TEMPERATURE CONTROL IN AN EXOTHERMIC BATCH REACTOR USING GENERIC MODEL CONTROL AND GLOBALLY LINEARIZING CONTROL

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ABSTRACT

A new model-based controller for the initial heat-up and subsequent temperature maintenance of exothermic batch reactors of two types (Series and Parallel reactions) is presented. The controller is developed using the Generic Model Control (GMC) framework, which provides a rigorous and effective way of incorporating a non-linear energy balance model of the reactor and the heat-exchange apparatus into the controller. Also presented is the design of the feedback controllers for trajectory tracking in a non-linear system, which is transformed into a linear system. This control law, referred as Globally Linearizing Control (GLC), is robust in the sense that small changes in it do not produce large steady state errors or loss of stability. The performance of both the control laws (GMC and GLC) is compared using two different exothermic batch reactors. GMC is found to be well suited for a system when there is no significant rate of change of the setpoint and GLC for the system when the setpoint changes exponentially. These two models are found to be much better than the Dual Control Model.

Key Words: Temperature control, Generic Model Control (GMC), Globally Linearizing Control (GLC), Batch Reactor Control, Dual Control Model.

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Introduction:

The initial heat up from ambient temperature and the subsequent temperature control of exothermic batch reactors have always proved to be a difficult control problem (Shinskey, 1979). Because the amount of heat released as the reaction mixture is heated up can become very large, very quickly the reaction may become unstable and cause the temperature to run away if the heat generated exceeds the cooling capacity of the reactor. This runaway can seriously cause risk to plant personnel and equipment and can, even in the best case, result in loss of the batch. Therefore, careful control of the rate of change of the reactor temperature and minimization of the temperature overshoot is required. On the other hand, from the production point of view, the heat up should be done as quickly as possible in order to reduce the overall cycle time of the reaction process. Therefore, any control strategy heat-up must balance the needs of production with use of safety and quality.

Traditionally, the problem has been approached through the use of open loop control theory to establish a priori, the optimal temperature profiles and of standard feedback control algorithms to achieve these profiles. The control action needed to bring the reactor contents to the desired set point were obtained by solving an optimal control problem with the objective of minimizing the time to reach the set point (Shinskey, 1979). The most commonly used strategy of this type in industry is the dual mode controller of Shinskey and Weinstein (1965), which uses standard PID controller for maintaining temperature. The main problem with approaches of this type is that the optimal switching criterion from heating to cooling, usually based on the reactor temperature, is determined a *priori* and is therefore only valid for a specific range of operating conditions. As heat-up proceeds in an openloop manner and no feedback from the reactor is used; there is no allowance for modeling errors or for changes in process parameters. The use of adaptive control algorithms would appear to offer promising solutions to this problem and there have been several attempts in this direction. The studies by Cluett et al. (1985) are a pointer in this direction. They used a single adaptive control for both heat-up and temperature maintenance but found that the algorithm did not handle the sharp change from the heat-up mode to the temperature maintenance mode very well. They state that the adaptation during the heat-up mode “misleads the operation of the adaptive system” and find that in practice, fully adaptive strategies give poor performance. In the end they effectively revert back to a dual-mode approach, where PID controller is simply replaced by an adaptive controller just for the temperature maintenance part of the profile. Therefore, the robustness concerns of Shinskey’s dual-mode controllers also apply to this controller.

