ANALYSIS AND TEMPERATURES CONTROL IN A TUBULAR CHEMICAL REACTOR

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Abstract

The paper deals with analysis and continuous-time adaptive control of a tubular chemical reactor with a countercurrent cooling as a non-linear single input – single output process. The output reactant temperature and the mean reactant temperature are chosen as the controlled outputs, and, the coolant flow rate as the control input. The parameters of its continuous-time external linear model are estimated via corresponding delta model The resulting controllers are derived using polynomial approach. The control system structure with two feedback controllers is considered. The approach is tested on a mathematical model of the tubular chemical reactor.

Key words

Tubular chemical reactor, nonlinear model, external linear model, delta model, polynomial method.

1 Introduction

Tubular chemical reactors are units frequently used in chemical and biochemical industry. From the system theory point of view, tubular chemical reactors belong to a class of nonlinear distributed parameter systems. Their mathematical models are described by sets of nonlinear partial differential equations (PDR). The methods of modelling and simulation of such processes are described eg. in [Luyben, 1989; Ingham *et al.*, 1994; Dostál *et al.*, 2008 and Severance, 2001].

It is well known that the control of chemical reactors, and, tubular reactors especially, often represents very complex problem. At all events, a previous analysis of the process behaviour is obligatory.

One possible method to cope with this problem is application of adaptive strategies based on an appropriate choice of a continuous-time external linear model (CT ELM) with recursively estimated parameters (see, e.g. [Rao and Unbehauen, 2005]). These parameters are consequently used for parallel updating of controller‘s parameters.

The paper deals with analysis and continuous-time adaptive control of a tubular chemical reactor with a countercurrent cooling as a non-linear single input – single output process. With respect to practical possibilities of a measurement and control, the output reactant temperature and the mean reactant temperatures are chosen as the controlled outputs, and, the coolant flow rate as the control input. The parameters of its CT ELM are estimated via corresponding delta model (see, e.g. [Middleton and Goodwin, 1990; Mukhopadhyay *et al.*, 1992; Stericker and Sinha, 1993]. The resulting controllers are derived using polynomial approach [Kučera, 1993]. The control system structure with two feedback controllers [Dostál *et al.*, 2007] is considered. The approach is tested on a mathematical model of the tubular chemical reactor.

2 Model of the Plant

Consider an ideal plug-flow tubular chemical reactor with a simple exothermic consecutive reaction $A \xrightarrow{k_1} B \xrightarrow{k_2} C$ in the liquid phase and with the countercurrent cooling. Heat losses and heat conduction along the metal walls of tubes are assumed to be negligible, but dynamics of the metal walls of tubes are significant. All densities, heat capacities, and heat transfer coefficients are assumed to be constant. Under above assumptions, the reactor model can be described by five PDRs

$$\frac{\partial c_A}{\partial t} + v_r \frac{\partial c_A}{\partial z} = -k_1 c_A \quad (1)$$

$$\frac{\partial c_B}{\partial t} + v_r \frac{\partial c_B}{\partial z} = k_1 c_A - k_2 c_B \quad (2)$$

$$\frac{\partial T_r}{\partial t} + v_r \frac{\partial T_r}{\partial z} = \frac{Q_r}{(\rho c_p)_r} - \frac{4U_1}{d_1(\rho c_p)_r}(T_r - T_w) \quad (3)$$

$$\frac{\partial T_w}{\partial t} = \frac{4}{(d_2^2 - d_1^2)(\rho c_p)_w}\left[d_1 U_1 (T_r - T_w) + d_2 U_2 (T_c - T_w)\right] \quad (4)$$

$$\frac{\partial T_c}{\partial t} - v_c \frac{\partial T_c}{\partial z} = \frac{4 n_1 d_2 U_2}{(d_3^2 - n_1 d_2^2)(\rho c_p)_c}(T_w - T_c) \quad (5)$$

with initial and boundary conditions

$$c_A(z,0) = c_A^s(z)\,,\ c_B(z,0) = c_B^s(z)\,,$$
$$T_r(z,0) = T_r^s(z)\,,\ T_w(z,0) = T_w^s(z)\,,$$
$$T_c(z,0) = T_c^s(z)$$
$$c_A(0,t) = c_{A0}(t)\,,\ c_B(0,t) = c_{B0}(t)\,,$$
$$T_r(0,t) = T_{r0}(t)\,,\ T_c(L,t) = T_{cL}(t)\,.$$

