NONLINEAR CONTROL OF A BATCH REACTOR IN THE PRESENCE OF UNCERTAINTIES

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Abstract: In this paper, we propose new control design strategies within the Generic Model Control (GMC) framework for tracking the pre-determined temperature profiles of a batch reactor. It is shown by simulation studies that the designed robust GMC controller is able to track the temperature reactor profile reasonably well, and its optimal performance is maintained in spite of large uncertainties.

Keywords: batch reactor, nonlinear control, uncertainties

1. PROBLEM FORMULATION

In recent years, the optimization, monitoring and control of batch processes have been an active research area as the emergence of generic drugs from the pharmaceutical industries are now pushed to be the first on the market (Bonvin, 1997; Y. Yabuki and MacGregor, 2002). A batch reactor is a typical process that exhibits challenging operational problems because of its highly nonlinear dynamics and its complex reaction kinetics and stoichiometry. As a result, the use of model-based technology to optimally operate the batch reactor should address simultaneously the nonlinear dynamics and the modelling errors due to the inability to model such complex reactions.

The operation of a batch reactor typically employs a process optimization and feedback control arrangement (Jutan and Uppal, 1984; M.V. Le Lann, 1999). Models are used in both optimization and control. Different approaches have been pursued to obtain a reliable kinetic and stoichiometric model. A *tendency modelling* has been the popular approach to capture the kinetics and stoichiometric of the reaction (C. Filippi and Georgakis, 1986). The minimum necessary and essential data for the reaction model development are: the total batch data, the reactor temperature, the initial compositions and the final concentration of different components. The model is used for the optimization of the batch operation to maximize either yields or some economic factors subject to some process constraints (e.g. rate of change in temperature, heat generated, etc.). The batch optimization is aimed at determining the temperature or additional reactant rate profiles. The profiles should be tracked optimally by the feedback control implemented for each batch cycle. Due essentially to the lack of on-line concentration measurements, in practice the problem of batch reactor control remains a problem of temperature control. Thus, the control performance is mainly dependent on the heating-cooling systems associated with the reactor.

We consider a batch reactor studied in (C.Kravaris and Chung, 1987). In the batch reactor, the following consecutive reaction is taking place:

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$$A \xrightarrow{k_1} B \xrightarrow{k_2} C \quad (1)$$

and the reaction model is given as:

$$\frac{dC_A}{dt} = -k_1(T)C_A^2, \quad \frac{dC_B}{dt} = k_1(T)C_A^2 - k_2(T)C_B, \quad (2)$$

with the initial concentrations of A and B are $C_A(0) = 1$ and $C_B(0) = 0$, and some parameters are defined as:

$$k_1(T) = A_{10}e^{(-E_1/RT)}; k_2(T) = A_{20}e^{(-E_2/RT)};$$
$$A_{10} = 1.1;\ E_1 = 2.09 \times 10^4;$$
$$A_{20} = 172.2;\ E_2 = 4.18 \times 10^4;$$
$$R = 8.31 \times 10^{-3};\ T_{min} = 25^oC;\ T_{max} = 125^oC$$

Batch cycle time is 1 hr. Within this cycle time, the feedback controller should be able to track the following reactor temperature profile $T_d(t)$, which is produced by the batch optimizer:

$$T_d(t) = 54 + 71e^{-2.5\times10^{-3t}}\ ^oC \quad (3)$$

subject to some operational constraints and uncertainties.

The critical step in designing the batch temperature control system is the choice of manipulated variable. The reactor temperature T can be controlled by regulating the steam temperature supplied into the heating jacket T_s and the flow rate of the coolant in the cooling coil F_c. The heat balance equation is:

$$\rho C_p V \frac{dT}{dt} = k_1(T)C_A^2(-\Delta H_1)V + k_2(T)C_B(-\Delta H_2)V + U_jA_j(T_s - T) - U_cA_c(T - T_c) \quad (4)$$
$$\frac{1}{U_c} = \frac{1}{4550F_c^{0.8}} + \frac{1}{10.8}$$

