

# Robust controller design for temperature tracking problems in jacketed batch reactors

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## Abstract

There is an increasing trend to employ advanced instrumentation and control strategies for batch processes where expensive products are being manufactured. In this paper, a robust nonlinear control strategy is developed for temperature tracking problems in batch reactors in the presence of parametric uncertainty. The controller has a multi-loop feedback configuration. An inner loop is designed for *approximate* input–output linearization of a nominal plant. The outer loop is designed for stability and robust performance by utilizing results from structured singular values ( $\mu$ -synthesis). It is shown via simulation of a temperature tracking problem in batch synthesis that the controller provides excellent tracking despite parametric uncertainty. © 2001 Elsevier Science Ltd. All rights reserved.

**Keywords:** Batch process; Robust nonlinear control; Temperature tracking

## 1. Introduction

Batch reactors are frequently used in the production of fine chemicals. The batch mode of operation is preferred when the production volume is low, when isolation is required for reasons of sterility or safety, and when the materials involved are hard to handle.

In batch processes, no material is added or removed during the course of the batch run; consequently, a large majority of batch control problems involve *temperature* control via a heating/cooling system. The batch temperature is typically regulated by using a jacket around the reactor in which a hot or cold fluid is circulated [1]. Control is achieved by manipulating the heat content from the jacket to the reactor.

In the past, the total value of products made in the batch mode was small and batch reactors were operated in open-loop fashion with very little instrumentation [2]. However, in the last decade, many chemical producers have moved from the relatively stable world of continuous plant

production to the more turbulent environment of multiproduct batch production in order to better adjust to changing market conditions [1]. Furthermore, for several high value products in the biotechnology and polymer industry, a shift in attitude from “quality means high purity” to “quality means low variability around a specification target” has been clearly observed [3]. This has provided the motivation for research in monitoring and control in batch reactors where the same trajectory needs to be followed from batch to batch. This trajectory is decided a priori either from plant experience or by solving a robust optimization problem [2].

In the area of process monitoring, there has been significant activity in academia as well as industry in developing new sensors for measuring or estimating reactor concentration in the past decade. For instance, the use of on-line mass spectrometry for measuring off-gas concentration is now standard practice in large-scale fermentors [4] and is used as a measure for cell mass concentration. Enzyme based biosensors are commonly used to quantify glucose and other components in bioreactors [5,6]. Advances in infra-red spectroscopy have made it possible to monitor organic species concentration on-line in a variety of applications [7–10]. The use of Raman spectroscopy to monitor complex chemical

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*Acronyms*

PMMA	Polymethylmethacrylate
MMA	Methylmethacrylate
AIBN	Azobisisobutyronitrile

I/O	Input/Output
PID	Proportional-integral-derivative
LF	Linear fractional
LFT	Linear fractional transformation

reactions has been effectively demonstrated in biological fermentations [11,12], inorganic reactions [13] as well as polymerization [14]. This development of sensor hardware has been accompanied by parallel research in software sensors. These sensors are designed on the basis of a mathematical model and can provide reliable on-line information on the process state variables. For instance, Schiler and Papadopoulou [15] developed a decoupled nonlinear estimator based on an Extended Kalman Filter for the real-time estimation of the chain-length distribution and conversions in a batch polystyrene reactor. Ellis et al. [16] applied a two-time-scale filtering technique to estimate the temperature, monomer conversion, initiator conversion, and the entire molecular weight distribution in a methyl methacrylate batch polymerization. Stephanopoulos and San [17] demonstrated the use of Kalman filtering to estimate the specific growth rate and cell mass in a batch fermentation using on-line off-gas data. A recent review of application of software sensors to chemical processes can be found in [18].

The availability of advanced instrumentation, especially of expensive products, has led to an increasing interest in developing advanced control strategies for temperature tracking problems in batch reactors. For instance, Ponnuswamy et al. [19] developed a linear quadratic regulatory controller designed on the basis of a linearized system for temperature control of a PMMA batch reactor. Tzounas and Shah [20] developed a discrete, adaptive pole-assignment control algorithm for batch polymerization. Soroush and Kravaris [21] utilized the input/output (I/O) framework in conjunction with an external PID controller to derive a globally linearizing controller for batch PMMA synthesis. Lakshmanan and Arkun [22] developed a self-scheduling, model predictive control technique by using multiple linear models, based on Extended Kalman Filtering and time varying parameters, and tested it, via simulation, on a semi-batch polymerization reactor.

In all these studies, it is necessary to have an accurate process model, or have closed-loop parameter estimation schemes in conjunction with the controller. However, in industrial batch processes, while the basic model *structure* can be developed from first principles, accurate values of kinetic parameters as well as the heat transfer coefficients are usually not available. In this paper, a novel methodology is presented for the design of a robust controller for tracking a pre-determined temperature trajectory in a batch reactor which accounts for parametric uncertainty in the kinetic parameters as well as the heat transfer coefficients.

The organization of the paper is as follows. In Section 2, the temperature trajectory tracking problem is formulated for a generalized jacketed batch reactor with arbitrary reaction kinetics. Plant-model mismatch due to uncertainty in the heat transfer coefficients as well as kinetic parameters are discussed. In Section 3, a multi-loop controller design methodology is presented. In this technique, the inner loop uses a *nominal* model, based on *nominal* parameter values, to *approximately* linearize the system in an input/output (I/O) sense. The outer loop is designed for both robust stability as well as nominal performance using recent results from robust control theory. In Section 4, this methodology is illustrated via simulation of the synthesis of polymethylmethacrylate (PMMA) in a batch reactor. Finally, in Section 5, conclusions of this work are discussed.

