

# Interval Identification - a Modelling and Design Technique for Dynamic Systems

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## Abstract

A new technique is presented to identify intervals for parameters and initial conditions for nonlinear dynamic systems based on an imprecise mathematical model and measurements of system variables. This technique employs a fuzz interval qualitative simulator for interval dynamical models and a qualitative description of measured signals, the episodes. These are based on the sign of the variable and of its first and second derivative. Episodes describe in a very simple and intuitive form the dynamic behaviour of the measured variable. By combining this qualitative with numerical information, a structure and parameter identification can be done in a very intuitive and explainable way.

This technique is used within a tool, *TAM-C*, to model and assess chemical processes involving exothermic chemical reactions.

Two applications of this technique are given: modelling of a chemical reaction system and safety assessment of an exothermic chemical process. The examples are based on real industrial and laboratory data.

## Introduction

Deriving models of dynamic processes is important for design, optimization and model-based monitoring and control in many engineering applications. Many systems are too complex or poorly understood to be completely modeled based on physical principles. Appropriate functions for parts of the equations which describe the system behaviour have to be found. This is usually done in an iterative procedure using a priori and empirical knowledge of the system to be modelled and measurements.

When a possible model candidate has been postulated, qualitative simulation techniques can be used to study the behaviour of that model without knowing the precise values for all model parameters, i.e. before running a time consuming quantitative parameter identification. This behaviour can then be compared to the observed behaviour of measured variables to check whether the candidate should be considered further.

Over the last decade, research on qualitative reason-

ing has produced many approaches to investigate such ill-defined systems, (Weld and de Kleer 1990). These approaches can be seen as an extension and generalization of traditional, quantitative modeling and simulation techniques, (Kuipers 1994). However, due to the inherent ambiguity of qualitative calculus, some of the set of behaviours produced by a qualitative simulator do not correspond to any of the possible behaviours of the underlying physical system. These spurious solutions make it difficult to apply qualitative simulation to large, complex systems. Reducing the amount of spurious solutions is an area of intense research. Recently, (Bonarini and Bontempi 1994) proposed a qualitative simulation approach, based on interval simulation, that does not generate spurious solutions.

In this contribution we use an interval simulation method as well to systematically identify possible model candidates, numerical ranges of the unknown parameters and initial conditions and thereby verifying the structure of the system equations. Qualitative interval simulation is also used to assess a worst case scenario of an exothermic process.

## Fuzzy and Interval Simulation

Fuzzy sets allow subjective or imprecise knowledge to be incorporated into models. A set of differential equations with fuzzy parameters and fuzzy initial conditions forms a fuzzy dynamical model. The analytic basis to handle and solve such a fuzzy dynamical model is provided by Zadeh's extension principle (Zadeh 1975) and Nguyen's identity (Nguyen 1978).

Several fuzzy qualitative simulation methods that generate solutions of fuzzy dynamical models have been proposed, e.g. Qua.Si I and II (Bonarini and Bontempi 1994), Qua.Si III (Bontempi 1996), FuSim (Shen and Leitch 1993), and FRenSi (Keller, Wyatt, and Leitch 1999). FRenSi, Qua.Si II, and Qua.Si III do a fuzzy simulation by splitting the fuzzy region, formed by the fuzzy values of system variables and model parameters, into  $\alpha$ -cuts using Nguyen's identity, i.e. the fuzzy simulation problem is transformed to several interval simulation problems. For these, all imprecise system variables and model parameters are represented by intervals. The intervals of each interval simulation problem

are combined to form a hypercube with the dimension  $n+k$  ( $n$  = model order;  $k$  = number of imprecise model parameters) and the evolution of this hypercube is simulated. In the special case that all initial conditions are intervals, it is demonstrated in (Bonarini and Bontempi 1994) that it is sufficient to generate the evolution of the external surface only to determine the model behaviour.

Integrating the hypercube avoids the introduction of spurious behaviours; only those system trajectories that are possible from the initial uncertainty and imprecision in the variables and parameters of the model are generated. This is due to the fact that interaction between the system variables is maintained over the entire simulation, see below.