There are two manipulated variables, T_s and F_c available for controlling the reactor temperature T. We will use a single parametric variable u as a combined manipulated variable for the temperature control, where u is defined as (Jutan and Uppal, 1984):

$$T_s = (T_{s,max} - T_{s,min})u + T_{s,min}$$
$$U_c = (U_{c,min} - U_{c,max})u + U_{c,max} \quad (5)$$

where the maximum and the minimum value of T_s and U_c are selected from the safety limits. Obviously, $u = 0$ denotes maximum cooling of the system while $u = 1$ represents the maximum heating. By substituting (5) into (4) and after some arrangement, we obtain:

$$\frac{dT}{dt} = \gamma_1 k_1(T)C_A^2 + \gamma_2 k_2(T)C_B + (a_1 + a_2T) + (b_1 + b_2T)u \quad (6)$$

where the parameters are defined as:

$$\gamma_1 = (-\Delta H_1)/\rho C_p,\ \gamma_2 = (-\Delta H_2)/\rho C_p$$
$$a_1 = (U_jA_jT_{s,min} + U_{c,max}A_cT_c)/\rho C_pV$$
$$a_2 = -(U_jA_j + U_{c,max}A_c)/\rho C_pV$$
$$b_1 = [U_jA_j(T_{s,max} - T_{s,min}) - (U_{c,max} - U_{c,min})A_cT_c]/\rho C_pV$$
$$b_2 = (U_{c,max} - U_{c,min})/\rho C_pV$$

and the constants are chosen as:

$$\rho C_p = 1000,\ \Delta H_1 = -4.18 \times 10^4;\ \Delta H_2 = -8.36 \times 10^4;$$
$$A_j/V = 30,\ A_c/V = 17,\ U_j = 1.16$$

The operational constraints are given by

$$T_{s,max} = 150,\ T_{s,min} = 70,\ T_c = 25 \quad (7)$$
$$F_{c,max} = 33.1 \times 10^5,\ F_{c,min} = 4.8 \times 10^5$$

Uncertainties in the batch reactor could be in terms of uncertain initial concentration of $A, C_A(0)$, reaction constants A_{10} and A_{20}, and the activation energies E_1 and E_2. Hence, the batch temperature control problem is formulated as follows: *Design a nonlinear controller that is able to track the temperature profile given in (3) subject to process constraints in (7) and large uncertainties in the initial concentration of A, reaction constants and the activation energies.*

In this work, we present a new robust Generic Model Control (GMC) design framework to optimally track the pre-determined temperature profile in the presence of uncertainties. The method is developed by optimizing the GMC parameters (τ and ξ) for the desired robust stability and performance levels.

2. STANDARD AND ROBUST GMC DESIGN

2.1 Standard GMC Design

GMC is a class of nonlinear control design that makes use of: a dynamic (nonlinear) model of a process, a reference system in terms of a desirable rate of change of the output variables, and a generation of an optimal control law to ensure closed-loop performance. A dynamic (nonlinear) model of the process is described as a set of differential equations:

$$\frac{dy}{dt} = f(y, u, d, \theta) \quad (8)$$

where y, u and d are the vectors of model outputs, inputs and measured disturbance variables, and θ is a vector of known process parameters. In general, f is a vector of known (or approximation of) nonlinear functional relationships of those variables. We never obtain an exact representation of the plant using (8). In other words, *process/model mismatch* inherently occurs when applying the GMC design, like other model-based design methods. The mismatch could be in the forms of structural mismatch (i.e. $f(.)$ is the result of model simplification) and/or parametric mismatch (i.e. θ represent partially known process parameters).

The basic idea of GMC design is to apply a reference system as a desirable rate of change of the controlled variables, $(\frac{dy}{dt})^*$. One reasonable choice of the reference system is:

$$(\frac{dy}{dt})^* = K_1(y^{sp} - y_o) + K_2 \int_0^{\tau} (y^{sp} - y_o)dt \quad (9)$$

Lee (Lee and Sullivan, 1988) discussed how the parameters K_1 and K_2 were chosen using simple techniques to accommodate the desired closed-loop performance. For example, to determine the i^{th} element of the diagonal matrices K_1 and K_2, the following simple rules can be applied:

$$k_{1i} = \frac{2\xi_i}{\tau_i}; \quad k_{2i} = \frac{1}{\tau_i^2} \quad (10)$$

The parameters ξ_i and τ_i specify the shape and speed of the desired closed-loop trajectory of the i^{th} controlled variable. It is obvious that the parameters of τ and ξ captures the desired closed-loop performance of GMC. No robustness objective is explicitly considered during the choice of K_1 and K_2. In the standard GMC design procedure, the robustness objective has been considered indirectly, and often in ad-hoc manner. No systematic procedure is available to explicitly address the robustness objective.