## 2. Problem formulation

The dynamics of a generalized jacketed batch reactor are given as follows:

$$\frac{d}{dt} \begin{bmatrix} x \\ T \\ T_j \end{bmatrix} = \begin{bmatrix} r(x, T, \theta) \\ s(x, T, \theta) - \alpha_1(T - T_j) \\ \alpha_2(T - T_j) + \alpha_3(T_\infty - T_j) \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ m \end{bmatrix} u \quad (1)$$

$$y = T \quad (2)$$

where the parameters  $\alpha_1$ ,  $\alpha_2$ , and  $\alpha_3$  are given by

$$\begin{aligned} \alpha_1 &= \frac{U_{ri}A_i}{m_r C_{pr}} \\ \alpha_2 &= \frac{U_{r0}A_0}{\rho_j V_j C_{pj}} \\ \alpha_3 &= \frac{U_j A_j}{\rho_j V_j C_{pj}} \end{aligned} \quad (3)$$

Here,  $x$  represents a vector of the states of the reaction (typically concentrations of reactants, intermediates, and products),  $T$  and  $T_j$  represent the reactor temperature and the jacket temperature, respectively, and  $T_\infty$  is the ambient temperature. The manipulated input,  $u$ , is the net heat (in units of power) added to the jacket using a combination of cooling water and electric heaters as shown in Soroush and Kravaris [21]. The

term  $U_{ri}$  represents the heat transfer coefficient between the reactor and jacket based on the inner area,  $U_{ro}$  represents the heat transfer coefficient between the reactor and jacket based on the outer area and  $U_j$  is the heat transfer coefficient between the jacket and surrounding. The terms  $A_i$  and  $A_0$  represent the inner and outer surface areas of the reactor and  $A_j$  represents the outer surface area of the jacket. The term  $m_r$  represents the mass of fluid in the reactor and  $C_{pr}$  and  $C_{pj}$ , the respective heat capacities of the fluids in the reactor and the jacket. The term  $m$  is the inverse of the heat capacity of the mass in the reactor. The vector  $r$  represents the kinetics of the reactions occurring in the reactor and  $s$  represents the heat generation due to reaction. The vector  $r$  represents the vector of kinetic parameters in the vector  $r$  and scalar  $s$  in Eq. (1).

In an engineering context, the basic model *structure* of Eq. (1) is chosen from first-principles considerations; however, the model *parameters* are computed so that the model predictions best fit the data. As most modeling runs are conducted on bench-scale reactors, there is plant-model mismatch in the production scale reactors due to changes in surface to volume ratio, mixing, wall catalysis, heat balance inaccuracies and unmeasured impurities [2]. In the specific model represented by Eq. (1), two sources of parametric uncertainty are considered:

1. *Uncertainty in heat transfer coefficients:* Due to imperfect mixing, the concentrations of the various reacting species will be non-uniform, especially near the reactor wall. Since each of these species has different heat conduction properties, the heat transfer coefficient between the heating/cooling fluid and the reaction mass will not be uniform over the entire heating surface. Also, it is not possible to precisely measure the value of the heat transfer coefficient on-line with present sensor technology. It may only be estimated empirically. This uncertainty in the exact value of the heat transfer coefficient may lead to a loss in controller performance.
2. *Uncertainty in kinetic parameters:* There are a large number of kinetic parameters in the functions  $r$  and  $s$  in Eq. (1) which need to be estimated from limited laboratory data. Due to changes in mass transfer characteristics in the production scale reactor, the apparent kinetic parameters may not match the values extracted from the bench scale reactor [23]. This uncertainty in kinetic parameter values can affect the performance of a controller designed on the basis of the process model.

### 3. Robust controller design

The control problem that we consider is the design of a controller that tracks a given temperature trajectory despite uncertainty in the model parameters,  $\theta$  and  $\alpha_i$ .

This control problem is considered under the following assumptions:

1. The *structure* of the reaction kinetics,  $r(x, T, \theta)$  and the reaction heat  $s(x, T, \theta)$  are known but the *exact parameter values* are not known.
2. The upper and lower bounds on the parameters  $\theta$  and  $\alpha_i$  are known and their allowable values represented by the sets  $\Theta$  and  $\alpha_i$ , respectively.
3. The system (1) is I/O linearizable with a well defined relative degree for all  $\theta \in \Theta$  and  $\alpha_i \in \alpha_i$ .
4. Measurements or estimates of the state  $(x, T, T_j)$  are available.