Here, t is the time, z is the axial space variable, c are concentrations, T are temperatures, v are fluid velocities, d are diameters, ρ are densities, c_p are specific heat capacities, U are heat transfer coefficients, n_1 is the number of tubes and L is the length of tubes. The subscript $(\cdot)_r$ stands for the reactant mixture, $(\cdot)_w$ for the metal walls of tubes, $(\cdot)_c$ for the coolant, and the superscript $(\cdot)^s$ for steady-state values.

The reaction rates and heat of reactions are nonlinear functions expressed as

$$k_j = k_{j0} \exp\left(\frac{-E_j}{RT_r}\right),\ j = 1, 2 \quad (6)$$

$$Q_r = (-\Delta H_{r1}) k_1 c_A + (-\Delta H_{r2}) k_2 c_B \quad (7)$$

where k_0 are pre-exponential factors, E are activation energies, (- ΔH_r) are in the negative considered reaction entalpies, and R is the gas constant.

The fluid velocities are calculated via the reactant and coolant flow rates as

$$v_r = \frac{4 q_r}{\pi n_1 d_1^2}\ ,\ v_c = \frac{4 q_c}{\pi (d_3^2 - n_1 d_2^2)} \quad (8)$$

The parameter values with correspondent units used for simulations are in Tab. 1.

From the system engineering point of view, $c_A(L,t) = c_{A\mathrm{out}}$, $c_B(L,t) = c_{B\mathrm{out}}$, $T_r(L,t) = T_{r\mathrm{out}}$ and $T_c(0,t) = T_{c\mathrm{out}}$ are the output variables, and, $q_r(t)$, $q_c(t)$, $c_{A0}(t)$, $T_{r0}(t)$ and $T_{cL}(t)$ are the input variables. Among them, for the control purposes, mostly the coolant flow rate $q_c(t)$ can be taken into account as the control variable, whereas other inputs enter into the process as disturbances. As the controlled outputs are considered the reactant output temperature $T_{r\mathrm{out}}$ and the mean reactant temperature given by

$$T_m(t) = \frac{1}{L}\int_0^L T_r(z,t)\, dz\ . \quad (9)$$

Tab. 1. Used Parameter Values

L = 8 m	n_1 = 1200
d_1 = 0.02 m	d_2 = 0.024 m
d_3 = 1 m	
ρ_r = 985 kg/m^3	c_{pr} = 4.05 kJ/kg K
ρ_w = 7800 kg/m^3	c_{pw} = 0.71 kJ/kg K
ρ_c = 998 kg/m^3	c_{pc} = 4.18 kJ/kg K
U_1 = 2.8 kJ/m^{2}s K	U_2 = 2.56 kJ/m^{2}s K
k_{10} = 5.61·10^{16} 1/s	k_{20} = 1.128·10^{18} 1/s
E_1/R = 13477 K	E_2/R = 15290 K
(-ΔH_{r1}) = 5.8·10^4 kJ/kmol	(-ΔH_{r2}) = 1.8·10^4 kJ/kmol

3 Computation Models

For computation of both steady-state and dynamic characteristics, the finite diferences method is employed. The procedure is based on substitution of the space interval $z \in <0, L>$ by a set of discrete node points $\{z_i\}$ for i = 1, … , n, and, subsequently, by approximation of derivatives with respect to the space variable in each node point by finite differences. The procedure is in detail described in [Dostál *et al.*, 2008].