By combining (9) and (8), the optimal GMC inputs, u^{opt} are generated by solving a minimization problem formulated as:

$$u^{opt} = arg \min_u \; J_{GMC} = \int_0^{\tau} \epsilon^T(t)\epsilon(t) \; dt \quad (11)$$

subject to: $u \in \mathcal{U}$. The objective function is defined as:

$$\epsilon(t) = [f(y_o, u, d, \theta) - (\frac{dy}{dt})^*] \quad (12)$$

The GMC control law is hence implemented as solving the optimization problem numerically at every sampling time by employing the model (8). Alternatively, an explicit solution of (11) is also possible only if the model (8) satisfies the nonlinear invertibility conditions.

2.2 Robust GMC Design

Consider the situation where there is no process/model mismatch and the nonlinear model (8) is completely invertible. This situation is referred to as the *ideal* case. In this ideal case, the dynamics from the reference rate of the process output change $\left(\frac{dy}{dt}\right)^*$ to the process output y_o (or *internal dynamics*) follows a pure integrator system $G = \frac{I}{s}$. The ideal closed-loop system is given by:

$$y_o = (sI - K)^{-1}K \; y^{sp} \quad (13)$$

where K is the diagonal transfer function matrix. This result shows a perfect disturbance rejection and decoupling of the outputs. Also, the stability and performance of the closed-loop system is dependent on $(sI - K)^{-1}K$. For the standard GMC design, the ideal closed-loop system (13) corresponds to a linear system $G = \frac{I}{s}$ under K, which corresponds to a PI controller (9).

The closed-loop analysis of the ideal case leads to the choice of a nominal model for designing an *optimally robust* GMC reference trajectory, K_{opt}. Samyudia and Lee (Samyudia and Lee, 2002) have used the integrator system $G = \frac{I}{s}$ as a nominal model, and then applied the H_∞ loop shaping design of McFarlane and Glover (McFarlane and Glover, 1992) for deriving K_{opt}, which is formulated as:

$$\left(\frac{dy}{dt}\right)^* = WK_\infty(y^{sp} - y_o) = K_{opt}(y^{sp} - y_o) \quad (14)$$

The stable transfer function matrix K_∞ is derived by minimizing the H_∞ norm of the following closed-loop transfer matrix:

$$H(G_s, K_\infty) = \begin{bmatrix} -SG_s & S \\ -K_\infty SG_s & K_\infty S \end{bmatrix} \quad (15)$$

where $S = (I - G_sK_\infty)^{-1}$ and $G_s = GW$. The elements of diagonal weighting function W follows a PI structure as:

$$w_i = \frac{k_i(s + z_i)}{s} \quad for \; i = 1, \cdots, n_y \quad (16)$$

where n_y is the number of outputs. Note that the choice of k_i and z_i can follow the simple rules of (10).

The GMC controller with the robust reference trajectory K_{opt} achieves an optimal robust stability margin $b_{[G,K_{opt}]} \leq \| H(G_s, K_\infty) \|_\infty^{-1}$.

In the presence of process/model mismatch, the internal dynamics can be different from $G = \frac{I}{s}$, say G_p. The robust closed-loop stability is determined using the following proposition:

Proposition 1. (Samyudia and Lee, 2002) Let $G = \frac{I}{s}$ be a nominal model for designing a robust GMC reference trajectory with a robust stability margin $b_{[G,K_{opt}]}$. The closed-loop system of GMC in the presence of process/model mismatch is guaranteed to be stable if and only if $b_{[G,K_{opt}]} > \delta_\nu(G, G_p)$, where G_p is the actual internal dynamics.

Proposition 1 was derived as a direct application of the robust stability conditions in terms of ν-gap metric (Vinnicombe, 1993). There are two interesting points to make concerning Proposition 1. Firstly, the smaller $\delta_\nu(G, G_p)$, the closer the achieved performance of the GMC controller would be to the ideal closed-loop performance as in (13). Secondly, for a specified performance objective as represented by the weighting function W, the robust reference trajectory of the GMC controller, K_{opt} can be designed for the maximum robustness level, $b_{opt} = \| H(G_s, K_\infty) \|_\infty^{-1}$.