It can be easily shown that the system described by (1) has a relative degree of (2). The diffeomorphism

$$\begin{bmatrix} \eta \\ \zeta_1 \\ \zeta_2 \end{bmatrix} = \begin{bmatrix} x \\ T \\ s(x, T, \theta) - \alpha_1(T - T_j) \end{bmatrix} \quad (4)$$

transforms the system described by (1) into the following normal form:

$$\dot{\eta} = r(\eta, \zeta_1, \theta) \quad (5)$$

$$\begin{aligned} \dot{\zeta}_1 &= \zeta_2 \\ \dot{\zeta}_2 &= a(\eta, \zeta_1, \theta, \alpha_i) + (\alpha_1 m)u \end{aligned} \quad (6)$$

where

$$\begin{aligned} a(\eta, \zeta, \theta, \alpha_i) &= \frac{\partial s}{\partial \eta} \cdot r(\eta, \zeta_1, \theta) - (\alpha_1 + \alpha_2 + \alpha_3)\zeta_2 - \alpha_1\alpha_3\zeta_1 \\ &+ \frac{\partial s}{\partial \zeta_1} \cdot \zeta_2 + (\alpha_1 + \alpha_3)s(\eta, \zeta_1, \theta) + \alpha_1\alpha_3T_\infty \end{aligned} \quad (7)$$

If the values of the parameters,  $\theta$  and  $\alpha_i$ , are known exactly, the nonlinear term  $a$  in the last equation of (6) can be cancelled off via state feedback. This results in a linear subsystem that can be designed for performance via pole placement. However, if the parameters,  $\theta$  and  $\alpha_i$ , are not precisely known, the diffeomorphism (4) has to be based on some nominal values  $\theta_0$  and  $\alpha_{i0}$ . Due to this, the nonlinear term,  $a$  is not exactly cancelled off which could lead to performance degradation if a conventional I/O design is used. Since bounds on the uncertain parameters can often be estimated, this information can be used to reduce performance degradation and robustness. This provides the motivation for using robust control techniques to account for this parametric uncertainty.

The issue of robust controller design in the I/O framework has attracted attention in the literature in the past decade. When the uncertainty in the model appears with the same relative degree as the control input, Kravaris

and Palanki [24] and Chou and Wu [25] developed Lyapunov based robust control strategies in the I/O linearization framework. Alternatively, if the uncertainty is predominantly parametric, adaptive control has been proposed by Marino et al. [26].

In this paper, we characterize the uncertainty due to inexact linearization in a suitable manner so that linear robust control techniques can be used in the outer loop. This approach does not require restrictive matching conditions (as in Kravaris and Palanki [24] and Chou and Wu [25]) and is thus applicable to a wider class of I/O linearizable systems. It is first shown how (1) is transformed if nominal values of the parameters  $\theta$  and  $\alpha_i$  are used. Then, the transformed uncertain system is characterized in a convenient, approximate linear form. Finally, a robust controller is designed for this system using structural singular value ( $\mu$  synthesis) techniques.

Consider the system represented by (1) with uncertainty in the parameters  $\theta$  and  $\alpha_i$ . Suppose that the nominal values of these uncertain parameters is  $\theta_0$  and  $\alpha_{i0}$ . Then, the *uncertain* system (1) can be characterized in terms of the *nominal* parameters,  $\theta_0$  and  $\alpha_{i0}$ , and an *additive* model for uncertainty as follows:

$$\begin{bmatrix} r(x, T, \theta) \\ s(x, T, \theta) - \alpha_1(T - T_j) \\ \alpha_2(T - T_j) + \alpha_3(T_\infty - T_j) \end{bmatrix} = \begin{bmatrix} r_0(x, T) \\ s_0(x, T) - \alpha_{10}(T - T_j) \\ \alpha_{20}(T - T_j) + \alpha_{30}(T_\infty - T_j) \end{bmatrix} + \begin{bmatrix} \delta r \\ \delta s - \delta\alpha_1(T - T_j) \\ \delta\alpha_2(T - T_j) + \delta\alpha_3(T_\infty - T_j) \end{bmatrix} \quad (8)$$

where  $r_0$  and  $s_0$  refer to the function values of  $r$  and  $s$  at the nominal values of the parameters and  $\delta r$  and  $\delta s$  refer to the deviation of the functions  $r$  and  $s$  from the nominal. We show in the theorem below that the uncertain system (1) under state feedback based on *nominal* values of the parameters  $\theta$  and  $\alpha_i$  results in a linear uncertain sub-system.

**Theorem 1.** *System (1) with an additive model of uncertainty of the form of (8) under the nominal transformation*

$$\begin{bmatrix} \eta \\ \zeta_1 \\ \zeta_2 \end{bmatrix} = \begin{bmatrix} x \\ T \\ s_0(x, T) - \alpha_{10}(T - T_j) \end{bmatrix} \quad (9)$$

and the nominal feedback law:

$$u = \frac{1}{\alpha_{10}m}(-a_0(\eta, \zeta) + v) \quad (10)$$

results in a linear uncertain subsystem of the form:

$$\begin{aligned} \dot{\zeta} &= A(\rho)\zeta + Bv + w_d d \\ y &= C\zeta \end{aligned} \quad (11)$$

where  $a_0$  is the function value of  $a$  at the nominal parameter values,  $\theta_0$  and  $\alpha_{i0}$ ,  $w_d$  is a linear time invariant weight,  $\|d_i\|_2 \leq 1$  are the non-linear perturbations represented as external bounded disturbances,  $v$ ,  $A$ ,  $B$ , and  $C$  are matrices of appropriate dimensions and  $\rho$  is the vector of uncertain parameters in the matrix  $A$ .