In the work reported here, the imprecision is exclusively represented by intervals. In the following we will always refer to intervals and interval dynamical models but it is important to note that the same can be applied to a wider class of fuzzy sets.

A simplified interval simulation algorithm has been developed. Equally distributed samples are taken from the initial region of uncertainty and integrated numerically. Since some initial conditions were known exactly, the interior of the initial region of uncertainty had to be sampled as well. From these simulations, the minimum and maximum values for each time point are extracted. Although this method generates an under-bound behaviour, good simulation results and a computationally efficient solution are achieved. It is only for external purposes, e.g. calculation of the model output, that the hypercube is mapped back to individual non-interacting interval values.

To demonstrate the above mentioned concept of interaction, which avoids spurious solutions, the following example is considered. Equations 1-3 are first evaluated using the well-known rules of non-interacting interval mathematics:

$$\mathcal{M} = \mathcal{A} + \mathcal{B} \quad (1)$$

$$\mathcal{N} = -(\mathcal{A} + \mathcal{B}) \quad (2)$$

$$\mathcal{Y} = \mathcal{M} + \mathcal{N} \quad (3)$$

In Equation 1 and 2 the model parameters  $\mathcal{M}, \mathcal{N}$  are calculated from the system parameters  $\mathcal{A}, \mathcal{B}$ . Without loss of generality the fuzzy values of  $\mathcal{A}, \mathcal{B}$  are defined as intervals  $\mathcal{A} = [0, 1], \mathcal{B} = [-1, 0]$ . The results from Equation 1 and 2 are then used in Equation 3, which yields  $\mathcal{Y} = [-2, 2]$ , i.e. beside the true solution  $[0, 0]$ , spurious solutions are obtained. In our approach we use the system parameters  $\mathcal{A}, \mathcal{B}$  directly in Equation 3:

$$\mathcal{Y} = \mathcal{A} + \mathcal{B} - (\mathcal{A} + \mathcal{B}) = [0, 0], \quad (4)$$

thus getting the only true solution. In the interval simulation problem mentioned above, interacting interval mathematics are used, hence avoiding spurious solutions as well.

### Interval Identification Approach

The interacting interval simulation techniques introduced above generate envelopes which enclose all phys-

ically possible solutions without introducing any spurious behaviours. However, for many applications not only the envelopes enclosing the measured or simulated variables at certain times are of interest, but as well - or even more - the (qualitative) development over time. The interval simulation techniques are not able to predict the possible shapes of curves within the region of uncertainty.

In Figure 1 such an envelope is shown together with

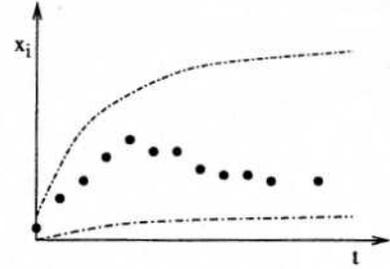


Figure 1: Sketch of an envelope (---) with measurement data of the respective variable ( $\bullet$ ). The envelope bounds the curve formed by the data points but cannot predict the (qualitative) temporal shape of that curve

noisy measurements of the same variable  $x_i$ . The measured variable has a maximum and decreases until it reaches a stationary value. This behavior is certainly very important, e.g. for modelling or process supervision. Even though all measured points are within the bounds calculated for that variable, interval simulation based solely on the system equations cannot predict this and other possible behaviours generated by the initial region of uncertainty. To overcome this problem, first a suitable form to represent the temporal shape of a variable qualitatively over time will be defined. Then an interval identification technique is deduced, which allows the detection of behaviours like the one in Figure 1. Finally, the way the interval identification technique is implemented is described.

### Qualitative Description of Measured Data

The procedure described here follows the concept presented in (King, Schaich, Munker, and Hellinger 1997). To overcome measurement noise which is usually present in real data the time series are smoothed with spline functions in a first step. Experimental and domain experience has been used to choose the type of smoothing function. These curves are then divided into sections of the same qualitative state.