Given the features of the robust GMC reference trajectory, K_{opt}, our new design methods are developed for the standard GMC controller, where the parameters τ and ξ are optimally adjusted such that (9) approximates K_{opt}. This attempt is motivated by the current practice that the GMC parameters τ and ξ are often adjusted in an ad-hoc manner to maintain the GMC performance in the presence of process/model mismatch. Our contribution of this work is therefore to establish a systematic procedure to optimally tune the GMC parameters τ and ξ such that the standard GMC controller satisfies the robustness objective.

2.3 Standard GMC Design for Optimal Robustness

As presented in Section 2.2, the robust GMC reference trajectory K_{opt} is different from the standard GMC reference trajectory because of the additional term K_∞. Since (9) and (14) are linear systems, we can measure their distance using the ν-gap metric as: $\delta_\nu(K_{opt}, K)$, where the ν-gap metric is a normalized measure that spans between zero and one. The smaller the distance, the closer the robustness of the standard GMC controller would be to the robust GMC controller with K_{opt}. This result leads to a systematic tuning of the standard GMC parameters τ and ξ for achieving an optimal robustness. The optimal GMC tuning is formulated as follows:

Procedure 1. Find the GMC parameters τ and ξ that minimize $\delta_\nu(K_{opt}, K)$, or mathematically:

$$\min_{0<\tau<\tau_H, 0<\xi<\xi_H} J_{RS} = \delta_\nu(K_{opt}, K(\tau, \xi)) \quad (17)$$

subject to: $J_{RS} < b_{opt}$.

This procedure can be applied for a given K_{opt}. The upper bounds, τ_H and ξ_H, are set by considering the closed-loop performance limits (e.g. speed and shape of responses). A reasonable set on the upper bounds τ_H and ξ_H makes the optimization problem convex. For the optimal values of τ^* and ξ^*, the achieved robustness of the standard GMC controller, b_{GMC} is guaranteed by:

$$\delta_\nu(G, G_p) < [b_{opt} - \delta_v(K_{opt}, K(\tau^*, \xi^*))] \approx b_{GMC} \quad (18)$$

where the ν-gap metric between the nominal model G and the actual internal dynamics G_p measures the process/model mismatch. Hence, by applying the new design procedure of (17), we are able to accommodate the robustness objective within the standard GMC design procedure by optimally tuning the parameters τ and ξ to satisfy the robust stability objective.

Note that translating $\delta_\nu(G, G_p)$, for example, to the range of parameter mismatch, however, would be difficult and be case-dependent. Our effort to estimate the actual process/model mismatch is to employ a closed-loop metric, which is calculated from a set of closed-loop data in response to a bounded power disturbance. For the worse-case disturbances, this metric is equivalent to $\delta_\nu(G, G_p)$.

2.4 Standard GMC Design for Robust Performance

The most important objective of any controller design is to maintain its ideal performance in spite of the presence of process/model mismatch. This is known as a *robust performance* objective. When designing the GMC controller for robust performance, the achieved closed-loop performance should be quantified and compared with the ideal performance. Hence, to achieve the robust performance property, we require a set of actual closed-loop data from which we compute a closed-loop metric as a measure of robust performance. So, the closed-loop metric is defined as:

$$\delta_\nu(\tau, \xi) := \frac{\| z(\tau, \xi) - z^* \|_S}{\| r \|_S} \quad (19)$$

where $z = \begin{bmatrix} y & \frac{dy}{dt} \end{bmatrix}^T$ is the measured data from the achieved closed-loop system where the plant is running under the standard GMC controller, $z^* = \begin{bmatrix} y^* & \frac{dy^*}{dt} \end{bmatrix}^T$ is the simulated data generated from the ideal closed-loop system where the robust GMC with K_{opt} is running for the nominal model G, r represents a typical disturbance, and $\| \, . \, \|_S$ denotes a bounded power (semi-norm) of a signal.

Since the closed-loop metric is evaluated for a particular disturbance r, this metric is not equivalent to $\delta_\nu(G, G_p)$. Recently, Date (Date, 2000) has shown that $\delta_\nu(G, G_p) := \sup_{r \in S_r} \delta_\nu(\tau, \xi)$, where S_r is a set of ℓ^1_∞ bounded signals. The ν-gap metric is therefore equivalent to the closed-loop metric evaluated for the worst-case disturbances. If we could identify what the worst case disturbances would be, and apply them to both achieved and ideal closed-loop loop systems, then the closed-loop metric in (19) would approach $\delta_\nu(G, G_p)$. This implies that we should have $\delta_\nu(\tau, \xi) \leq \delta_\nu(G, G_p)$.