**Proof.** Define the following vectors:

$$f_0 = \begin{bmatrix} r_0(x, T) \\ s_0(x, T) - \alpha_{10}(T - T_j) \\ \alpha_{20}(T - T_j) + \alpha_{30}(T_\infty - T_j) \end{bmatrix} \quad (12)$$

$$\delta f = \begin{bmatrix} \delta r \\ \delta s - \delta\alpha_1(T - T_j) \\ \delta\alpha_2(T - T_j) + \delta\alpha_3(T_\infty - T_j) \end{bmatrix} \quad (13)$$

$$f = \begin{bmatrix} r(x, T, \theta) \\ s(x, T, \theta) - \alpha_1(T - T_j) \\ \alpha_2(T - T_j) + \alpha_3(T_\infty - T_j) \end{bmatrix} \quad (14)$$

$$g = \begin{bmatrix} 0 \\ 0 \\ m \end{bmatrix} \quad (15)$$

$$h = T \quad (16)$$

Applying the nominal coordination transformation (9) on Eq. (1) results in the following system:

$$\begin{aligned} \dot{\eta} &= r_0(\eta, \zeta_1) + \delta_r \\ \dot{\zeta}_1 &= \zeta_2 + \Delta_1 \\ \dot{\zeta}_2 &= \alpha_0 + \Delta_2 + (\alpha_{10}m)u \\ y &= \zeta_1 \end{aligned} \quad (17)$$

where

$$\begin{aligned} \Delta_1 &= L_{\delta f} h \\ \Delta_2 &= L_{\delta f} L_f h \\ a_0 &= L_{f_0}^2 h \end{aligned} \quad (18)$$

Applying the nominal state feedback, (10) to Eq. (17) results in the following system:

$$\begin{aligned} \dot{\eta} &= r_0(\eta, \zeta_1) + \delta_r \\ \dot{\zeta}_1 &= \zeta_2 + \Delta_1 \\ \dot{\zeta}_2 &= \Delta_2 + v \\ y &= \zeta_1 \end{aligned} \quad (19)$$

By a formal Taylor's series expansion, we write

$$\Delta_1 = \delta_{11}(\theta, \alpha_i)\zeta_1 + \delta_{12}(\theta, \alpha_i)\zeta_2 + \tilde{\delta}_1(\eta, \zeta, \theta, \alpha_i) \quad (20)$$

$$\Delta_2 = \delta_{21}(\theta, \alpha_i)\zeta_1 + \delta_{22}(\theta, \alpha_i)\zeta_2 + \tilde{\delta}_2(\eta, \zeta, \theta, \alpha_i) \quad (21)$$

where  $\delta_{11}$ ,  $\delta_{12}$ ,  $\delta_{21}$ ,  $\delta_{22}$  are the first order terms with respect to  $\zeta_1$  and  $\zeta_2$  in the Taylor series expansion and  $\tilde{\delta}_1$  and  $\tilde{\delta}_2$  contain the higher order terms. Then the last three equations of the system (19) can be put in the following form:

$$\frac{d}{dt} \begin{bmatrix} \zeta_1 \\ \zeta_2 \end{bmatrix} = \begin{bmatrix} \delta_{11}(\theta, \alpha_i) & \delta_{12}(\theta, \alpha_i) \\ \delta_{21}(\theta, \alpha_i) & \delta_{22}(\theta, \alpha_i) \end{bmatrix} \begin{bmatrix} \zeta_1 \\ \zeta_2 \end{bmatrix} + \begin{bmatrix} 0 \\ 1 \end{bmatrix} v + \begin{bmatrix} \tilde{\delta}_1 \\ \tilde{\delta}_2 \end{bmatrix} \quad (22)$$

$$y = \zeta_1 \quad (23)$$

This is of the form of Eq. (11)

With the uncertain linearized system, (22) and (23), it is now possible to use linear robust control theory for designing stabilizing controllers. The following three step procedure is followed.

### Step 1. Reduction to standard form

A linear fractional representation (LFR) of the uncertain system is found using the procedure given in Cockburn and Morton [27]. This is necessary to pull-out the uncertain parameters from the state-space equations into a block diagonal perturbation to obtain an equivalent system where the state-space matrices do not depend on the uncertain parameters. The closed loop system is then reduced to the standard feedback form shown in Fig. 1. The  $P$ -block represents the interconnection of the linearized nominal system, scaling weights and performance weights.  $\Delta_u$  represents the parametric and unstructured uncertainty in the system. Nominal performance is represented as an  $H_\infty$  norm constraint by connecting the exogenous inputs and outputs with a performance block

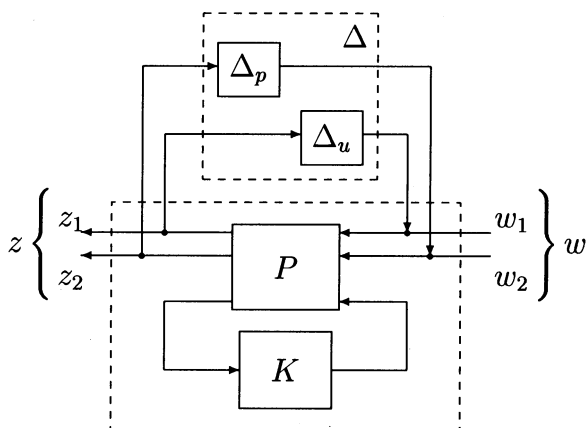


Fig. 1. General interconnection structure for  $\mu$ -synthesis.

$\Delta_p$  which is absorbed into the perturbation block  $\Delta = \text{diag}(\Delta_p, \Delta_u)$  represents the controller to be designed.  $w_2$  represents the exogenous input signals which include the desired tracking signals and disturbances (if any).  $z_2$  represents the output “errors” which typically includes weighted error signals to be minimized.

