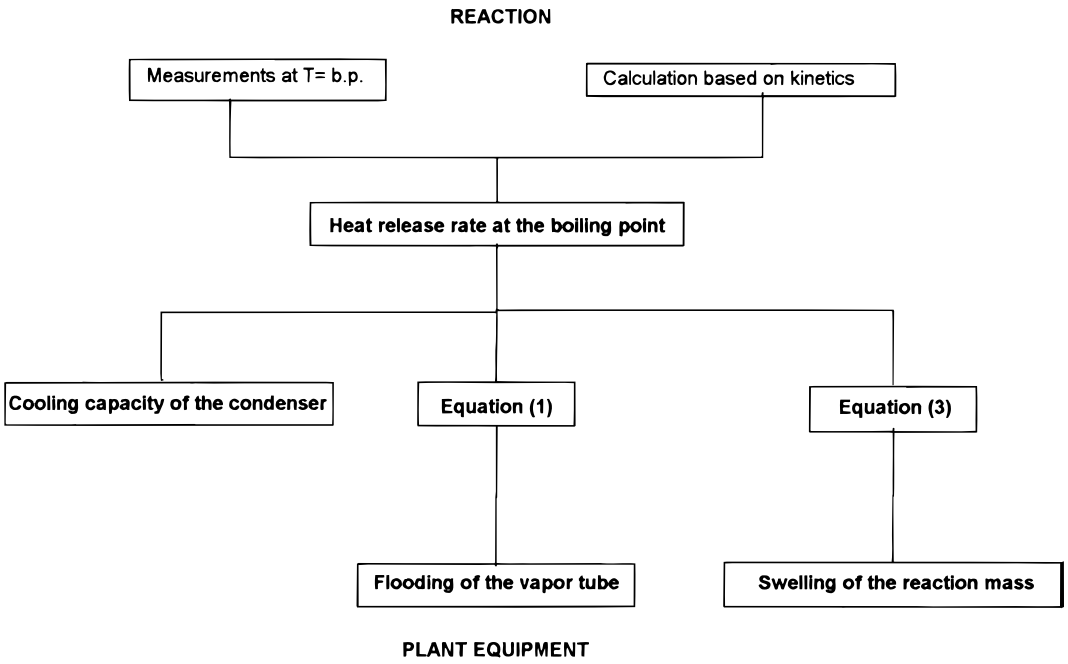

***Figure 2.*** **Systematic assessment of the behavior of a reaction mass at the boiling point.**

enthalpy of vaporization, kJ·kg$^{-1}$; $\rho_G$ = specific mass of vapor, kg·m$^{-3}$; $s$ = cross section area of vapor tube, m$^2$; 4.52 = constant, mass flux, kg·m$^{-2}$·s$^{-1}$; $3.37 \times 10^6$ = constant, heat flux, W·m$^{-2}$.

**Swelling of the Reaction Mass.** The swelling of the reaction mass can be estimated using the Wilson correlation. This correlation was first established for air in water. The correlation is easy to use and was found (experimentally) to describe with sufficient accuracy the swelling of a liquid by bubbles of its vapor:

$$\alpha = K\left(\frac{\rho_G}{\rho_L - \rho_G}\right)^{0.17} (D_H^*)^{-0.1} (j_G^*)^a \tag{3}$$

with

$$\alpha = \frac{H_B - H_0}{H_B} \tag{4}$$

$$D_H^* = \frac{D_H}{\sqrt{\dfrac{\sigma}{g(\rho_L - \rho_G)}}} \tag{5}$$

$$j_G^* = \frac{j_G}{\sqrt{g\dfrac{\sigma}{\sqrt{g(\rho_L - \rho_G)}}}} \tag{6}$$

and

$$\text{if } j_G^* < 2,\ K = 0.68 \text{ and } a = 0.62$$

$$\text{if } j_G^* \geq 2,\ K = 0.88 \text{ and } a = 0.40$$

where $H_B$ = height of boiling liquid, m; $H_0$ = height of liquid before boiling, m; $\sigma$ = surface tension, kg·s$^{-2}$; $\rho_G$ = specific mass of vapor, kg·m$^{-3}$; $\rho_L$ = specific mass of liquid, kg·m$^{-3}$; and $D_H$ = hydraulic diameter of the reactor, m.

The correlation allows one to calculate the maximum admissible heat release rate for given plant equipment or to design equipment for the requirements of a given process. Both capabilities are based on easily accessible physicochemical properties of the boiling solvent and on geometric data of the reactor.