This result has an interesting implication to our GMC design. The GMC parameters τ and ξ

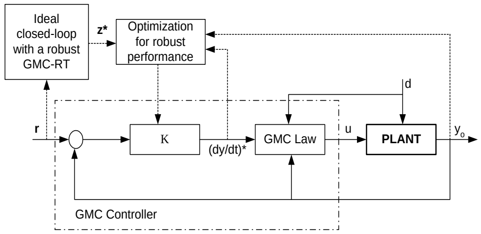

Fig. 1. GMC control design for robust performance

can now be obtained for a robust performance objective in response to the disturbance r.

Procedure 2. An optimal design of the standard GMC controller for robust performance with respect to a disturbance r follows a two step procedure as:

(1) Design a stabilizing GMC controller using either (17) or Lee and Sullivan's method.
(2) Re-tune the GMC parameters τ and ξ by solving the following optimization:

$$\min_{\tau>0,\xi>0} J_{RP} = [\delta_\nu(\tau,\xi) + \delta_\nu(K_{opt}, K(\tau,\xi))] \quad (20)$$

subject to: $J_{RP} < b_{opt}$.

The constraint represents the robust stability condition, which means that the robust performance objective is achieved only if the robust stability condition is satisfied. Also, the constraint is to guarantee that we have a stabilizing controller at each iteration when solving the optimization (20).

By following the above two step procedure, the achieved robust performance level is indicated by $J_{RP}(\tau^*, \xi^*)$, where τ^* and ξ^* are the optimal solutions to the optimization problem of (20). The smaller $J_{RP}(\tau^*, \xi^*)$ as compared to b_{opt}, the closer the achieved closed-loop performance would be to the ideal closed-loop performance. This means that the controller can effectively handle the process/model mismatch. Fig. 1 illustrates a schematic diagram of the robust GMC controller. The outer loop is a data-driven optimizer to optimally tune the GMC parameters τ and ξ by solving the optimization problem (20). The inner loop is the closed-loop system where a (*to be updated*) GMC controller is implemented in the actual plant. Both loops are running at different sampling rates, where the inner loop is running faster than the outer loop.

The process noise or unmeasured disturbance are assumed to be uncorrelated with the excitation signal r. Also, the power of the excitation signal is large enough to ensure a high signal to noise ratio.

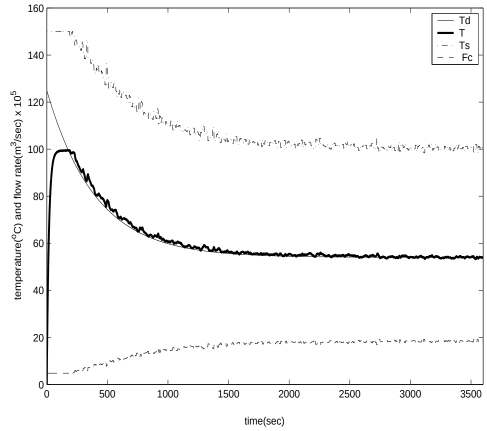

Fig. 2. Robust GMC controller with K_{opt}.

3. APPLICATION TO THE BATCH REACTOR

The new GMC design procedures were applied to the batch temperature control problem. In the simulation, we applied a $\pm 100\%$ uncertainty in the initial concentration of A, $C_A(0)$ and the reaction constants, A_{10} and A_{20}, and a $\pm 50\%$ uncertainty in the activation energies E_1 and E_2. In the GMC nonlinear model, the concentration dynamics were not considered. Further, measurement noise was introduced as a zero-mean random numbers with variance 25, and a zero-mean random numbers with variance 0.056 was added to the heat balance equation.

Fig. 2 shows the ideal responses of the robust GMC controller with K_{opt}, which was designed for an optimal robustness b_{opt}=0.705. The responses are reasonably good in tracking the temperature profile while satisfying the operational constraints.

The responses of the standard GMC controller with the parameters $\tau = 141.4$ and $\xi = 1.07$, are presented in Fig. 3. The responses are stable, but worse and more sensitive to noise as compared to the responses of the robust GMC (or RGMC). To improve the performance of the standard GMC controller, we applied Procedure 1. The optimization process is shown in Fig. 4. The optimal GMC parameters were obtained as $\tau^* = 140$ and $\xi^* = 7.00$. The responses of the optimal robustly tuned GMC controller are presented in Fig. 5. The responses are improved significantly and achieve almost the same responses as the RGMC controller.

