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THERMALLY SAFE OPERATION OF A COOLED SEMI-BATCH REACTOR. SLOW LIQUID-LIQUID REACTIONS.

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Abstract
Thermally safe operation of a semi-batch reactor (SBR) implies that conditions leading to strong accumulation of unreacted reactants must be avoided. All thermal responses of a SBR, in which a slow liquid-liquid reaction takes place, can be represented in a diagram with the kinetics, cooling capacity and potential temperature rise as the keyfactors. Slow reactions taking place in the dispersed phase were found to be more prone to accumulation than reactions in the continuous phase. An overheat situation can develop after the reactants have accumulated in their "own" phase due to a slight overcooling.

Keywords
semi-batch reactor, semi-batch reaction, liquid-liquid system, limits of safe operation, runaway.

1. Introduction

The safe operation of a semi-batch reactor has been investigated in detail for homogeneous reaction systems by Hugo and Steinbach [1, 2, 3]. They clearly showed that runaway reactions can suddenly occur in exothermic reaction systems after a severe accumulation of unreacted material. Key factors in the process of accumulation are the maximum temperature rise in the absence of cooling, the cooling capacity and the reaction rate at the start. In a diagram covering the above key factors they have indicated important reaction patterns such as poor conversion, severe accumulation followed by a runaway or sufficiently high reaction rate right from the start.

In this study we will report on the behaviour of heterogeneous liquid-liquid reaction mixtures in a semi-batch reactor.

2. Mathematical model for liquid-liquid reactions in a semi-batch reactor

The mass balance

In an indirectly cooled semi-batch reactor component B is present right from the start and the second component A is added at a constant feed rate until a desired stoichiometric ratio has been reached. The components A and B are either pure or diluted with inert solvents. A and B react under the formation of the products C and D. The heat of the reaction is removed by a flow of coolant through a cooling coil or a jacket. The general set-up of such a cooled semi-batch reactor is sketched in Fig. 1. The temperature in the reactor and the concentrations of components A and B as functions of time can be found by solving the heat and mass balances over the reactor.

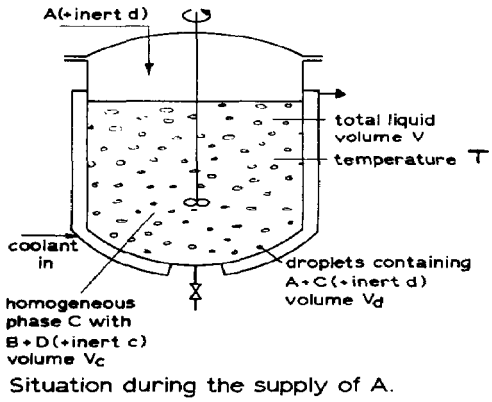


Fig. 1: The operation of a heterogeneous liquid-liquid semibatch reactor.

We will make a few important assumptions:
- volumes are additive.
- no phase inversion occurs during the reaction.
- the amount of a component in the phase to which it does not "belong" is very small compared to the amount in its own phase.
- the reaction rate is first order in the concentration of the reactants A and B, and reaction only takes place in one phase.
- the reaction equation is written as

$$\nu_A A + \nu_B B \rightarrow C + \nu_D D \tag{1}$$

  Components B and D remain in the continuous phase, the phase already present at the start of the batch. Components A and C remain in the dispersed phase which is formed as soon as the supply of component A has been started. Component C is the desired product.
- the product of the heat transfer area and overall heat transfer coefficient UA is proportional to the liquid volume in the reactor.
- the starting temperature in the reactor is equal to the mean coolant temperature T_c. The latter temperature remains constant.

The initial volume V_{ro} of phase c is present at the start of the supply period, t = 0:

$$V_{ro} = \frac{n_{Bo}}{c_{Bo}} \tag{2}$$

where n_{Bo} is the number of kmoles of B in the reactor at t=0 and c_{Bo} the molar concentration of B in kmol/m^3 at t = 0. The phase d containing A is supplied at a constant feed rate ϕ_{VD} m^3/s and it contains C_{AD} kmol/m^3 of component A. If the phase c contains initially $c_{Bo} \cdot V_{ro}$ kmoles of B then after a time t_D a stoichiometric amount of A has been supplied if:

$$\phi_{VD}\, C_{AD}\, t_D = \frac{\nu_A}{\nu_B}\, C_{Bo}\, V_{ro} \tag{3}$$

A dimensionless time θ is now introduced by dividing the time t by t_D:

$$\theta = t\, \frac{\nu_B}{\nu_A}\, \frac{\phi_{VD}\, C_{AD}}{C_{Bo}\, V_{ro}} \tag{4}$$