A more encouraging strategy was proposed by Jutan and Uppal (1984), who used a model based approach to estimate the current amount of heat being released in the reactor at any given moment in time. This information was used in a feedforward control structure designed to counterbalance the effect of heat released. In order to compensate for modeling errors and for the lack of a precise estimate if the heat released, they combined the feedforward controller with a feedback controller. Although this approach overcomes many of the problems of the open-loop strategies, the control performance reported by the author could be improved further. The reactor is not smoothly delivered to the desired temperature, and there is the presence of significant overshoot in the reactor temperature. These effects may be attributed to the linearization necessary to implement the feedback control action and to the manner in which the feedforward and feedback effects are added. The subsequent interest in batch process control has been shifted to the design of efficient controller configurations by linearizing the nonlinear input/output models and finding the manipulations required in the inputs. Global input/output Linearizing Control (Kravaris and Chung, 1987), GLC, is one of such attempts which involves complex mathematical understanding. GLC is applied to two exothermic batch reactors in the present study. A new model-based controller design for the heat-up and the temperature maintenance of the above exothermic batch reactors is also presented, which is derived from the Generic Model Control (GMC) algorithm of Lee and Sullivan (1988). Two types of reactions (Series and Parallel) are considered. The energy released in the reactor due to the reaction is treated as a disturbance and the ways and means by which one can determine its value is discussed. The online estimator is very effective than depending on the reaction kinetics. Both the control algorithms are compared for the reactors and the results show that the GMC is better in both the cases.

Exothermic Batch Reactor:

Batch reactor processes offer some of the most interesting and challenging problems in modeling and control because of their inherent dynamic nature. Although most large-scale chemical processes have traditionally been operated in a continuous mode, many batch processes are still used in the production of smaller-volume specialty chemicals and pharmaceuticals. The batch chemical reactor has inherent kinetic advantages over continuous reactors for some reactions (primarily those with slow rate constants). The wide use of digital process control computers has permitted automation of batch processes and made them more efficient and less labor intensive. The batch reactor configuration considered in the present study is shown in Fig.1. Reactant is charged into the vessel. Steam is fed into the jacket to bring the reaction mass up to a desired temperature. Then cooling water must be added to the jacket to remove the exothermic heat of reaction and to make the reactor temperature follow the prescribed temperature-time curve. This temperature profile is fed into the temperature controller as a setpoint signal. The setpoint varies with time.

Estimation of the heat released for the controllers:

The success of the GMC temperature controller is largely dependent on the ability to measure, estimate, or predict the heat released, Q, at any given period in time. There are three main techniques of estimating Q on-line: (1) direct use of detailed kinetic models, (2) deterministic on-line energy balances, and (3) empirical heat-released estimators (Juba and Hamer, 1986). For most reaction systems of industrial interest, the first approach often proves not to be feasible because of the lack of good kinetic models. Deterministic on-line energy balances can also have drawbacks. The main problem is often the assumption that the heat held in the reactor walls is small. If the heat capacity of the reactor walls is not small, then a deterministic energy balance requires the solution of a system of coupled differential equations with several unobservable states such as the wall temperatures. Furthermore, the number of process parameters increases and there may be difficulty in obtaining good estimates for all of them. Juba and Hamer (1986) used an empirically developed discrete-time transfer-function model of the reactor. The model was determined experimentally by simulating heat generation by the injection of steam into a reactor full of water. They used time series analysis to develop a transfer function relating the reactor temperature to the jacket inlet temperature and the heat generation. This model was then inverted to obtain an estimate of the heat released. This method has the advantage of accounting for all the dynamics of the reactor, but has the disadvantage that the resulting model is specific of the reaction/reactor system.

In the present study, since it is the simulation of the exothermic batch reactor, we cannot use the on-line heat estimator but rely on the kinetics of the reactions. We minimized the problems of unknown process parameters by choosing to estimate rather than Q itself. By solving for Q, the number of parameters needed to be determined is minimized to the single group. In addition, it is the only parameter left in the GMC control algorithm, so effectively one parameter characterizes both the estimator and the controller. Since the equations to be solved involve differentiation terms, it is easy to solve them using the Explicit Numerical Differentiation Algorithm. In this work, Euler Algorithm is used which is simpler than Runge-Kutta Algorithm, in spite of its lesser accuracy, as the reactors under consideration do not require very accurate values as there is a possibility of various errors such as noise etc, in the estimation. The details are reported elsewhere (Jyotsna, 1997).