4 Steady-state Characteristics

Steady-state characteristics were computed from discretized model with zero time derivatives using fixed point iterations algorithm.

The dependences of output concentrations and temperatures on the coolant flow rate in the steady-state for $c_{A0}^s = 2.85$, $c_{B0}^s = 0$, $T_{r0}^s = 323$, $T_{c0}^s = 293$ and $q_r^s = 0.15$ are shown in Figs. 1, 2. The nonlinearity of all characteristics is evident.

5 Dynamic Characteristics

The dynamic charakteristics were investigated for both supposed controlled outputs and selected step changes of the control input in the neighbourhood of the chosen operating point $q_c^s = 0.27\ \mathrm{m^3/s}$, $T_{rout}^s = 326.10\,\mathrm{K}$ and $T_m^s = 334.44\,\mathrm{K}$. All variables were considered as deviations from their steady values

$$\Delta q_c = q_c(t) - q_c^s\,,\ \Delta T_{r\,\mathrm{out}}(t) = T_{r\,\mathrm{out}}(t) - T_{r\,\mathrm{out}}^s\,,$$

$$\Delta T_m(t) = T_m(t) - T_m^s\,.$$

Simulated step responses are in Figs. 3 and 4.

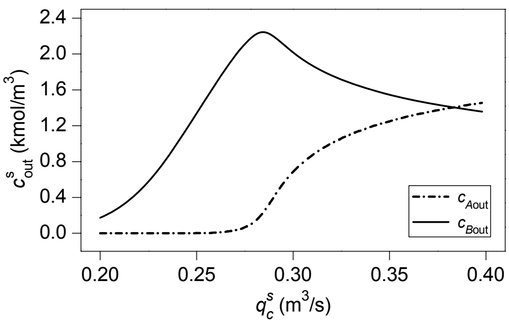

Figure 1. Dependence of output concentrations on the coolant flow rate.

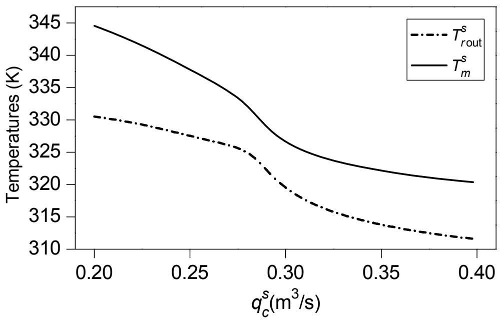

Figure 2. Dependence of reactant output and mean temperatures on the coolant flow rate.

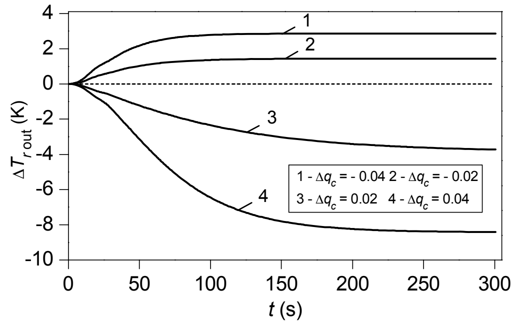

Figure 3. Reactant output temperature step responses.

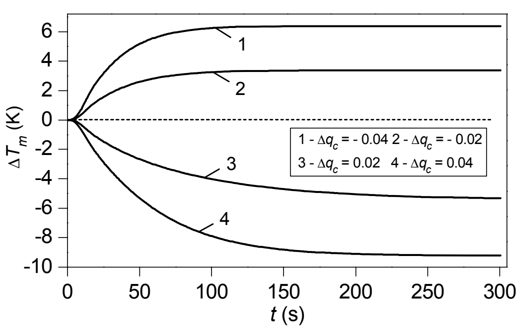

Figure 4. Reactant mean temperature step responses.