The stoichiometric ratio is reached if θ = 1. In this study we will assume that at θ = 1 the supply of A is indeed stopped. Excess or underdelivery of A is obtained by stopping at θ > 1 or θ < 1 respectively. The relative volume increase ε during the supply period is defined as:

$$\varepsilon = \frac{\phi_{VD} t_D}{V_{ro}} = \frac{\nu_A}{\nu_B}\, \frac{C_{Bo}}{C_{AD}} \tag{5}$$

The following statements are valid if θ > 1:
i) for εθ read ε
ii) for $(\theta - \zeta_B)$ or $\left(\frac{\theta - \zeta_B}{\theta}\right)$ read $(1 - \zeta_B)$
The total volume V at the time t can now be found as:

$$V = V_{ro} + \phi_{VD}\, t = V_{ro}\, (1+\varepsilon\theta) \tag{6}$$

It is required to determine the individual volumes of phases c and d, as the concentrations of A and C are referred to phase d and those of B and D to phase c. A simple approach is to assume:

$$V_c = V_{ro} \tag{7}$$

The dispersed volume V_d is given by:

$$V_d = \varepsilon\theta \quad V_{ro} \tag{8}$$

Heat balance
The ratio of specific heats will be introduced as:

$$R_H = \frac{(\rho c_p)_D}{(\rho c_p)_o} = \frac{(\rho c_p)_d}{(\rho c_p)_c} \tag{9}$$

The conversion ζ_B of component B - present right from the start - is defined as

$$\zeta_B = \frac{n_{Bo} - n_B}{n_{Bo}} \tag{10}$$

and the heat of reaction will be expressed in the adiabatic temperature rise $\Delta T_{ad,o}$ based on the initial volume in the reactor

$$\Delta T_{ad,o} = \frac{-\Delta H_R\, n_{Bo}}{(\rho c_p)_o\, V_{ro}\, \nu_B} \tag{11}$$

Alternatively, ΔT_{ad} can be based on the supplied volume at θ = 1 (symbol: $\Delta T_{ad,D}$) or the total volume at θ = 1 (symbol: ΔT_{ad}):

$$\Delta T_{ad,D} = \frac{-\Delta H_R n_{Bo}}{\nu_B (\rho c_p)_D V_D} = \frac{\Delta T_{ad,o}}{R_H \varepsilon} \tag{12a}$$

$$\Delta T_{ad} = \frac{-\Delta H_R n_{Bo}}{\nu_B (\rho c_p)_o V_{ro}(1+\varepsilon R_H)} = \frac{\Delta T_{ad,o}}{(1+\varepsilon R_H)} \tag{12b}$$

The heat balance (absorption = production - cooling + input) is now:

$$(\rho c_p)_o V_{ro}(1+\varepsilon\theta R_H)\frac{dT}{dt} = \Delta T_{ad,o}(\rho c_p)_o V_{ro}\frac{d\zeta_B}{dt} - (UA)_o(1+\varepsilon\theta)(T-T_c) - \phi_{VD}(\rho c_p)_D(T-T_D) \tag{13}$$

In Equation (13) all temperatures and $\Delta T_{ad,o}$ are made dimensionless by dividing them by a reference temperature T_R, yielding a dimensionless temperature T and a dimensionless adiabatic temperature rise $\Delta T_{ad,o}$. Multiplying all terms of Equation (13) by $\frac{t_D}{T_R(\rho c_p)_o V_{ro}(1+\varepsilon\theta R_H)}$ yields:

$$\frac{dT}{d\theta} = \frac{1}{1+\varepsilon\theta R_H}\left[\Delta T_{ad,o}\frac{d\zeta_B}{d\theta} - \varepsilon\left\{\frac{(UA)_o(1+\varepsilon\theta)(T-T_c)t_D}{(\rho c_p)_o V_{ro}\varepsilon} + R_H(T-T_D)\right\}\right] \tag{14}$$