The block-diagonal uncertainty block  $\Delta_u$  is determined by  $\delta_{11}$ ,  $\delta_{12}$ ,  $\delta_{21}$  and  $\delta_{22}$  in (22). The input vector  $w_2$  is determined by the temperature setpoint and two disturbance inputs induced by  $\tilde{\delta}_1$  and  $\tilde{\delta}_2$ . The output vector  $z_2$  is determined by the tracking error signal, that is, the difference between setpoint and reactor temperature and the control signal generated by the controller  $K$ . In addition scaling weights are chosen so that the norm on the input and output signals is unity. Performance weights are chosen to determine the desired tracking accuracy and the bandwidth of the controller. For more details see Section 4.

### Step 2. Controller design via optimization

The controller design is posed as the following min-max optimization problem:

Find a stabilizing controller  $K$  such that  $\|T_{z_2w_2}\|_\infty$  is minimized over all perturbations  $\Delta_u \in \Delta_u$

where  $T_{z_2w_2}$  is the transfer function from  $w_2$  to  $z_2$  and  $\Delta_u$  is the set of allowable perturbations determined by the nature and size of the uncertainty. Here  $\Delta_u = \text{diag}(\theta I_{n_0}, \alpha_1 I_{n_1}, \alpha_2 I_{n_2}, \alpha_3 I_{n_3}, \alpha_4 I_{n_4})$  where  $I_{n_i}$  is the  $n_i \times n_i$  identity matrix and  $n_i$  is determined by the Linear Fractional Representation of the uncertainty. The bounding set  $\Delta_u$  defines the range of values that each uncertain parameter or block is allowed to take and is determined by  $\theta$  and  $\alpha_i$ ,  $i = 1, \dots, 3$ .

This problem is equivalent to finding a stabilizing controller that minimizes  $\mu_\Delta(T_{z_w})$ , the structured singular value of  $T_{z_w}$  with respect to  $\Delta = \text{diag}(\Delta_u, \Delta_p)$  where  $\Delta_p$  is a full complex matrix with dimensions determined by  $w_2$  and  $z_2$  [28]. Since the computation of the structured singular value is NP-hard, in practice a controller is designed to minimize the standard upper bound on the structured singular value,  $\hat{\mu}_\Delta(T_{z_w}) \inf_{D \in \Delta'} \|DT_{z_w}D^{-1}\|_\infty$  where  $\Delta'$  is the set of all LTI stable systems with stable inverse that commute with  $\Delta$ . Since  $T_{z_w} = \mathcal{F}_l(P, K)$ , for continuous LTI systems

$$\hat{\mu}_\Delta(T_{z_w}) = \sup_{\omega} \inf_{D \in \Delta'} \bar{\sigma}\{D\mathcal{F}_l(P, K)D^{-1}(j\omega)\} \quad (24)$$

For fixed  $K$  and  $\omega$ , this problem is convex in  $D$  and for fixed  $D$  it is convex in  $K$ . Synthesis of the controller is carried out by  $D$ - $K$  iteration, which is a practical approximation to  $\mu$ -synthesis [29]. The  $K$  step involves fixing  $D$  and finding a stabilizing controller  $K$  such that  $\|D\mathcal{F}_l(P, K)D^{-1}\|_\infty$  is minimized. This is a standard  $H_\infty$

optimization problem that can be solved using the results in Glover et al. [30] or Gahinet and Apkarian [31]. The  $D$  step involves fixing  $K$  and finding a matrix  $D_\omega$  that commutes with  $\Delta$ ; such that  $\bar{\sigma}\{D_\omega \mathcal{F}_l(\bar{G}, K)(j\omega) D_\omega^{-1}\}$  is minimized at each  $\omega \in \Omega$ , where  $\Omega$  is a frequency grid properly chosen and  $\bar{P}$  represents the new  $P$ -block with the  $D$  scales of previous iterations absorbed. This is a convex minimization problem that can be solved using the results of Fan and Tits [32]. The  $D$ - $K$  iterations are repeated until  $\hat{\mu}$  cannot be reduced further. The controller  $K$  corresponding to this (local) minimum is the desired stabilizing controller. If  $\hat{\mu} < \gamma$ , where  $\|\Delta\|_\infty \leq \gamma^{-1}$  then the controller is stabilizing and a successful design has been obtained.

*Step 3. Reduction of controller order via balanced residualization*

The controller,  $K$ , from step 2 is typically of a high order due to the dynamic  $D$  scales. Thus, it is customary to reduce the order of the controller. In this work, balanced residualization is used as it preserves the low frequency behavior of the controller [33,34]. The controller state-space matrix is first balanced with respect to the controllability and observability Gramians. This helps remove unobservable and/or uncontrollable modes. The balanced form is then residualized to the smallest possible order while preserving the  $\mu$  characteristics of the original controller.

**4. Illustrative example: synthesis of PMMA**

In this section, the robust nonlinear control methodology developed in the previous section will be implemented on a temperature tracking problem in the synthesis of PMMA in a batch reactor.

The synthesis of PMMA in a batch reactor has been studied extensively in the literature. The kinetic model structure for this process is available in the literature (see, for instance, [35] and the references therein). Vickers et al. [14] developed a sensor based on Raman spectroscopy for monitoring the concentration of both the monomer as well as polymer in real time.