The effect of different initial GMC parameters when solving the optimization of Procedure (2) was also investigated. For example, another set of initial GMC parameters was chosen as $\tau = 100$ and $\xi = 7.07$. Then, the same optimal GMC parameters $\tau^* = 140$ and $\xi^* = 7.00$ were obtained. This indicates the convexity of the optimization

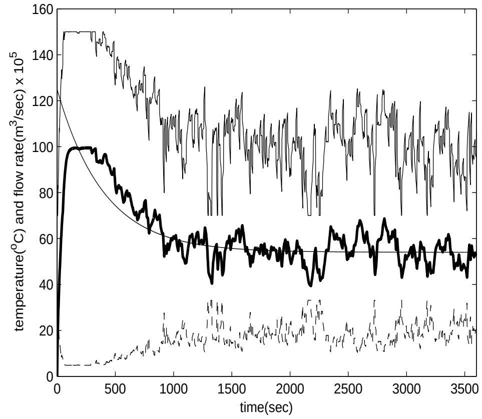

Fig. 3. Standard GMC controller.

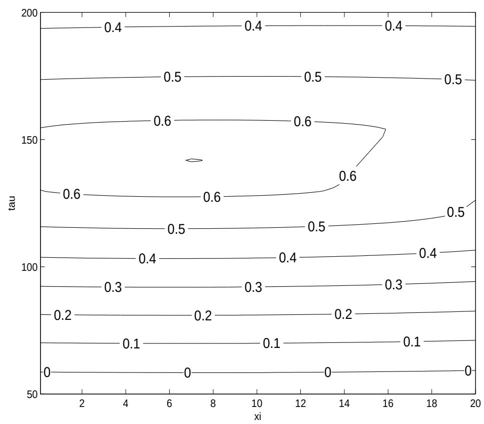

Fig. 4. Contour $b_{GMC(\tau,\xi)}$.

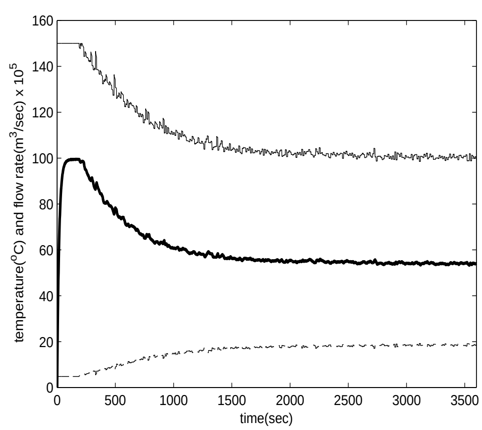

Fig. 5. Optimally tuned GMC controller

problem in (14). This is partially because of the reasonable choice of τ_H and ξ_H.

The GMC design procedure for robust performance was then followed for the batch temperature control problem. The optimization process is depicted in Fig. 6. The optimal parameters were obtained as $\tau^* = 140$ and $\xi^* = 7.00$, which are the same as obtained for robust stability. This result shows that for the batch reactor control problem, the optimal GMC parameters for robust stability achieve a robust performance property. As indicated by a faster change of the optimization

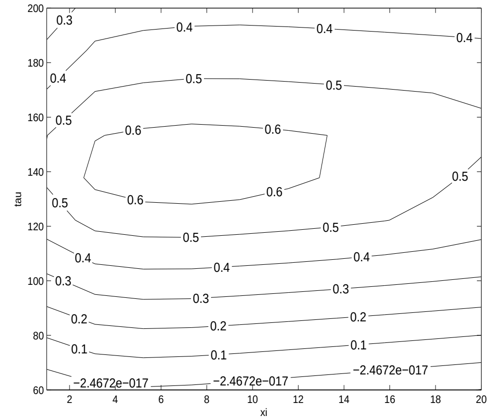

Fig. 6. Contour $(b_{opt} - J_{RP})$

contour in Fig. 6 than in Fig. 4, the feasible range of the GMC parameters for robust performance is smaller than that for robust stability.

4. CONCLUSIONS

With the application to a batch reactor control problem, new procedures to the robust nonlinear GMC control design have been presented in this paper. The new design procedures have been used to robust optimally tune the standard GMC parameters. As shown by simulation studies, the performance of robust nonlinear GMC controllers was reasonably well in tracking the batch reactor's temperature trajectory in spite of the presence of large uncertainties in the initial conditions and process parameters.

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