6 CT and Delta External Linear Model

For the control purposes, the controlled outputs and the control input are defined as

$$y_1(t) = \Delta T_{rout} = T_{r\,\mathrm{out}}(t) - T_{r\,\mathrm{out}}^s\,, \qquad (10)$$

$$y_2(t) = \Delta T_m(t) = T_m(t) - T_m^s\,,\ u(t) = 10\,\frac{q_c(t) - q_c^s}{q_c^s}\,.$$

These expressions enable to obtain variables of approximately the same magnitude.

For both controlled outputs, the second order CT ELMs have been chosen in the form of the second order linear differential equation

$$\ddot{y}(t) + a_1\dot{y}(t) + a_0 y(t) = b_0 u(t) \qquad (11)$$

or, in the transfer function representation as

$$G(s) = \frac{Y(s)}{U(s)} = \frac{b_0}{s^2 + a_1 s + a_0}\,. \qquad (12)$$

Establishing the δ operator

$$\delta = \frac{q-1}{T_0} \qquad (13)$$

where q is the forward shift operator and T_0 is the sampling period, the delta ELM corresponding to (20) takes the form

$$\delta^2 y(t') + a_1'\delta y(t') + a_0' y(t') = b_0' u(t') \qquad (14)$$

where t' is the discrete time. When the sampling period is shortened, the delta operator approaches the derivative operator, and, the estimated parameters a', b' reach the parameters a, b of the CT model as shown in [Stericker and Sinha, 1993].

7 Delta ELM Parameter Estimation

A procedure of the recursive CT ELM parameter estimation via a corresponding delta model can be briefly described in following steps:

Substituting $t' = k-2$, equation (14) may be rewriten to the form

$$\begin{aligned}\delta^2 y(k-2) + a_1'\delta y(k-2) + a_0' y(k-2) &= \\ = b_0' u(k-2).\end{aligned} \qquad (15)$$

In the paper, the recursive identification method with exponential and directional forgetting according to [Bobál *et al.*, 2005] was used.

Establishing the regression vector

$$\boldsymbol{\Phi}_\delta^T(k-1) = \left(-\delta y(k-2) \quad -y(k-2) \quad u(k-2)\right) \qquad (16)$$

the vector of delta model parameters

$$\boldsymbol{\Theta}_\delta^T(k) = \left(a_1'\ a_0'\ b_0'\right) \qquad (17)$$

can be recursively estimated from the ARX model

$$\delta^2 y(k-2) = \boldsymbol{\Theta}_\delta^T(k)\boldsymbol{\Phi}_\delta(k-1) + \varepsilon(k) \qquad (18)$$

8 Control System Design

The control system with two feedback controllers is considered as shown in Fig. 5. Here, w is the reference signal, v denotes the load disturbance, e is the tracking error, u_0 is the output of the controller, y is the controlled output and u is the control input.

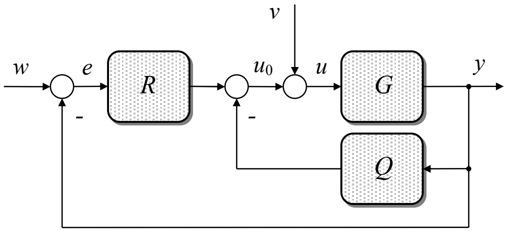

Figure 5. Control system with two feedback controllers.

In general therms, G represents an ELM with the transfer function

$$G(s) = \frac{b(s)}{a(s)} \tag{19}$$

and, Q and R are feedback controllers with transfer functions

$$Q(s) = \frac{\tilde{q}(s)}{\tilde{p}(s)}, \quad R(s) = \frac{r(s)}{\tilde{p}(s)} \tag{20}$$

where $\tilde{q}$ and $\tilde{p}$ are polynomials in s. Both w and v are considered to be step functions with transforms

$$W(s) = \frac{w_0}{s}, \; V(s) = \frac{v_0}{s}. \tag{21}$$

The controller design appears from the polynomial approach and the pole assignment method. The resulting controllers obtained by a solution of polynomial equations ensure the control system internal properness and stability as well as asymptotic tracking of step references and step load disturbance attenuation.