The synthesis of PMMA in a batch reactor is modeled as follows [35]:

$$\frac{d}{dt} \begin{bmatrix} C_m \\ C_i \\ T \\ T_j \end{bmatrix} = \begin{bmatrix} \left(1 + \varepsilon \frac{C_m}{C_{m0}}\right) R_m \\ R_i + \varepsilon \frac{C_m}{C_{m0}} R_m \\ \frac{\alpha_0 k_P \xi_0 C_m}{1 + \varepsilon \frac{C_m}{C_{m0}}} - \alpha_1 (T - T_j) \\ \alpha_2 (T - T_j) + \alpha_3 (T_\infty - T_j) \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ 0 \\ m \end{bmatrix} u \tag{25}$$

where  $C_m$  and  $C_i$  are the concentrations of MMA and AIBN.  $R_m = -C_m \xi_0 (k_p + k_{fm})$  and  $R_i = -k_i C_i$  are the production rates of MMA and AIBN respectively.  $\xi_0$  is the concentration of the live polymer chains and is given by

$$\xi_0 = \sqrt{\frac{2fk_i C_i}{k_t}}$$

where  $f$  is the initiator efficiency.  $k_i$ ,  $k_p$ ,  $k_{fm}$  and  $k_t$  are the reaction rate constants for initiation, propagation, chain transfer to monomer, and termination, respectively. The gel and glass effects are included as

$$k_t = \frac{k_{t0}}{1 + \frac{\xi_0 k_{t0}}{Dk_{ot}}}$$

where

$$D = \exp\left(\frac{2.3(1 - \phi_p)}{A(T) + B(1 - \phi_p)}\right)$$

$\phi_p$ , the volume fraction of the polymer in the reactor, is given by

$$\phi_p = \frac{\frac{\mu_1}{\rho_p}}{\frac{\mu_1}{\rho_p} + \frac{C_m M_m}{\rho_m} + \frac{C_s M_s}{\rho_s}}$$

All other rate constants, except  $k_p$ , follow the Arrhenius law.  $\varepsilon$  is the volume expansion factor and is given by

$$\varepsilon = \phi_{m0} \left(\frac{\rho_m}{\rho_p}\right)$$

where  $\phi_{m0} = C_{m0} M_m / \rho_m$  is the volume fraction of the monomer at the start of reaction. The volume of the reacting mass changes as

$$V = V_0(1 + \varepsilon x_m)$$

where  $x_m$ , the fractional conversion of the monomer, is given by

$$x_m = \frac{1 - \frac{C_m}{C_{m0}}}{1 + \varepsilon \frac{C_m}{C_{m0}}}$$

$\alpha_0$ ,  $C_s$  and  $\mu_1$  are given by

$$\alpha_0 = \frac{(-\Delta H_p)V_0(1 + \epsilon)}{mC}$$

$$C_s = \frac{\phi_{s0}\rho_s}{M_s} \left( \frac{1 + \epsilon \frac{C_m}{C_{m0}}}{1 + \epsilon} \right)$$

and

$$\mu_1 = \frac{M_m}{1 + \epsilon} (C_{m0} - C_m)$$

The above model is in the form of Eq. (1) hence, the theory developed in the previous section can be applied directly. The objective of the controller is to track a pre-specified temperature trajectory despite parametric uncertainty. This desired temperature profile is maintained by circulating heating/cooling fluid in a jacket around the polymerization reactor.

PID controllers are a popular commercial choice for many process control applications. However, there is no systematic procedure (such as Ziegler–Nichols or Cohan-Coons method) to tune a conventional PID controller for this problem due to the absence of a steady state. One could perform exhaustive simulations and try various values of PID controller parameters to find a PID controller that results in desirable performance for all combinations of uncertainties in the process parameters. This procedure is not only time consuming, but also comes with no guarantees that such a PID controller could be found. This provides the motivation to use the systematic procedure developed in the previous sections to this tracking problem.

The reactor temperature profile determined in Krothapally and Palanki [36] will be used as the desired set-point trajectory to be tracked. Tracking this trajectory results in a weight average molecular weight of 400,000 which is the desired end-point specification. The loading concentrations of MMA and AIBN corresponding to this trajectory are 6.01 and 0.13 kmol m<sup>-3</sup> respectively. The values of the various model parameters used in this paper are taken from Soroush and Kravaris [21] and are listed in Table 1. In this paper, it is assumed that the parameters,  $\alpha_1$  and  $\alpha_2$ , and the propagation rate constant,  $k_p$ , are imprecisely known. A parametric sensitivity analysis was conducted and it was found that the above-mentioned parameters have a significant effect on the dynamics of the system.

For simulation of the plant, the following expressions for  $\alpha_1$ ,  $\alpha_2$  and  $k_p$  are used [35]

$$\alpha_1(x_m) = \alpha_{10}(1 + \epsilon x_m)[a + (1 - a)\exp(-\mathcal{B}x_m^c)] \quad (26)$$

where  $x_m$  is the monomer conversion;