In Eqn. (14) the term $\frac{(UA)_o t_D}{(\rho c_p)_o V_{ro}\varepsilon}$ is called the dimensionless cooling capacity μ by Hugo and Steinbach [1, 2, 3]. μ still contains the important operating variable t_D, and therefore is not a "fundamental" group. Therefore we prefer to split μ into two terms according to:

$$\mu = \frac{(UA)_o}{\varepsilon(\rho c_p)_o V_{ro} k_R C_{Bo}} \; k_R C_{Bo} t_D = U^* \, Da \tag{15}$$

where k_R is the reaction rate constant at the reference temperature T_R, Da the Damköhler number representing the total supply period and U^* the cooling capacity. Further the latter two terms in Eqn. (14) can be combined to one single expression by introducing the dimensionless average cooling temperature T_o:

$$T_o = \frac{U^* Da(1+\varepsilon\theta)\; T_c + R_H T_D}{U^* Da(1+\varepsilon\theta) + R_H} \tag{16}$$

with $T_D = T$ for $\theta > 1$. Hence the final expression for the heat balance is:

$$\frac{dT}{d\theta} = \frac{1}{1+\varepsilon\theta R_H}\left[\Delta T_{ad,o}\frac{d\zeta_B}{d\theta} - \varepsilon(R_H + U^* Da(1+\varepsilon\theta))(T-T_o)\right] \tag{17}$$

In Eqn. (17) implicit or explicit expressions for $\frac{d\zeta_B}{d\theta}$ can easily be substituted. Explicit expressions can be derived for cases where the reactants have only a low solubility in the phase to which they do not belong, and as long as there is no transition to a different kinetic regime during the reaction. The partial mass balances in case of low mutual solubility read

$$\frac{dn_B}{dt} = -\nu_B \, r \, V \tag{18}$$

and

$$\frac{dn_A}{dt} = -\nu_A \, r \, V + \phi_{VD} \, C_{AD} \tag{19}$$

where r is the reaction rate in kmol/s m^3 liquid volume. The expression for r must reflect the phase where the reaction occurs! The bulk concentrations of A and B in the phases d and c respectively are

$$C_{Ad} = \frac{n_A}{V_d} = \frac{(1-\zeta_A)n_{Bo}\frac{\nu_A}{\nu_B}\theta}{V_d} = \frac{(\theta-\zeta_B)n_{Bo}\frac{\nu_A}{\nu_B}}{V_d} \tag{20}$$

$$C_{B_c} = \frac{n_B}{V_c} = \frac{(1-\zeta_B)n_{Bo}}{V_c} \tag{21}$$

Due to the low solubilities $C_{Ac} \approx 0$ and $C_{Bd} \approx 0$. Furthermore

$$\frac{d\zeta_B}{d\theta} = t_D \frac{d(1-\frac{n_B}{n_{Bo}})}{dt} = \frac{t_D}{n_{Bo}} \cdot -\left(\frac{dn_B}{dt}\right) = \frac{t_D}{n_{Bo}} \; \nu_B \, r \, V \tag{22}$$

Rate constants are made dimensionless by dividing them by k_R, the value of the rate constant at the reference temperature T_R:

$$\kappa = \frac{k}{k_R} = \exp\left(-\frac{E}{RT} + \frac{E}{RT_R}\right) \tag{23}$$

The dimensionless activation energy is given by

$$\gamma = \frac{E}{RT_R} \tag{24}$$

Combination of Eqs. (24) and (23) yields

$$\kappa = \exp(\gamma(1-\frac{1}{T})) \tag{25}$$

The distribution coefficients will be defined such that a low value means a low solubility in the other phase:

$$m_A = \frac{C_{Ai,c}}{C_{Ai,d}} \quad \text{and} \quad m_B = \frac{C_{Bi,d}}{C_{Bi,c}} \tag{26}$$

Table 1 gives a survey of the correlations for the slow reactions, including the necessary checks on the validity of the calculations.

kinetic regime	reaction rate r (kmoles/m^3.s)	expression for $\frac{d\zeta_B}{d\theta}$	definition of Da in previous column	necessary check on the validity of the expressions [4]
slow reaction in the continuous phase. Component A is transferred through the interface	$m_A C_{Ad} k C_{Bc}(1-\varepsilon_d)$	$\nu_A \kappa Da \frac{(1-\zeta_B)(\theta-\zeta_B)}{\varepsilon\theta}$	$t_D k_R m_A C_{Bo}$	$\phi = \frac{1}{k_L}\sqrt{k C_B D_A} < 0.3$ $\frac{C_{Ac}}{C_{Ai,c}} > 0.95$
slow reaction in dispersed phase. Component B is transferred through the interface	$m_B C_{Bc} k C_{Ad} \varepsilon_d$	$\nu_A \kappa Da(1-\zeta_B)(\theta-\zeta_B)$	$t_D k_R m_B C_{Bo}$	$\phi = \frac{1}{k_L}\sqrt{k C_A D_B} < 0.3$ $\frac{C_{Bd}}{C_{Bi,d}} > 0.95$
homogeneous reaction system	$k C_A C_B$	$\nu_A \kappa Da \frac{(1-\zeta_B)(\theta-\zeta_B)}{1+\varepsilon\theta}$	$t_D k_R C_{Bo}$	no checks at all