The procedure to obtain admissible controllers can be briefly described as follows:

Establishing the polynomial t as

$$t(s) = r(s) + \tilde{q}(s) \tag{22}$$

the control system stability is ensured when polynomials $\tilde{p}$ and t are given by a solution of the polynomial Diophantine equation

$$a(s)\tilde{p}(s) + b(s)\,t(s) = d(s) \tag{23}$$

with a stable polynomial d on the right side. Evidently, the roots of d determine poles of the closed-loop.

Taking into account the transform of the tracking error

$$E(s) = \frac{1}{d}\left[(a\tilde{p} + b\tilde{q})W(s) - b\tilde{p}\,V(s)\right] \tag{24}$$

and both transforms (20), the asymptotic tracking and load disturbance attenuation are provided by polynomials $\tilde{p}$ and $\tilde{q}$ having the form

$$\tilde{p}(s) = s\,p(s), \;\; \tilde{q}(s) = s\,q(s). \tag{25}$$

Then, the transfer functions of controllers (20) take forms

$$Q(s) = \frac{q(s)}{p(s)}, \quad R(s) = \frac{r(s)}{s\,p(s)}. \tag{26}$$

A stable polynomial $p(s)$ in denominators of (26) (excepting the integrating part) ensures the stability of controllers.

Now, the polynomial t can be rewritten into the form

$$t(s) = r(s) + s\,q(s). \tag{27}$$

Taking into account solvability of (23) and condition of internal properness of the control system, the degrees of polynomials in (23) and (27) can be easily derived as

$$\deg t = \deg r = \deg a, \;\; \deg q = \deg a - 1,$$
$$\deg p \geq \deg a - 1, \;\; \deg d \geq 2\deg a. \tag{28}$$

Denoting deg $a = n$, polynomials t, r and q have forms

$$t(s) = \sum_{i=0}^{n} t_i s^i, \; r(s) = \sum_{i=0}^{n} r_i s^i, \; q(s) = \sum_{i=1}^{n} q_i s^{i-1} \tag{29}$$

where their coefficients fulfill equalities

$$r_0 = t_0, \;\; r_i + q_i = t_i \;\text{ for }\; i = 1,\ldots,n \tag{30}$$

Then, unknown coefficients r_i and q_i can be obtained by a choice of selectable coefficients $\beta_i \in \langle 0,1 \rangle$ such that

$$r_i = \beta_i t_i, \;\; q_i = (1-\beta_i)\,t_i \;\text{ for }\; i = 1,\ldots,n. \tag{31}$$

The coefficients β_i split a weight between numerators of transfer functions Q and R.

The controller parameters then follow from solution of the polynomial equation (23) and depend upon coefficients of the polynomial d.

For the second order model (12) with $\deg a = 2$, the controller's transfer functions take specific forms

$$Q(s) = \frac{q_2 s + q_1}{s + p_0}, \quad R(s) = \frac{r_2 s^2 + r_1 s + r_0}{s\,(s + p_0)} \tag{32}$$

where

$$r_1 = \beta_1 t_1, \; r_2 = \beta_2 t_2, \; q_1 = (1-\beta_1)\,t_1,$$
$$q_2 = (1-\beta_2)\,t_2. \tag{33}$$

In this paper, the polynomial d with roots determining the closed-loop poles is chosen as

$$d(s) = n(s)\,(s+\alpha)^2 \tag{34}$$

where n is a stable polynomial obtained by spectral factorization

$$a^*(s)\,a(s) = n^*(s)\,n(s) \tag{35}$$

and α is the selectable double pole.

Note that a choice of d in the form (34) provides the control of a good quality for aperiodic controlled processes.

Now, it follows from the above introduced procedure that tuning of the controllers can be performed by a suitable choice of selectable parameters β and α.