(De Kleer and Brown 1984) defined a set of qualitative numbers as the sign of the respective quantitative values, i.e.  $+, 0$  and  $-$ . Based on this, the qualitative state of a continuous quantitative variable  $x(t)$  is defined as the triplet of the qualitative value of the variable  $v$  and the first  $dv$  and the second  $ddv$  derivative of the vari-

able, (Cheung and Stephanopoulos 1990, Coghill 1992).

$$v = \begin{cases} + & \text{if } x(t) > 0 \\ 0 & \text{if } x(t) = 0 \\ - & \text{if } x(t) < 0 \end{cases}$$

$$dv = \begin{cases} + & \text{if } x'(t) > 0 \\ 0 & \text{if } x'(t) = 0 \\ - & \text{if } x'(t) < 0 \end{cases}$$

$$ddv = \begin{cases} + & \text{if } x''(t) > 0 \\ 0 & \text{if } x''(t) = 0 \\ - & \text{if } x''(t) < 0 \end{cases}$$

A time interval, in which this triplet does not change, is called an episode. If any of the above properties changes value, a new episode starts. The time at which this change between two episodes occurs, is the transition time. The temporal shape of any variable is described here with a sequence of episodes, called a history of episodes or qualitative history and associated transition times.

All combinations for  $dv$  and  $ddv$ , which are physically possible, are shown in Figure 2. Thus, all possible

Type	A	B	C	D	E	F	G
$x$							
$dv$	+	-	-	+	+	-	0
$ddv$	-	-	+	+	0	0	0

Figure 2: Episodes

episodes are defined by the types from Figure 2 and the sign of the value itself denoted by a superscript, e.g.  $A^+$  or  $D^-$ .

Thus, with this procedure, noisy, quantitative informa-

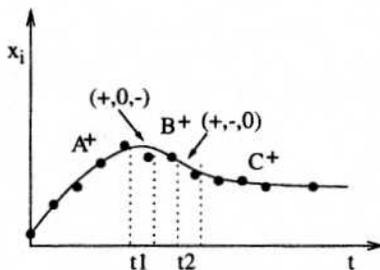


Figure 3: Abstracting the noisy, quantitative measurement information ( $\bullet$ ) of Figure 1 into a qualitative form by smoothing ( $-$ ) and division into Episodes ( $A^+B^+C^+$ ).

tion can be transformed into a simple qualitative representation, which contains important features of the original time series. In Figure 3 the smoothed curve

reaches a maximum value for the transition time  $t_1$  (first pair of dotted lines), then decreases until it changes its curvature at  $t_2$  (second pair of dotted lines) and reaches an equilibrium value. Numerical values of the transition times can be calculated, however,  $t_1$  and  $t_2$  are treated as intervals too. This accounts for the imprecision and bias introduced by using a smoothing function to describe the behaviour of the variable.

### Extension of the Interval Simulation

In order to use this qualitative description based on episodes, the interval simulation technique has to be extended to include the generation of information, with which the observed episodes can be validated.

The process under consideration is described by a system of ordinary differential equations, Equation 5.

$$\frac{d\underline{X}(t)}{dt} = \underline{f}(t, \underline{X}(t), \underline{P}), \quad \underline{X}(t=0) = \underline{X}_0 \quad (5)$$

$\underline{X}(t)$  is the vector of state variables (dimension  $n$ ) and  $\underline{P}$  the vector of parameters (dimension  $k$ ). The elements of the variable vector  $X_i(t)$ , the initial conditions  $X_{i,0}$  ( $i = 1 \dots n$ ), and parameters  $P_j$  ( $j = 1 \dots k$ ) are intervals, i.e. the region of uncertainty has the dimension  $N = n + k$ . All elements of the vector of the right-hand side  $\underline{f}$  are continuous and differentiable. Since all variables and parameters are expressed as intervals Equation 5 is an interval differential equation (IDE).