Table 1: expressions for the conversion rate $\frac{d\zeta_B}{d\theta}$ for various situations

The expressions for $\frac{d\zeta_B}{d\theta}$ were derived by evaluating Eqn. (22) for the relevant reaction rate r, using Eqs. (20) and (21). The homogeneous reaction system was included for comparison purposes. For that case the concentration definitions were adapted by taking V instead of V_d or V_c. The expressions in Table 1 are based on a second order reaction.
Eqn. (17) and the relevant expressions for $\frac{d\zeta_B}{d\theta}$, in the form of two simultaneous differential equations, were solved numerically using a 4th order Runge & Kutta integration method [5], with a variable integration step to increase the calculation speed and accuracy. The computer results are data sets [T, ζ_B, θ].
For the interpretation the relative number of kmoles M of A and B, and the dimensionless concentrations Γ of A and B, were also found useful:

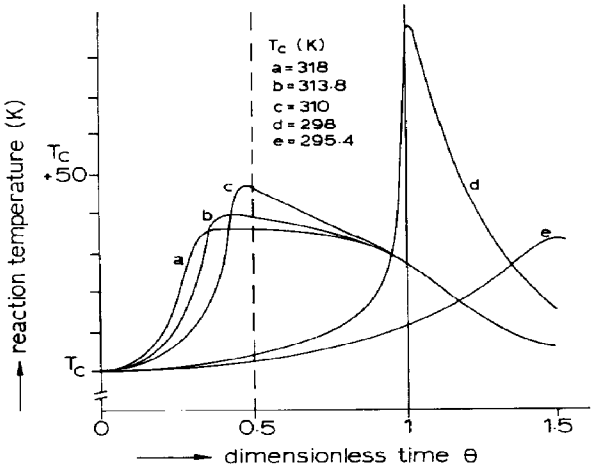
$$M_A = \frac{n_A}{n_{Bo}\frac{\nu_A}{\nu_B}} = \frac{n_{Bo}\frac{\nu_A}{\nu_B}(\theta-\zeta_B)}{n_{Bo}\,\nu_A/\nu_B} = \theta - \zeta_B \quad \text{and} \quad M_B = \frac{n_B}{n_{Bo}} = 1 - \zeta_B$$

$$\Gamma_{Ad} = \frac{C_{Ad}}{C_{AD}} = \frac{n_A}{V_{ro}\,\varepsilon\theta\,C_{AD}} = \frac{n_{Bo}\frac{\nu_A}{\nu_B}(\theta-\zeta_B)}{V_{ro}\varepsilon\theta\frac{\nu_A}{\nu_B}\frac{C_{Bo}}{\varepsilon}} = \frac{\theta-\zeta_B}{\theta} \quad \text{and} \quad \Gamma_{Bc} = \frac{C_B}{C_{Bo}} = 1 - \zeta_B \tag{27}$$

3. The accumulation criterion

There is no easy guide as to what is an acceptable accumulation of unreacted reagent. Only infinitely fast reactions in a SBR will show no accumulation! A situation which is considered "safe enough" will show no temperature jump and no sudden conversion of most of the available reactants and no large accumulation; but basically the choice of a quantifiable criterion to describe such a "safe enough" situation is arbitrary. Intuitively, we feel that keeping the reaction temperature below a realistic target temperature is more important than a sharp limitation of the accumulated mass of M_A or the conversion rate $\frac{d\zeta_B}{d\theta}$. Figure 2 is helpful in elucidating what is happening in a SBR. The reaction in this system is carried out at stepwise increasing coolant temperatures T_c. The kinetic regime corresponds to a slow reaction in the dispersed phase. Figure 2 shows that the temperature courses in cases of sufficient initial reaction rate (here for $T_c \geq 313.8$ K) do not basically differ. The reaction temperature seems to

stay close to an as yet undefined target temperature T_m. Around T_c = 313 K a modest temperature excursion developes but the reaction temperature stays in the neighbourhood of the target temperature. Around T_c = 300 K, there is a large overheating of the reaction mixture and the reactor temperature comes close to $T_c + \Delta T_{ad}$, as most of the reaction heat is liberated in a short time. ΔT_{ad} for this system is 122 K, according to Eqn. (12b). If $T_c \leq$ 295 K the reaction does not ignite anymore due to overcooling of the reaction mixture. Obviously the target temperature T_m is the steady state temperature for a well ignited reaction.
Steinbach [1] derived the target temperature from the heat balance by stating that $\frac{dT}{d\theta} = 0$ and $\frac{d\zeta_B}{d\theta} = 1$. The latter condition means that all of component A is consumed immediately as soon as it is supplied. The condition $\frac{dT}{d\theta} = 0$ is not valid in our case as the cooling capacity increases during the supply period, yielding a slightly decreasing target temperature. This is faintly visible in Fig. 2.