A systematic procedure for the assessment of the safety of chemical reactions at the boiling point is presented in Figure 2. This procedure allows one to predict the behavior of a reactor at the boiling point. As an example, for a 6.3 m$^3$ stirred tank filled with 6.3 m$^3$ of acetone, the maximum allowable heat release rate at boiling is 35 kW with a 200 mm vapor tube (the diameter of the vapor tube is the limiting factor) and 68 kW with a 300 mm vapor tube (the swelling of the reaction mass is the limiting factor).

Such considerations allow one to adapt the equipment or the process, i.e., the degree of filling of the reactor, to the safety requirements. This kind of measure often allows one to run processes under safe conditions whereas a classical assessment would consider them to be critical.

## 5. TMRad and Self-Accelerating Reactions

**Time to Maximum Rate.** As explained in the Introduction, the time to maximum rate can be used to estimate the probability of triggering a decomposition reaction:

$$\text{TMRad} = \frac{C_p R T_0^{\,2}}{q_0 E_a}\ [\text{s}] \tag{7}$$

with $C_p$ = heat capacity of reaction mixture [J·kg$^{-1}$·K$^{-1}$]; $R$ = ideal gas constant [=8.314 31 J·mol$^{-1}$·K$^{-1}$]; $T_0$ = initial temperature of the runaway [K]; $q_0$ = heat release rate at $T_0$ [W·kg$^{-1}$]; and $E_a$ = activation energy [J·mol$^{-1}$].

This approximation (7) was established for reactions of zero order. The error is low for other reaction orders if the reaction in question is very exothermic. In this case, the temperature increase is high even at low conversion and the reaction rate is almost independent of the conversion.

A decomposition reaction, however, often has an autocatalytic mechanism. Such a reaction can be formally

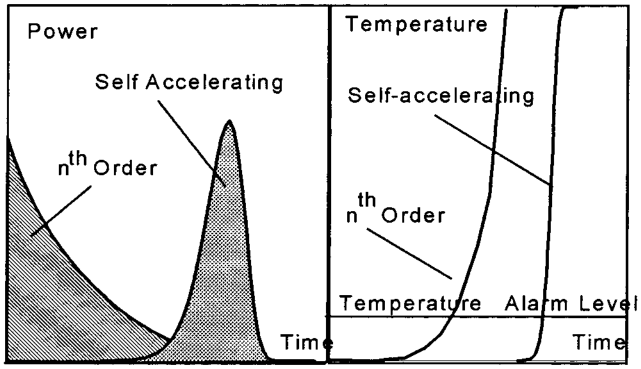

***Figure 3.*** **Comparison of an *n*th-order reaction with a self-accelerating reaction.**

represented by a mechanism involving two parallel steps: the first one, the initiation reaction, is a first-order reaction, whereas the second one is a second-order, Prout−Tompkins type of reaction:

$$A \xrightarrow{k_1} B$$

$$A + B \xrightarrow{k_2} 2B$$

The reaction seems sometimes to be preceded by an induction time where no exothermic effect can be observed. In this case, one could calculate the activation energy and the TMRad using the maximum heat release rate and neglecting the induction time. This would lead to unnecessarily short induction times and therefore to excessive safety margins in terms of time. The apparent risk could eventually prevent an otherwise interesting procedure from being commercially exploited.

Therefore an estimation method for the time to explosion under adiabatic conditions in the case of an autocatalytic decomposition reaction was developed.[5]

The method must be reliable and easy to use. It should require only instruments found in thermal safety laboratories like differential scanning calorimeters (DSC)[6,7] and possibly an accelerating rate calorimeter (ARC).[8]

**Special Aspects of Autocatalytic Reactions with Respect to Safety.** Reactions often follow an *n*th-order kinetic law. Under isothermal conditions, i.e., under conditions where the temperature remains constant, the heat release rate decreases uniformly in time. In the case of autocatalytic decomposition, the behavior is quite different (Figure 3). An acceleration of the reaction rate with time is observed. The corresponding heat release rate passes through a maximum and then decreases again. The acceleration period is often preceded by an induction time where no thermal signal and therefore no noticeable conversion can be observed. Hence an isothermal DSC experiment immediately shows to which type a reaction belongs.

In the case of an adiabatic runaway these two types of reactions will lead to totally different temperature versus time curves: with *n*th-order reactions the temperature increase starts immediately after the cooling failure, while with autocatalytic reactions the temperature remains stable during the induction period and suddenly increases very sharply as shown in Figure 3. For the design of emergency measures, it is very important to know to which of the two types a decomposition reaction belongs. For example, temperature alarms will work only with decomposition reactions following a *n*th kinetic order law, as only in these cases are the prewarning times sufficiently long.