Table 1  
Values of the model parameters

$k_{r0} = Z_{r0}\exp(\frac{-E_{r0}}{RT})$	$k_{p0} = Z_{p0}\exp(\frac{-E_{p0}}{RT})$
$k_{\theta t} = C_i(0)Z_{\theta t}\exp(\frac{-E_{\theta t}}{RT})$	$k_{\theta p} = Z_{\theta p}\exp(\frac{-E_{\theta p}}{RT})$
$k_{fm} = Z_{fm}\exp(\frac{-E_{fm}}{RT})$	$k_i = Z_i\exp(\frac{-E_i}{RT})$
$A(T) = 0.17 - 8.21 \times 10^{-6}(T - T_{gp})^2$	$B = 0.03$
$Z_{r0} = 9.8 \times 10^7 \text{ m}^3 \text{ kmol}^{-1} \text{ s}^{-1}$	$E_{r0} = 2.94 \times 10^3 \text{ kJ kmol}^{-1}$
$Z_{p0} = 4.92 \times 10^5 \text{ m}^3 \text{ mol}^{-1} \text{ s}^{-1}$	$E_{p0} = 1.83 \times 10^4 \text{ kJ kmol}^{-1}$
$Z_{\theta t} = 1.45 \times 10^{20} \text{ m}^3 \text{ kmol}^{-1} \text{ s}^{-1}$	$E_{\theta t} = 1.46 \times 10^5 \text{ kJ kmol}^{-1}$
$Z_{\theta p} = 3.02 \times 10^{13} \text{ m}^3 \text{ kmol}^{-1} \text{ s}^{-1}$	$E_{\theta p} = 1.17 \times 10^5 \text{ kJ kmol}^{-1}$
$Z_{fm} = 4.66 \times 10^9 \text{ m}^3 \text{ kmol}^{-1} \text{ s}^{-1}$	$E_{fm} = 7.45 \times 10^4 \text{ kJ kmol}^{-1}$
$Z_i = 1.05 \times 10^{15} \text{ s}^{-1}$	$E_i = 1.29 \times 10^5 \text{ kJ kmol}^{-1}$
$T_{gp} = 3.87 \times 10^2 \text{ K}$	$-\Delta H_p = 5.78 \times 10^4 \text{ kJ kmol}^{-1}$
$R = 8.35 \text{ kJ kmol}^{-1} \text{ K}^{-1}$	$\rho_i = 9.15 \times 10^2 \text{ kg m}^{-3}$
$M_i = 1.64 \times 10^2 \text{ kg kmol}^{-1}$	$f = 0.58$
$C = 2.2 \text{ kJ kg}^{-1} \text{ K}^{-1}$	$\rho_m = 9.15 \times 10^2 \text{ kg m}^{-3}$
$m = 1.26 \text{ kg}$	$\rho_p = 1.2 \times 10^3 \text{ kg m}^{-3}$
$\rho_s = 8.42 \times 10^2 \text{ kg m}^{-3}$	$M_s = 9.21 \times 10^1 \text{ kg kmol}^{-1}$
$M_m = 1.00 \times 10^2 \text{ kg kmol}^{-1}$	$\mathcal{B} = 7.0$
$V_0 = 1.34 \times 10^{-3} \text{ m}^3$	$T_\infty = 2.93 \times 10^2 \text{ K}$
$a = 0.2$	$\phi_{s0} = 0.3$
$c = 3.0$	$\alpha_{20} = 8.0 \times 10^{-4} \text{ s}^{-1}$
$\alpha_{10} = 3.8 \times 10^{-3} \text{ s}^{-1}$	$\alpha_4 = 6.64 \times 10^{-2} \text{ K kJ}^{-1}$
$\alpha_3 = 3.7 \times 10^{-4} \text{ s}^{-1}$	

$$k_p = \frac{k_{p0}}{1 + \frac{\xi_0 k_{p0}}{Dk_{\theta p}}} \quad (27)$$

$$\alpha_2(x_m) = \alpha_{20}(1 + \epsilon x_m)[a + (1 - a)\exp(-\mathcal{B}x_m^c)] \quad (28)$$

The controller is designed based on the nominal parameter values,  $\alpha_{1n}$ ,  $\alpha_{2n}$  and  $k_{pn}$ , which are given as follows:

$$\alpha_{1n} = 2.25 \times 10^{-3} \text{ s}^{-1} \quad (29)$$

$$k_{pn} = 112.0242 + 444.0225 \exp(-1.3C_m) \text{ m}^3 \text{ kmol}^{-1} \text{ s}^{-1} \quad (30)$$

$$\alpha_{2n} = 4.5 \times 10^{-4} \text{ s}^{-1} \quad (31)$$

Scaling weights,  $W_{\alpha 1} = 1.75 \times 10^{-3} \text{ s}^{-1}$ ,  $W_{k_p} = 125.1769 \text{ m}^3 \text{ kmol}^{-1} \text{ s}^{-1}$  and  $W_{\alpha 2} = 3.5 \times 10^{-4} \text{ s}^{-1}$  are used to capture the bounds on  $\alpha_1$ ,  $k_p$ , and  $\alpha_2$  as

$$\alpha_1 = \alpha_{1n} + W_{\alpha 1} \delta_{\alpha 1} \quad (32)$$

$$k_p = k_{pn} + W_{k_p} \delta_{k_p} \quad (33)$$

$$\alpha_2 = \alpha_{2n} + W_{\alpha 2} \delta_{\alpha 2} \quad (34)$$

such that  $|\delta_{\alpha 1}| \leq 1$ ,  $|\delta_{k_p}| \leq 1$ , and  $|\delta_{\alpha 2}| \leq 1$ . In terms of the weights, the uncertainty in the plant becomes:

$$\delta f = \begin{bmatrix} -\left(1 + \varepsilon \frac{C_m}{C_{m0}}\right) C_m \xi_0 W_{kP} \delta k_P \\ -\left(\varepsilon \frac{C_m}{C_{m0}}\right) C_m \xi_0 W_{kP} \delta k_P \\ \frac{\alpha_0 \xi_0 C_m}{1 + \varepsilon \frac{C_m}{C_{m0}}} W_{kP} \delta k_P - (T - T_j) W_{\alpha 1} \delta \alpha_1 \\ (T - T_j) W_{\alpha 2} \delta \alpha_2 \end{bmatrix} \quad (35)$$

The uncertainty resulting from inexact linearization can be found by substituting the above expression in (18). The bounds on the parametric uncertainty are obtained using expressions (26), (27), and (28). However, in general, one would get bounds on the parametric uncertainty from experimental data or from operator experience in the absence of a high-fidelity model.