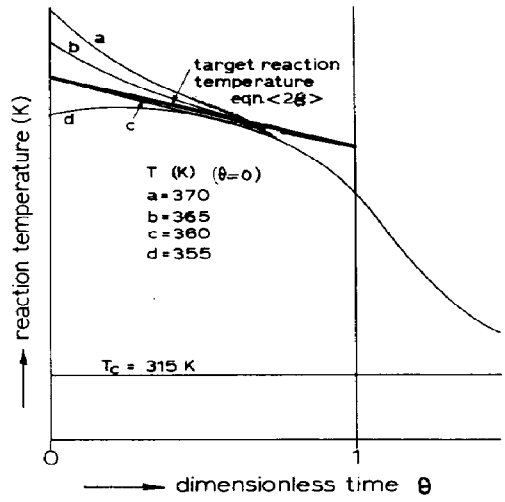


Fig. 2: Reactor temperature versus time for varying coolant temperature, other conditions remain the same. $\varepsilon = 0.35$, $\Delta T_{ad,o} = 0.55$, $\gamma = 38$, $Da = 0.4$, $R_H = 1$, $U^* Da = 10$
Fig. 3: Reactor temperature versus time for batch start-up temperatures near the steady state temperature for instantaneous reactions.

Fig. 3 represents the effect of higher starting temperature for the reaction system as in Fig. 2 and with T_c = 315 K (taking T_c = 315 K in Fig. 2 yielded a modest temperature excursion but the T_m line was not exceeded).
In Fig. 3 a smooth target line with a slightly negative slope emerges. For engineering and calculation purposes it is approximated very well by

$$T_m = T_c + \frac{1.05\Delta T_{ad,o}}{\varepsilon(R_H + U^* Da(1+\varepsilon\theta))} \tag{28}$$

Eqn. (28) replaces the solution of Eqn. (17) for $\frac{d\zeta_B}{d\theta} = 1$ and for the interval $0 < \theta < 1$, for any realistic combination of ε, R_H, $\Delta T_{ad,o}$ and $U^* Da$. Evidently, the target temperature is the steady state temperature for an instantaneous reaction if the reactor contents at $\theta = 0$ are already heated up to the steady state temperature.
In all calculation runs it was found that the temperature-based accumulation criterion, reading "the reactor temperature just touches but does not intersect the T_m-line", works adequately and yields the following results: the maximum value of M_A is between 0.1 and 0.2 and the maximum $\frac{d\zeta_B}{d\theta}$ just after the accumulation is usually 2.5 ± 1.0. A possible reason for the success of this criterion (though not seeming accurate as the warming-up period is neglected) is that the form of the T_m vs. θ curve allows a small temperature excursion just before the reaction temperature is "brought back" by the cooling system.
The events of interest for the operation of a SBR and for the design of its cooling system are shown in Fig. 4, where the course of the reactor temperature is plotted as a function of time. In case 1 the target temperature T_m is approached during the major part of the supply period, the reaction is well ignited. For cases 2, 3 and 4 the reaction mixture is strongly cooled and the target temperature is approached only once, for case 2 during, for case 3 at the end of and for case 4 after the supply period. As the target temperature T_m is not exceeded we just have avoided dangerous conditions. In case 5 the coolant temperature is low and strong cooling occurs. This results in a strong accumulation of reactants and a sudden ignition causing a temperature excursion far above the target line. It is obvious that these runaways should be prevented at all costs.

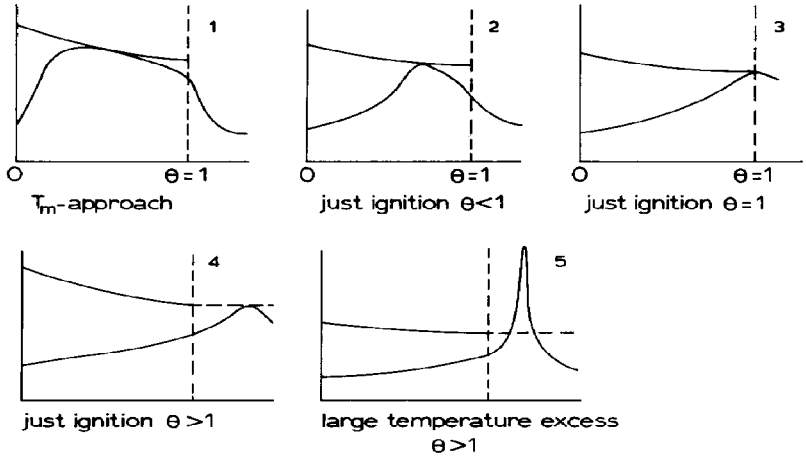


Fig. 4: Characteristic reactor temperature profiles.