9 Simulation Results

The control simulations for the reactant output temperature are shown in Figs. 6 – 8. Simulations were performed in the neighbourhood of the operating point $q_c^s = 0.27\ \mathrm{m}^3/\mathrm{s}$, $T_{rout}^s = 326.10\,\mathrm{K}$.

For the start (the adaptation phase), a P controller with a small gain was used in all simulations.

The effect of the pole α on the control responses is transparent from Fig. 6 and 7. Here, two values of α were selected. The control results show sensitivity of the controlled output and control input to α. Obviously, careless selection of this parameter can lead to oscillatory controlled output or even to unstability. Further, a increasing α leads to higher values and changes of the control input. The effect of β_2 on the controlled output is shown in Fig. 8.

The control simulations for the reactant mean temperature shown in Figs. 9 – 14 were performed in the neighbourhood of the operating point $q_c^s = 0.27\ \mathrm{m}^3/\mathrm{s}$ and $T_m^s = 334.44\,\mathrm{K}$ under the same references and constraints on the control input as in the previous case. Present results again demonstrate an possibility to determine a form and speed of the controlled output as well as an amplitude of the control input and its changes. For instance, the control inputs in Figs. 12 and 14 show their high sensitivity to a choice of the parameters β. This fact may be very important in a practical control.

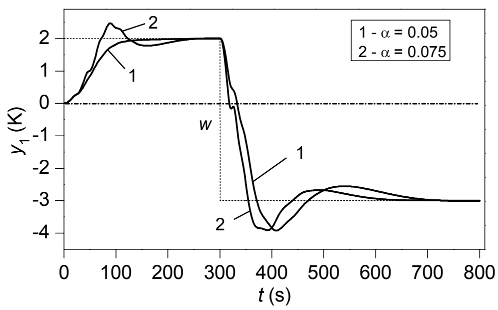

Figure 6. Controlled output y_1 – dependence on α.($\beta_1 = \beta_2 = 1$).

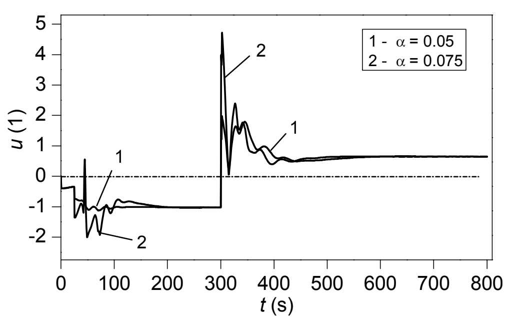

Figure 7. Control input – dependence on α ($\beta_1 = \beta_2 = 1$).

Conclusions

In this paper, one approach to the continuous-time

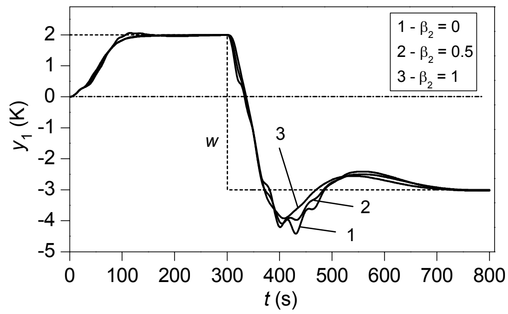

Figure 8. Controlled output y_1 – effect of β_2 (β_1= 1).

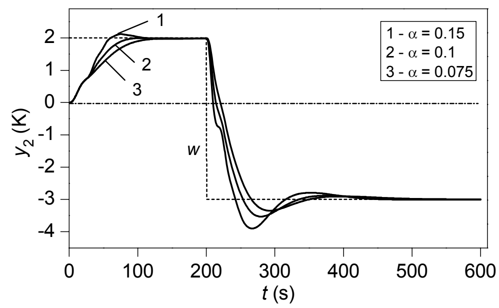

Figure 9. Controlled output y_2 – dependence on α ($\beta_1 = \beta_2 = 1$).