In order to not only compare the envelopes but as well the (qualitative) shapes of the measured variables, the first and second derivative must be determined together with the values of the measured variables. The differential equation system describing the process under consideration, Equation 5, is differentiated once, yielding:

$$\frac{d^2 \underline{X}(t)}{dt^2} = \frac{\partial \underline{f}}{\partial t} + \frac{\partial \underline{f}}{\partial \underline{X}} \underline{\dot{X}} \quad (6)$$

with the following initial condition:

$$\underline{\dot{X}}(t=0) = \underline{f}(0, \underline{X}_0, \underline{P}) \quad (7)$$

Finally, Equations 5 and 6 can be rewritten as:

$$\frac{d\underline{Z}(t)}{dt} = \underline{g}(t, \underline{Z}(t), \underline{P}), \quad \underline{Z}(t=0) = \underline{Z}_0 \quad (8)$$

with

$$\underline{Z}_i = \begin{cases} X_i & \text{for } i = 1, \dots, n \\ \dot{X}_{i-n} & \text{for } i = (n+1), \dots, 2n \end{cases} \quad (9)$$

It should be noted, that no additional uncertainties are introduced by differentiating Equation 5, since the relationships between the variables in Equation 5 and 6 are conserved when  $\underline{f}$  is differentiated analytically. Since  $N$  is not increased, it is not necessary to differentiate Equation 6 again to calculate the second derivative.  $\ddot{\underline{X}}$  is calculated by Equation 6.

If an interval simulation is done for Equation 8 every point of the state hypercube corresponds to a consistent triplet  $\underline{X}$ ,  $\underline{\dot{X}}$ , and  $\underline{\ddot{X}}$  of the original problem stated

in Equation 5. This extended interval simulation now yields the envelopes for  $\underline{X}$ ,  $\dot{\underline{X}}$ , and  $\ddot{\underline{X}}$ , which have to be evaluated together. Figure 4 shows a sketch of these combined envelopes. The qualitative history of the measured variable  $A^+B^+C^+$  can now be compared with the envelopes of  $\dot{X}_i$ ,  $\ddot{X}_i$ , and  $\ddot{\ddot{X}}_i$ . The first episode  $A^+$  is consistent with the behaviour generated by the IDE since the regions  $X_i$ ,  $\dot{X}_i$ , and  $\ddot{X}_i$  cover, include the signs of this episode. The same is true for the change from episode  $A^+$  to  $B^+$ , which corresponds to the crossing of the abscissa by the envelope of  $\dot{X}_i$  within the time interval  $t_1$ . However, the transition from  $B^+$  to  $C^+$  can not be explained by the given IDE, since the envelope for  $\ddot{\ddot{X}}_i$  covers only negative values for the time interval  $t_2$ . Based on this, it can be concluded that the IDE

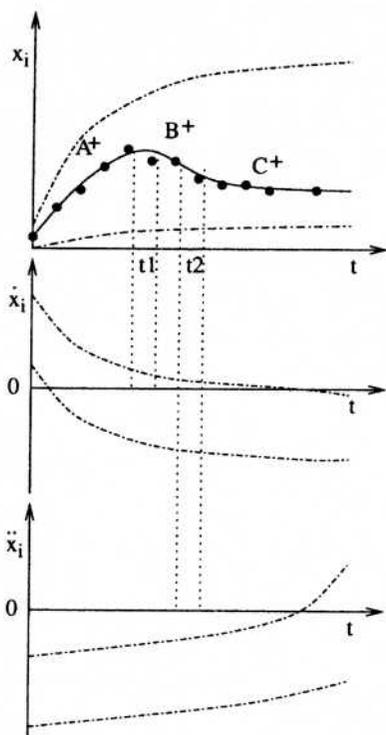


Figure 4: Sketch of the combined envelopes for  $X_i$ ,  $\dot{X}_i$ , and  $\ddot{\ddot{X}}_i$  (- · -) with the transition time intervals  $t_1$  and  $t_2$  (· · ·) indicating the changes of the qualitative temporal shape of the smooth curve (-) from Figure 3

which created the envelopes  $X_i$ ,  $\dot{X}_i$ , and  $\ddot{\ddot{X}}_i$  can not explain the observed data points (•) in Figure 4. In the following step, the intervals for the parameters and initial conditions are varied, if this is physically possible (see below). That way, all combinations of intervals which can explain the observed data are identified. If no such interval is found, the functional structure of the IDE is not capable of reproducing the observed process dynamics.