4. Development of the boundary diagram

A diagram indicating the boundaries between the various types of thermal behaviour of fig. 4 should be based on the system parameters. Eqn <17> for the heat balance gives a key to the required combination of these parameters, because the following combinations appear in it: $\Delta T_{ad,o}$ and $\varepsilon(R_H+U^*Da)$ A similar analysis of the equations for the conversion rate yields the combinations R_H, ν_A Daκ and again ε. As a first approach the combinations a and b used by Hugo and Steinbach [1,2,3] will be applied for the construction of a diagram:

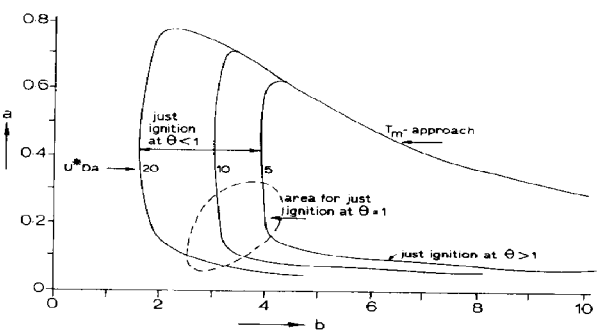
$$a = \frac{\text{reactivity at } \theta = 0}{\text{initial cooling capacity}} = \frac{\nu_A Da\ \kappa_c}{\varepsilon(R_H+U^*D_a)} = \frac{\nu_A Da.\ \exp(\gamma(1-\frac{1}{T_c})}{\varepsilon(R_H+U^*Da)}$$

and

$$b = \frac{\text{potential temperature rise}}{\text{initial cooling capacity}} = \frac{E}{RT_c^2}\frac{\Delta T_{ad,o}T_r}{\varepsilon\ (R_H+U^*Da)} = \qquad (29)$$

The diagram for a slow reaction in the dispersed phase

Figure 5 is based on a calculational analysis of the characteristic phenomena. The conversion rate for this kinetic regime is given by $\frac{d\zeta_B}{d\theta} = \nu_A \kappa Da\ (1-\zeta_B)(\theta-\zeta_B)$ and the applied range of parameters was $0.3 \leq \varepsilon \leq 0.75$, $0.3 \leq \Delta T_{ad,o} \leq 0.7$, $32.5 \leq \gamma \leq 44$, $0.025 \leq Da\ \nu_A \leq 8$, U^*Da-values 5, 10 and 20, and $R_H = 1$. A smooth diagram also emerges if one takes b equal to $\frac{E}{RT_c}\frac{\Delta T_{ad,o}}{\varepsilon(R_H+U^*Da)}$ or a/b on the vertical axis. In the latter case the T_m-approach line comes fairly close to the "just ignition" line except for $2<b<4$. No real improvements were found possible by taking other combinations and therefore the original definitions of a and b by means of equation (29) were maintained.



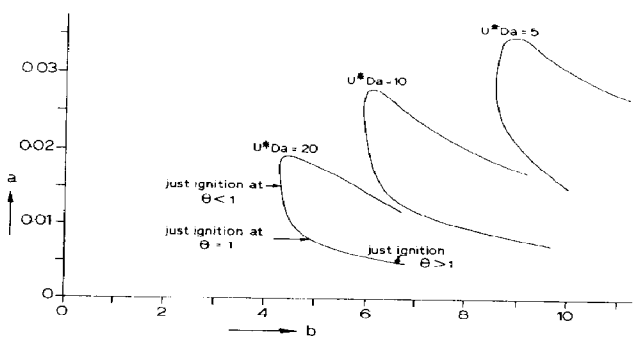


Fig. 5: Boundary diagram for a slow reaction in the dispersed phase, $R_H = 1$.
Fig. 6: Boundary diagram for a slow reaction in the continuous phase, $R_H = 1$.

The diagram for a slow reaction in the continuous phase

The conversion rate is now given by $\frac{d\zeta_B}{d\theta} = \nu_A \kappa\ Da\ \frac{(1-\zeta_B)(\theta-\zeta_B)}{\varepsilon\theta}$
Fig. 6 represents the boundary diagram for a slow reaction in the continuous phase for about the same range of parameter values. Again $R_H = 1$ was taken.