Among different rate equations describing self-accelerating reactions, the following simple equations have been shown to be satisfactory for our purpose in the field of process safety:

$$A \xrightarrow{k_1} B \qquad \text{slow initiation reaction}$$

$$A + B \xrightarrow{k_2} 2B \qquad \text{fast autocatalytic reaction}$$

$$r = \frac{d[B]}{dt} = k_1[A] + k_2[A][B] \tag{8}$$

The simplification (reaction order and stoichiometric coefficients) will in general underestimate the adiabatic runaway time of reactions of higher orders. This can be tolerated for safety reasons.

**Determination of Kinetic Parameters from DSC Experiments.** The heat release rate of a chemical reaction is a function of both temperature and conversion rate. The complete thermokinetic description of a decomposition reaction involves therefore the knowledge of both factors separately. By using a series of isothermal measurements, where the temperature is kept constant, the conversion rate as function of time can be measured separately.

The instantaneous heat release rate, as measured by DSC, is proportional to the conversion rate:

$$\frac{dq}{dt} = -\Delta H_R \frac{dX}{dt} \tag{9}$$

The kinetic parameters from the model presented above (eq 8), i.e., both rate constants, $k_1$ and $k_2$, and the activation energies, $E_{a1}$ and $E_{a2}$, must be determined. The rate equation can be written

$$\frac{dB}{dt} = k_1[A] + k_2[A][B] \tag{10}$$

$$\text{if } [B] = X[A]_0\text{, then } [A] = [A]_0 - X[A]_0$$

and eq 10 becomes

$$\frac{dX}{dt} = k_2(1 - X)\left(X + \frac{k_1}{k_2[A]_0}\right) \tag{11}$$

Depending on the initial concentration of B, different types of thermograms are obtained. The initial concentration of B, the catalyst, is directly responsible for the "degree of autocatalysis". For a low initial concentration of B, the thermogram presents no initial heat release rate. Such a reaction is called a reaction with a high degree of autoca-

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[6] Eigenmann, K. *Chimia* **1976**, *30*, 12, 545−546.
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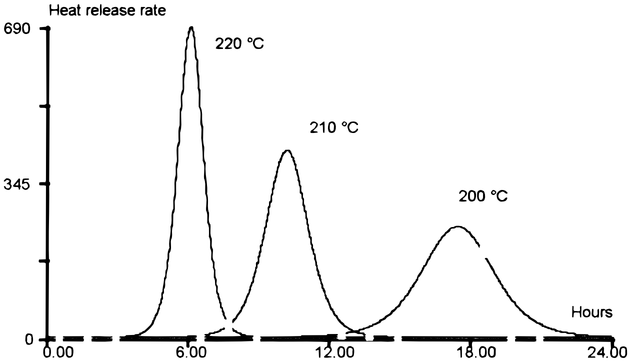

***Figure 4.*** **Isothermal DSC thermograms of an autocatalytic reaction with a high degree of autocatalysis.**

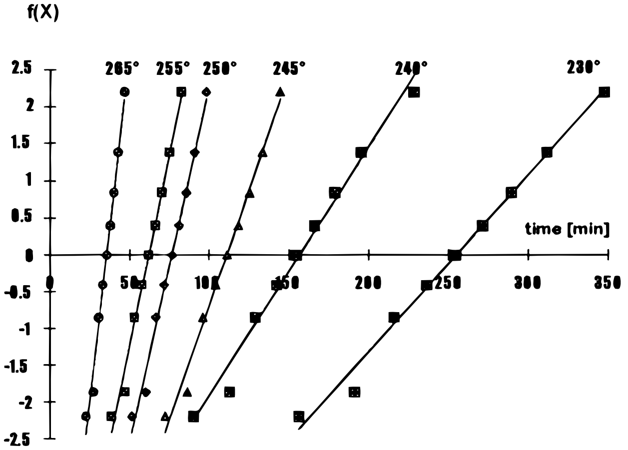

***Figure 5.*** **Determination of kinetic parameters for reactions with a high degree of autocatalysis.**

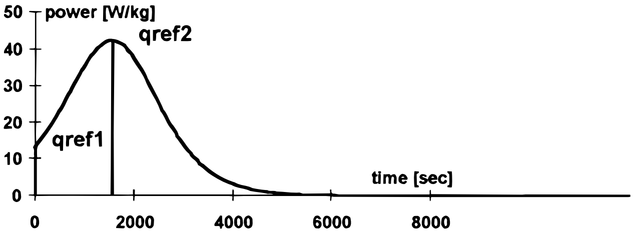

***Figure 6.*** **Heat release rate of an autocatalytic reaction with a low degree of autocatalysis.**

talysis (Figure 4). If the concentration $[B]_0$ is higher, the thermogram presents an initial heat release rate, and a low degree of autocatalysis is attributed to the reaction. Both types of reactions require different evaluation methods.