## Implementation of the Interval Identification Technique

Currently, only the signs which the envelopes cover are checked against the respective episodes. This is done with a certain margin of error. It does not make sense to check the numerical values of the first and second derivatives of the spline function against the ranges the respective episodes cover, because the smoothing of the measurement data is a biased and data-only driven procedure, whereas the mathematical model used to generate the envelopes, contains structural knowledge of the system.

In the current version, the interval identification technique has been implemented using a simplified version of the interval simulation algorithm. Equally distributed samples are taken from the initial region of uncertainty and integrated numerically. From these simulations, the minimum and maximum values for each time point and observed variables are extracted. Through the number of samples the approximation error can be influenced.

For efficiency reasons, only the original Equation 5 is integrated and the first  $\dot{x}_i(t_k)$  and second  $\ddot{x}_i(t_k)$  derivatives of the measured state or non-state variables are calculated from a five point Lagrange interpolation of  $x_i(t_k)$ .

The interval identification technique is used within *TAM-C* (*Tool for the Automatic Modelling of Chemical reaction systems*), a software tool which automates the modelling process of exothermic chemical reactions, see Figure 5. All procedures depicted in a dashed box in Figure 5 are integrated in *TAM-C* and run without any interaction by the user. Therefore, the process of building adequate mathematical models of reaction systems is substantially accelerated. The qualitative techniques used are described in detail in (Schaich and King 1999, Schaich, Munker, Hellinger, and King 1998, King et al. 1997).

Models with different rate equations beginning with simple expressions for formal kinetics are set up for the investigated reaction system in an automated procedure. A priori rule-based knowledge is used at this stage to restrict the amount of possible models.

The interval identification technique has been implemented as an alternative to an order of magnitude simulation, a non-interacting interval simulation algorithm. To verify if a postulated model is a possible candidate for subsequent quantitative identification, the described qualitative representations of the measured variables are extracted from measured data. Those qualitative models, which do not generate behaviors corresponding to the qualitative phases of measured variables, are rejected. In the following step, the substantially more time-consuming quantitative structure and parameter identification is applied only to the remaining candidates, which can at least qualitatively describe the measured data. For this the interval identification also gives a first rough estimate of the unknown parameters.

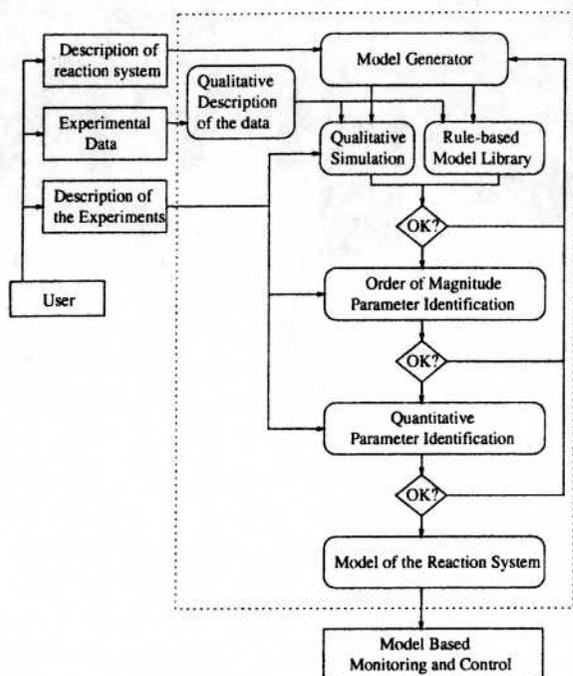


Figure 5: Modelling process in *TAM-C*, (Schaich and King 1999)

### Drawbacks of the Interval Identification Technique

In the current version a drawback of the proposed technique is that it can not be proved, that the envelopes calculated encapsulate all physically possible behaviors. This is because the simulator samples the initial region of uncertainty. However, the sampling simulation was chosen for its efficiency, since in *TAM-C* all possible combinations of parameter intervals are studied which amounts to up to several thousand interval identification runs.