The influence of different specific heats of the phases

The influence of the specific heats of the phases was checked for a slow reaction in the dispersed phase with $U^*Da = 20$ and three values for R_H namely 0.4, 1 and 2.5. If one starts with an inorganic phase, to which an organic phase is supplied, R_H is probably close to the lower value, in the reversed situation close to the higher value, see Fig. 7.

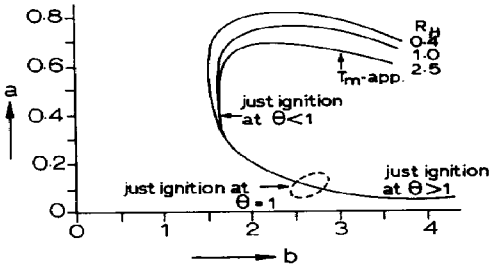


Fig. 7: Boundary diagram for a slow reaction in the dispersed phase for varying values of R_H, $U^*Da = 20$.

A combined diagram for slow reaction in a homogeneous system, in the dispersed phase and in the continuous phase.

The boundaries for the "homogeneous reaction" regime were derived while taking into account the increase in the cooling capacity during the supply period. See Fig. 8 for a comparison of the three cases. We observe that the enclosed area is largest for the liquid-liquid system where the reaction takes place in the dispersed phase. In the areas enclosed by the boundary lines overheating can occur.

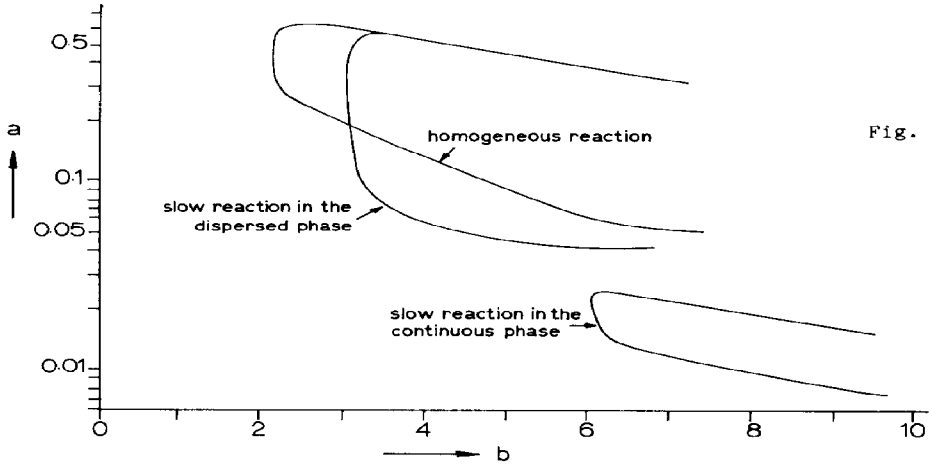


Fig. 8: Boundary diagrams for homogeneous and heterogeneous SBR's, with $R_H = 1$ and $U^*Da = 10$.

General interpretation of the boundary diagrams

The temperature excursion above the target temperature is relatively small if $b<b_{min}$, see Fig. 9. The dashed line is the route through the diagram for a given combination ε, Da, U^*Da, $\Delta T_{ad,o}$, R_H, γ if only T_c is varied. Fig. 10 explains what happens during a runaway event: now the reaction rate is slow during the greater part of the supply period but just sufficiently high to bring the temperature up. The reactants A and B accumulate in their own phase until suddenly the reaction ignites and all reaction heat is liberated in a very short time.

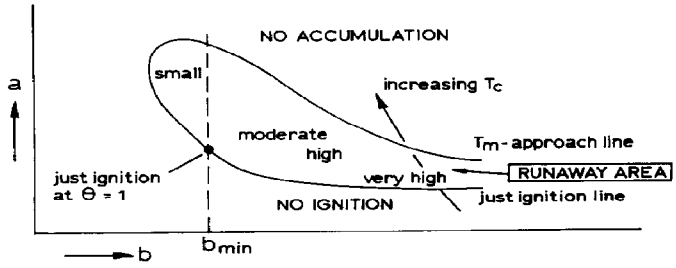


Fig. 9: Safety conditions for a SBR in a boundary diagram.