Two batch reactors (one with series reaction and the second with parallel reaction) are simulated using GMC and GLC for both SISO and MISO models. The SISO Model of Series Reaction and its control with both GMC and GLC are detailed here. Similar treatment is given for MISO Model of Series reaction, SISO Model of Parallel reactions, and MISO Model of Parallel reactions.

SISO Model of Series Reaction:

The reaction considered is: $A \longrightarrow B \longrightarrow C$ (1)

$R_1 = k_1 C_A^2$ (2)

$R_2 = k_2 C_B$

From the process dynamics, the state equations are:

$$\frac{dC_A}{dt} = k_1 C_A^2 \tag{3}$$

Results and Discussion:

The simulation results are presented in Figs. 2-9. The results for the reactor I (Series reaction) are shown in Figs. 2-5. In Fig. 2, the setpoint of the reactor temperature is decreasing exponentially to maximize the yield of ‘B’ and minimize ‘C’. Initially the reactor temperature has to be more than that after some time. The controller adjusts the jacket temperature to the maximum allowed (maximum heating) and when the reaction starts at about 10 min., because of the heat of reaction the temperature of the reactor increases enormously if not controlled. GMC predicts the future and even before the reaction starts the jacket temperature is reduced to the minimum to avoid the overshoot (maximum cooling), which is very dangerous. As the heat of reaction gradually reduces, the jacket temperature has to be increased in order to maintain the reactor temperature at setpoint. The reactor temperature could not reach the setpoint initially, as the change from the initial temperature to the maximum required is too large for the controller constants to achieve. It can be only achieved at the cost of certain overshoots later on. It takes relatively a lot of time for the reactor to settle at the setpoint. In the case of GLC, the controller can effectively take the reactor temperature (T_r) to even the maximum temperature of the setpoint without any later overshoots. Fig.3 shows the close movement of T_r to the setpoint. This is more effective than GMC in such cases. Even in the MISO model, though there are some initial setbacks in T_r for GLC, after 5 min., of time the reactor followed the setpoint with almost less than 0.05% error (see Fig. 4 and 5).

For the parallel reaction type reactor (II), where the setpoint is for the reactor is constant at 95^oC, since the rate of change of temperature is not large, GMC tracked the required temperature within 20 min. Without any overshoots with the same PI constants as can be seen from Figs. 6 and 8. The jacket temperature setpoint also need to be reached by jacket in order to meet the reactor setpoint. GMC has managed the task without any error more than 0.05%. The reaction started at 20 min. and the controller has started to detect the expected change at around 5-min. and carefully reduced the jacket temperature setpoint from then. This is not possible with the conventional controllers. GLC is not effective in this case since there is an overshoot of more than 15^oC before it slowly reached 95^oC. Since the reaction runaway temperature is only 100^oC, GLC is not advisable with the chosen constants. But probably when the constants are changed from the present values the danger can be avoided (see Fig. 7).

The comparison of both the GMC and GLC models are presented in the Figs. 9 and 10 for clearer insight.

Conclusions:

A model-based control strategy using the Generic Model Control (GMC) algorithm was developed and applied to the heat-up and subsequent temperature control in an exothermic batch reactor. GMC provides a method in which nonlinear feedforward and feedback effects can be combined properly. We also simulated a perfect model of batch reactor and using the Global Linearizing Control (GLC) linearized the input/output equations and controlled the reactor using the PI controller. The PI constants were chosen by trial-and-error since there is no particular solution for the characteristic equation.

For both the heat-up and maintenance stages of the reactor without shifting over to a different control strategy, it can be maintained using only one algorithm. This is very useful since there is no time lag for changing and but it takes care of the heat-up at the minimum time only.

GMC is well suited for a system when there is no too large rate of change of the setpoint and GLC for the system when the setpoint changes exponentially. In the former case there might be a chance of reaction temperature overshoot if the controller constants are changed to track. These models are much better than the Dual Control Model described by Shinskey (1979).

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