The interval identification technique presented here is independent of the underlying simulation algorithm and can be replaced by any alternative fuzzy or interval simulator. An interacting interval simulator which uses optimization techniques to determine the envelopes is currently under development. This will improve the performance of the interval identification technique as well as guarantee that all possible behaviours are found.

### Applications

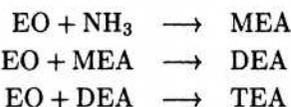
In the first application, a parameter identification for a three step reaction system is performed. The initial ranges of the parameters are too wide to be evaluated directly with a gradient based method. Therefore, more narrow subintervals are formed and with interval identification combinations of subintervals are identified, which can explain the observed behaviour.

The second application comprises a structure and parameter identification of an exothermic reaction and a subsequent safety assessment.

As mentioned above, the approximation error for the calculated envelopes can be influenced through the number of samples. For the two applications a sample number of 10 for each parameter was sufficient to yield an error below 0.1%.

### Identification of valid parameter ranges

Ethylenoxide (*EO*) reacts with ammonia (*NH<sub>3</sub>*) yielding monoethanolamine (*MEA*), diethanolamine (*DEA*), and triethanolamine (*TEA*), (Steiner 1993):



Assuming mass action the following simple rate equations are formed:

$$\begin{aligned} r_1 &= k_1 c_{\text{EO}} c_{\text{NH}_3} \\ r_2 &= k_2 c_{\text{EO}} c_{\text{MEA}} \\ r_3 &= k_3 c_{\text{EO}} c_{\text{DEA}} \end{aligned}$$

where  $c_i$  denotes the concentrations of the different compounds ( $i = \text{EO}, \text{NH}_3$ , etc.). The unknown kinetic rate constants  $k_1$ ,  $k_2$ , and  $k_3$  had to be determined, given measurement data for  $c_{\text{MEA}}$ ,  $c_{\text{DEA}}$ , and  $c_{\text{TEA}}$ . As mentioned above, the initial ranges of the estimated parameters were too wide to be evaluated directly with a gradient based method. Therefore, narrow subintervals for the parameters were formed and with interval identification combinations of subintervals were identified, which explained the observed behaviour. The found combinations of subintervals were the starting point for the subsequent parameter identification. The smoothed data for the measured concentrations  $c_{\text{MEA}}$ ,  $c_{\text{DEA}}$ , and  $c_{\text{TEA}}$  resulted in the qualitative episodes and transition times given in Table 1. The

	Qualitative History	Transition time intervals [h]	
$c_{\text{MEA}}$	$A^+ B^+ C^+$	[0.2 ... 0.3]	[0.42 ... 0.52]
$c_{\text{DEA}}$	$D^+ A^+$	[0.01 ... 0.11]	
$c_{\text{TEA}}$	$D^+ A^+$	[0.19 ... 0.29]	

Table 1: Qualitative episodes and transition times for the measured concentrations  $c_{\text{MEA}}$ ,  $c_{\text{DEA}}$ , and  $c_{\text{TEA}}$

initial, very rough estimate for all parameters was the interval [1 ... 11] l/mole/h, which was estimated from the overall turnover of this process. This range was divided into subintervals of width 2 l/mole/h for each parameter and all 125 possible combinations were evaluated in an automatic procedure using interval identification with an interacting and a non-interacting simulator. Only with an interacting simulator the interval

identification technique was able to find only the true combination,  $k_1=[3 \dots 5]$ ,  $k_2=[1 \dots 3]$ , and  $k_3=[1 \dots 3]$ , see Figure 6.

This identified set of intervals provided the starting point for the subsequent quantitative parameter identification in which the following values were determined:  $k_1=4.0244$  l/mole/h,  $k_2=2.471$  l/mole/h, and  $k_3=1.486$  l/mole/h. The quantitative parameter identification was done with a quasi-newton algorithm and the weighted sum of all three residuals as objective function.

