

Application of QR techniques within an integrated tool for automated modelling of chemical reaction systems

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Motivation Model based methods for process control and supervision have been known for many years. In the field of process industries, these methods allow the safe operation of plants with growing complexity and higher efficiency. Nevertheless, such model-based systems didn't find wide acceptance in industry, mainly because of the efforts and costs that are needed to find the structure of an adequate mathematical model within an usually extremely nonlinear domain.

This contribution wants to show, how QR techniques, implemented in an integrated software tool, may support the process of finding adequate mathematical models especially for safety critical chemical reaction systems.

Modelling task and modelling situation The chemical conversion of one or several educts into one or several products is described by a reaction rate r , which depends on parameters like the concentration of the participating substances c_i and the reaction temperature T . Usually, several of such reaction steps occur simultaneously, resulting in a reaction network, where a product of a certain step may be the educt of another and vice versa. Quite often not all of the substances are known at the beginning of an investigation. Substances are fed into or taken out of the reactor. The heat release of the exothermic reactions depends on the reaction rates: $\dot{Q}_j = \dot{Q}_j(r_j)$. It can be controlled by a cooling system. If T increases too much, secondary extremely exothermic reactions may take place, resulting in a runaway or explosion of the reaction system.

The first step in the modelling process is "gathering information" in experiments. After running the reactions at defined conditions in the laboratory and continuously measuring certain temperatures, statements about the temporal behaviour of the heat evolution rate of the reaction $\dot{Q}$ can be gained.

The most difficult task that the modeller has to solve follows, i.e. to describe the time dependancy of the reaction rates r_j of each of the reaction steps by the time dependancies of the already mentioned quantities ($c_i, T, \dots$) in the context of a dynamical model.

Structures and parameters of the functional relationships $r_j = r_j(c_i, T, \dots)$ have to be selected in such a way, that the observed system behaviour can be represented by this model in a numerical simulation.

Numerical optimization support is only available for the last modelling step, which is finding "optimal" parameter values of a given kinetic model. The art of modelling, however, lies in the selection of adequate functional structures. Only very experienced modellers will find a satisfying model design within a few iterations. Moreover, modelling and identification requires time, because usually the kinetic functions of each model design have to be handcoded for simulation and parameter identification. Therefore, the modelling success is not always guaranteed.

Requirements for an integrated modelling tool and the task for QR In order to make it possible also for non-modelling-experts to find a "good" mathematical model for a complex reaction system, it is necessary to integrate and automate as many steps of the whole modelling procedure in a software tool as possible. Starting with the acquisition of data the tool should be able to analyze this data, propose structures for the occurring reaction steps and kinetic functions and identify the free model parameters on its own. However, if the user does have his own modelling experience, it is reasonable to make use of that knowledge, too, thus shorten the modelling run and/or gain a reaction model of higher quality. He should be able to enter suggestions into the system through an appropriate interface. Furthermore, the software tool has to supply the knowledge and experience that in the traditional way the modeller brings in.

This last mentioned feature can be realized by a library of building blocks for certain reaction steps, for experimental devices, for model fragments and other components. The task "parameter identification" is solvable by integration of commercially available optimization and simulation software, if a certain model structure once is chosen. Accessing the correct data at the correct time throughout the whole modelling process requires an intelligent data management for the integrated tool.

The essential task, the detection of possible reaction patterns and structures for the kinetic functions, is solvable by application of QR techniques.

Application of Qualitative Reasoning Currently our group is developing a modelling tool in the proposed integrated way. Within this program, Qualitative Reasoning supports the modelling process in different ways:

- "Qualitative Reasoning" is exactly, what the modeller does, when he looks at the measured data of temperature, heat or concentration values. He tries to detect different episodes in the reaction process and associate them with reaction patterns and kinetic functions that he knows. Within the tool, such associations between certain reaction kinetics and their corresponding qualitative behaviour are stored in a library. So a subset of possible reaction patterns and kinetics can be selected by a simple search procedure automatically.

If adequate models aren't found in the library another approach has to be chosen:

- The experimentally determined overall heat evolution rate $\dot{Q}(t)$ is the sum of the heat evolution rates of all single reaction steps. The program has to solve the inverse qualitative problem: "The sum of which qualitative temporal behaviours of $\dot{Q}_j(r_j(t))$ equals $\dot{Q}(t)$?". For each possible solution it then tries to find appropriate functional relationships $r_j = r_j(c_i, T, \dots)$, based on the qualitative histories of measured T - and c_i -values. If the qualitative simulation shows discrepancies, only little time is lost and the next qualitative model can be checked.

The common goal of both approaches is to detect subsets of possible reaction kinetics by computational "in-expensive" qualitative methods quickly, and to pass only this subset of models to the usually very time consuming parameter identification procedure. Thus much more models can be tested within a certain time and the propability to find a "good" model will increase, especially in the domain of the extremely non-linear kinetics of safety critical reaction systems. Because of the described simplification of the whole modelling procedure, it can be expected that model based methods will find wider acceptance in the future.