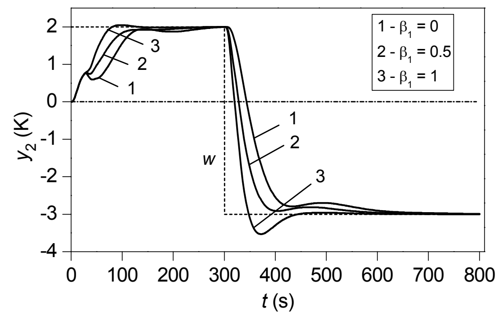

Figure 10. Controlled output y_2 – effect of β_1 (β_2= 0).

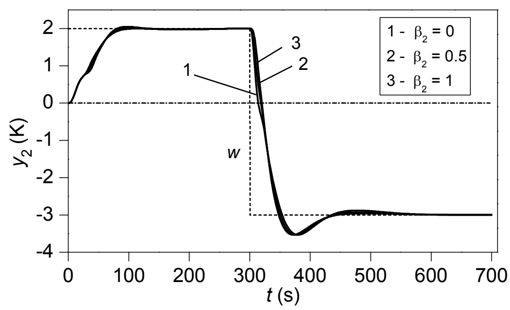

Figure 11. Controlled output y_2 – effect of β_2 (β_1= 0).

adaptive control of the output and mean reactant temperatures in a tubular chemical reactor was proposed. The control strategy is based on a preliminary steady-state and dynamic analysis of the process behaviour and on the assumption of the temperature measurement at the output as well as along the reactor. The proposed algorithm employs an alternative continuous-time external linear model with parameters obtained through recursive parameter estimation of a corresponding delta model. The resulting continuous-time controllers are derived using the polynomial approach and given by a solution of a polynomial Diophantine equation. Tuning of their parameters is possible either via the parameter affecting the closed-loop poles or by a choice of selectable coefficients splitting a weight between numerators of controllers' transfer functions. The presented method has been tested by computer simulation on the nonlinear model of the tubular chemical reactor with a consecutive exothermic reaction. The results demonstrate the applicability of the presented control strategy.

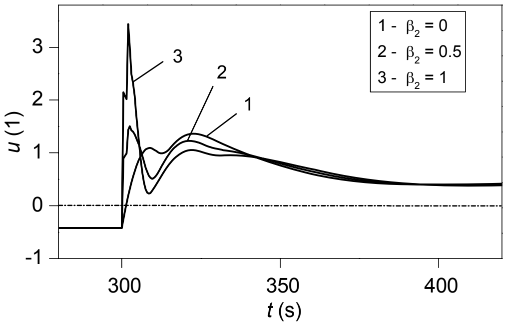

Figure 12. Control input – effect of β_2 (β_1= 0).

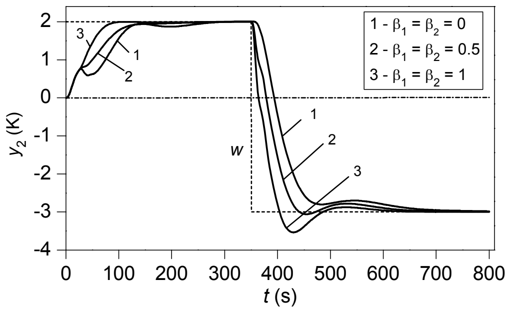

Figure 13. Controlled output y_2 – effect of β_1, β_2.

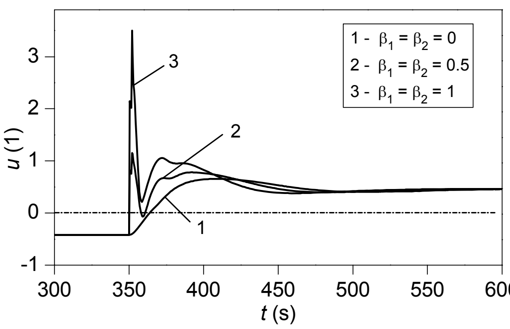

Figure 14. Control input – effect of β_1, β_2.

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