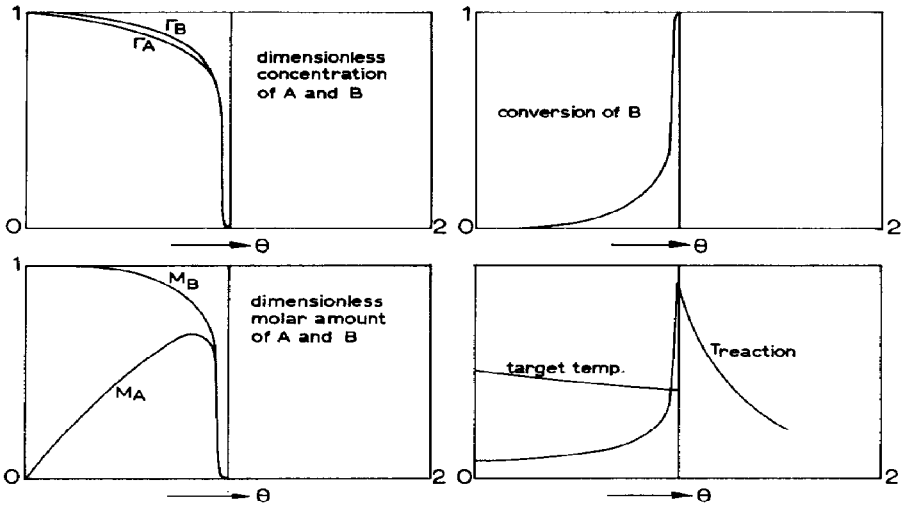


Fig. 10 Detailed analysis of a runaway event. Actual screendumps. Kinetic regime: slow reaction in the dispersed phase. $\varepsilon = 0.3$, $Da = 0.3$, $\gamma = 44$, $U^* Da = 10$, $\Delta T_{ad,o} = 0{,}5$.

5. Final remarks

The desirable operating condition is no accumulation. The main parameters dosing time and cooling temperature can be obtained from the relevant diagrams if the kinetics of the reaction is fully known.

A more empirical method would be the use of heat flow vs. time plots of a reaction carried out in a (practically) isothermal reaction calorimeter [6,7]. Further studies [8] show that:

- a reaction system at the brink of dangerous accumulation has a specific heat flow vs. time picture.
- the "slow" reaction approach is no longer valid if the distribution coefficients for A or B become smaller than approx. 0.01, because if B or A have a lower solubility the reaction rate constant to prevent accumulation must be so large that the assumption of $\phi < 0.3$ - basis for the model - is no longer valid.
- the simplified expressions for the reaction rates are valid if there are no larger concentration drops in the films than 5%. For a typical liquid-liquid dispersion with $a = 20.000\ m^2/m^3$ [9] this is the case if the distribution coefficients for A or B are not smaller that 0.005 to 0.01.
- fast reactions can only show a moderate form of accumulation if the distribution coefficients are very small, typically less than 10^{-4}.

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Notation

Normal symbols

A	area of cooling jacket or cooling coil	m^2
a	reactivity parameter specific area of dispersed phase	m^2/m^3
b	potential temperature rise	--
C	molar concentration	$kmol/m^3$
c_p	heat capacity	J/kgK
Da	Damköhler number	--
E	activation energy	J/kmol
ΔH_R	reaction enthalpy	J/kmol
k	rate constant for a specified phase	$m^3/kmol.s$
m	distribution coefficient	--
M	relative amount of kmoles of a specified compound	--
n	total number of kmoles of a specified compound in the reactor	kmol
R	gas constant = 8.314 J/kmol K	J/kmol K
r	reaction rate	$kmol/m^3s$
T	temperature	K
t	time	s
ΔT_{ad}	adiabatic temperature rise	K
U_*	overall heat transfer coefficient	W/m^2K
U	dimensionless cooling capacity	--
V	liquid volume in the reactor	m^3

Subscripts

o	at the start of the supply period
c	continuous phase or coolant
d	dispersed phase
D	dosed component, dosing
crit	critical
R	(at the) reference temperature
d	adiabatic

Greek or specific symbols

Γ	relative concentration	--
γ_p	E/RT_R, dimensionless activation energy	--
ε	relative volume increase at the end of the supply period	--
ε_d	volume fraction of the dispersed phase	--
ζ	conversion	--
θ	dimensionless time t/t_D	--
κ	k/k_R, dimensionless reaction rate constant	--
μ	cooling number of Hugo and Steinbach	--
ν	stoichiometric coefficient	--
ρ	density	kg/m^3
R_H	$\frac{(\rho c_p)_D}{(\rho c_p)_o} = \frac{(\rho c_p)_d}{(\rho c_p)_c}$ ratio of specific heats	--
T	T/T_R, dimensionless temperature	--
D	diffusivity	m^2/s
ϕ_v	volumetric flow rate	m^3/s
ϕ	Hatta number	--