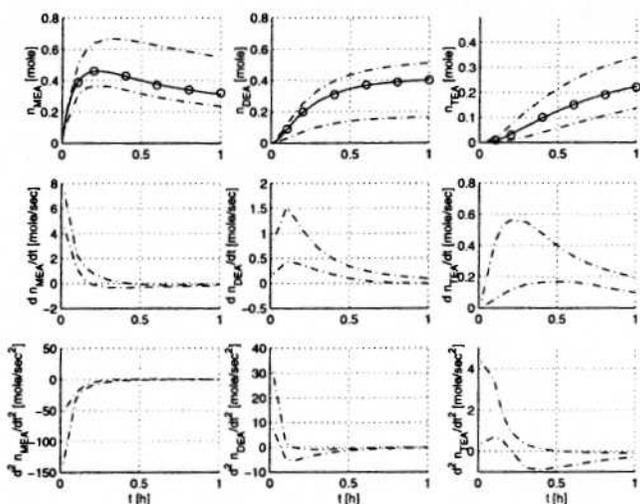
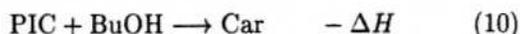


Figure 6: The combined envelopes of the value, first and second derivative for MEA, DEA, and TEA (---) with the measured data (o) and the simulated curve with the identified parameters (-)

### Assessment of Safety Critical Reactions

The assessment of the safety of exothermic processes is based on the dynamics of the heat evolution, which is described by the kinetic rate equation of the chemical reaction. The standard experimental technique to gain insight into this dynamic is thermal analysis. For most industrial exothermal batch- or semi-batch processes this thermal signal (temperature or heat evolution rate) is the only time series measurable in practice, because often all occurring compounds are generally difficult to analyse, highly toxic or exist only for a very short time or under extreme conditions.

(Leonhardt 1997b) compared isothermal, isoperibolic and adiabatic calorimeters and a power-compensated DSC by running experiments of a simple reaction in each of them. In this model reaction phenylisocyanate (PIC) and 2-butanol (BuOH) with toluene as a solvent form carbamate (Car):



First, a structure and parameter identification for the kinetic rate equation was done automatically with TAM-C. It was based on the description of the isoperibolic experiments in (Leonhardt 1997b) and the data of isoperibolic experiments at different temperatures given by (Leonhardt 1997a). The first rate equation, proposed by the model generator (which always starts with the least complex possible rate equation for the system under investigation), which was not rejected by the rule-

based model library was:  $r = k_{\infty} e^{-\frac{E}{RT}} c_{\text{PIC}} c_{\text{BuOH}}$ . Three out of 125 possible combinations for the unknown parameters  $k_{\infty}$ ,  $E$ , and  $-\Delta H$ , were not rejected by interval identification. However, the combinations found were rejected by the subsequent quantitative parameter identification. Although the simulated evolution showed the same qualitative behaviour, the quantitative deviations exceeded the allowed error tolerance. Thus, by using interval identification, it was shown, that within the full range of the initially proposed intervals for the parameters only three narrow combinations can create the observed qualitative behaviour. This reduction of the search space avoided more time-consuming quantitative identification runs. Moreover, with this technique it was possible to automatically detect that the chosen kinetic expression was unable to explain experimental data. Without this quantitative assessment it would not be possible to automatically explain why a qualitative identification does not converge. This was necessary, however, as the main goal of TAM-C is the automatic modelling of reaction systems. It should be avoided that a human expert is responsible to stop a non-converging identification run. The next rate equation proposed by TAM-C was able to reproduce the observed behaviour within the given error tolerance,  $r = k_{\infty} e^{-\frac{E}{RT}} c_{\text{PIC}}^n c_{\text{BuOH}}^m$ . This result is identical to the one given by (Leonhardt 1997b). Furthermore, (Leonhardt 1997b) made a systematic study, using different types of calorimeters and found different kinetic parameters, depending on the type of calorimeter. For each type of calorimeter, several experiments were carried out under identical initial conditions but different courses of temperature. Subsequently, the kinetic parameters of the performed experiments were determined for each calorimeter in an uniform manner by evaluating several measurements simultaneously. However, a simultaneous evaluation of measurements from different calorimeters was not done. Instead, the following averaged equation was deduced, which accounts explicitly for the differences of individual identification runs:

$$r = k(300 \text{ K}) e^{-\frac{E}{R} \left[ \frac{1}{300 \text{ K}} - \frac{1}{T} \right]} c_{\text{PIC}}^n c_{\text{BuOH}}^m \quad (11)$$

with

$$\begin{aligned} n &= 1.05 \pm 0.1 & - \\ k(300 \text{ K}) &= (1.33 \pm 0.3) \times 10^{-4} & \text{mole}^{1-2n} \text{l}^{2n-1} \text{s}^{-1} \\ E &= 41 \pm 3 & \text{kJ mole}^{-1} \\ -\Delta H &= 85 \pm 5 & \text{kJ mole}^{-1} \end{aligned}$$

To assess the effect of these imprecisions, this rate equation was used in a simple design case study using an interacting simulator. In practice, such an exothermic process would be realized in a semi-batch reactor with a controlled cooling jacket, keeping the reactor isothermal.

Based on this, the following worst case scenario was studied:

- Complete cooling failure
- All compounds already in the reactor

A complete cooling failure means that the reactor exhibits an adiabatic behaviour. The maximum adiabatic temperature rise is given by:

$$\Delta T_{ad} = \frac{\Delta H X}{m c_p (1 + b)} \quad (12)$$

with X as the overall turnover and the b-factor, accounting for the heat capacity of the vessel to be  $b \approx 0$ . However, it is important to know with which rate and acceleration this maximum temperature is reached. Since the given kinetic parameters are imprecise, this was studied with an extended interval simulations, as proposed above, see Figure 7. The fastest rate, with

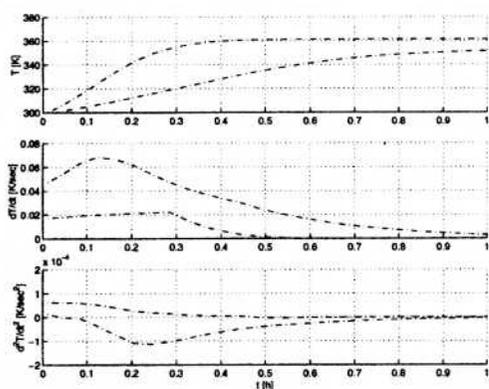


Figure 7: Assessment of the Temperature evolution in case of a cooling failure for the carbamate formation reaction

which the temperature would increase, is for the setup used in Figure 7, 4.2 K/min. Thus, the extended interval simulation is an ideal tool to study such scenarios.

### Conclusion

The objective of this paper was to introduce interval identification, a technique to identify intervals of parameters and initial conditions for nonlinear dynamic systems based on an imprecise mathematical model and measurements of system variables.

First, the evolution of the measured data is described by representative smoothing functions. The smoothed curve is divided into sections of the same qualitative behaviour defined by episodes, i.e. by the sign of the

value and the first and second derivative. The evolution of the measured data is described by the sequence of episodes.

Next, an interacting interval simulator is used to calculate numeric envelopes for the measured variables and their first and second derivative.

Finally, in the interval identification step the qualitative sign information represented by the episodes is checked against the numerically calculated envelopes. If the envelopes bound the behaviour represented by the qualitative history, the identification is successful. Otherwise the assumed interval differential equation cannot create the qualitative dynamic behaviour observed.

Two different applications were presented: A parameter identification of a three-step reaction system in which the interval identification technique proved to be more efficient than a non-interacting simulator by identifying the correct set of intervals.

And a structure and parameter identification of an exothermic reaction, which was subsequently used for an assessment of the safety using an imprecise representation of the kinetic equation.

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