**Reactions with a High Degree of Autocatalysis.** In this case, $k_1 \ll k_2[A]_0$ and the rate equation (11) can be linearised:

$$\ln \frac{X}{1-X} = \ln X_0 + k_2[A]_0 t = f(X) \tag{12}$$

Plotting $f(X)$ as a function of time allows one to compute the slope, i.e., $k_2[A]_0$. The value of $k_1$ can be deduced from the point at which $f(X) = 0$, since

$$X_0 = \frac{k_1}{k_2[A]_0} \tag{13}$$

$k_1$ can be obtained from this point (Figure 5).

**Reactions with a Low Degree of Autocatalysis.** Self-accelerating reactions of this type present an initial heat release rate in the isothermal DSC thermograms (Figure 6).

The value of the rate constant of the initiation reaction, $k_1$, can be obtained directly from the initial heat release rate, $q_{ref1}$:

$$k_1 = \frac{q_{ref\,1}}{-\Delta H_r} \tag{14}$$

The heat release rate at the peak maximum, $q_{ref\,2}$, is obtained for a conversion of $X_{max} \approx 0.5$ and since

$$q_{ref\,2} = -\Delta H_r k_2 [A]_0 (1 - X_{max})^2 \tag{15}$$

$$k_2 = \frac{4 q_{ref\,2}}{-\Delta H_r [A]_0} \tag{16}$$

**Prediction of Time to Explosion.** The use of more realistic kinetic data instead of the zero-order assumption allows one to predict more accurate times to maximum rate, and as shown in the example of Figure 7, a factor of more than 10 is obtained: the zero-order approximation leads to a time to maximum rate of about 1 h whereas the real kinetic data lead to more than 10 h. In this case the decomposition is by far less critical at 475 K than the short-cut would predict. Such factors are not exceptional with autocatalytic reactions.

Such considerations often allow one to run processes under safe conditions without any drawback for process safety. In the case shown in Figure 7, the relatively long induction period can be used to take countermeasures allowing one to regain thermal control of the reaction. As

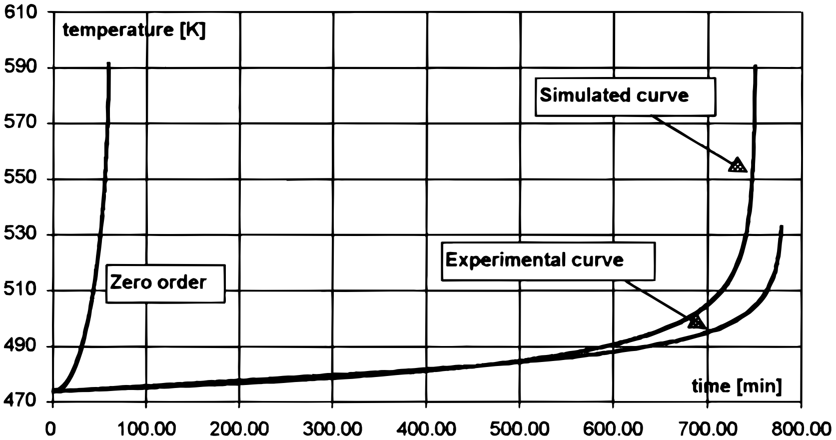

***Figure 7.*** **Adiabatic runaway curves of autocatalytic reactions compared with zero-order approximation.**

the kinetic behavior depends strongly on factors like the thermal history and the amount of impurities in the sample, these extrapolations are strictly valid for the sample in question only.

**Conclusion.** The tools and methodologies presented in this paper were recently developed at Ciba's Central Safety Research Laboratories. After an initial period where the development essentially consisted of the identification of possible instrumental techniques or their adaptation to safety analysis, developments in progress now are more focused on the refinement of the techniques and tools which help the final user to become familiar with these techniques and efficient in performing the risk assessment of the processes of interest.

Present trends in the specialty chemical industry show that the chemistry applied becomes more and more sophisticated, involving complex reaction systems, and further that the requirements of environmental protection become more and more demanding. Both trends indicate a clear need for a more comprehensive optimization of the processes.

In the future, numerous technical problems associated with the control of complex reactions, for example, with heterogeneous reaction systems or with sophisticated workup technologies, will present new safety problems which must be solved in an economical and efficient way. Future research and development and training programs must take these facts into account. These programs will also require a stronger collaboration between industry and universities to ensure long-term safe industrial development.

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[⊗] Abstract published in *Advance ACS Abstracts,* November 1, 1997.