First, a controller based on a *conventional* I/O linearization is implemented, where it is assumed that there is no uncertainty in the parameters. An inner loop is designed by assuming nominal values for the parameters to linearize the plant and the two poles in the outer loop are placed at  $-0.1$ . Fig. 2. shows the results of this design.

It is found that when there is no uncertainty in the parameters (i.e.) both the plant as well as the controller have nominal values  $\alpha_{1n}$ ,  $\alpha_{2n}$  and  $k_{Pn}$ , the desired set-point trajectory is very well tracked and results in the desired weight average molecular weight of 400,000 at the end of the batch time. However, when the true parameter values,  $\alpha_1$ ,  $\alpha_2$  are  $k_P$  used in the plant while nominal values,  $\alpha_{1n}$ ,  $\alpha_{2n}$  and  $k_{Pn}$  are used in the controller, the set-

point is not well tracked which results in the production of “off-spec” product with a weight average molecular weight of 385,204. This provides the motivation to develop a robust controller that tracks the desired set-point despite parameter uncertainty.

Using Theorem 1, system (25) can be represented as the following uncertain linear system:

$$\frac{d}{dt} \begin{bmatrix} \zeta_1 \\ \zeta_2 \end{bmatrix} = A \begin{bmatrix} \zeta_1 \\ \zeta_2 \end{bmatrix} + \begin{bmatrix} 0 \\ 1 \end{bmatrix} v + \begin{bmatrix} d_1 \\ d_2 \end{bmatrix} \quad (36)$$

where

$$\begin{bmatrix} \zeta_1 \\ \zeta_2 \end{bmatrix} = \begin{bmatrix} T \\ L_{f0h} \end{bmatrix} = \begin{bmatrix} \frac{\alpha_0 k_{Pn} \xi_0 C_m}{1 + \varepsilon \frac{C_m}{C_{m0}}} T + \alpha_{1n} (T_j - T) \end{bmatrix} \quad (37)$$

and the expressions for  $A$ ,  $d_1$ , and  $d_2$  are given in the Appendix A.  $d_1$  and  $d_2$  are characterized as external disturbances. Using the values of the system parameters from Table 1, the limits on the states,  $[C_m \ C_i \ T \ T_j]^T$ , are determined by simulation. These values are used to determine the bounds,  $W_{d1}$ , and  $W_{d2}$  on the terms,  $d_1$  and  $d_2$ , and are found to be  $6.24 \times 10^{-1}$ , and,  $9.83 \times 10^{-4}$  respectively. Weights are chosen on the different signals for scaling and for capturing the desired accuracy of tracking. A performance weight,  $W_e$ , is attached to the exogenous output (error signal) and a scaling weight,  $W_w$ , is attached to the exogenous input (optimal trajectory). The weights used in this example, are

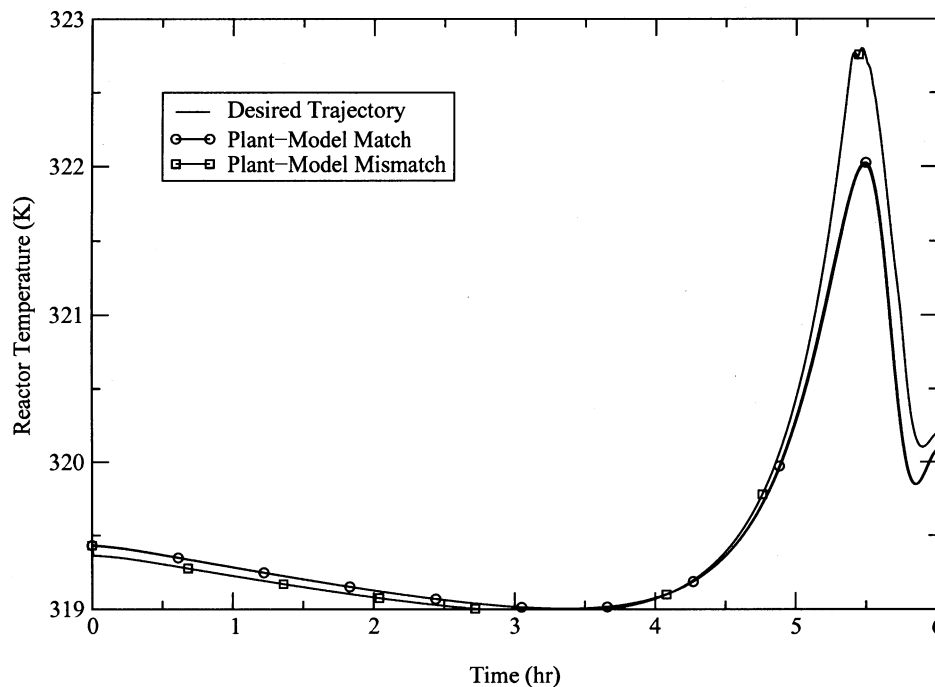


Fig. 2. Implementation of conventional I/O linearizing controller.

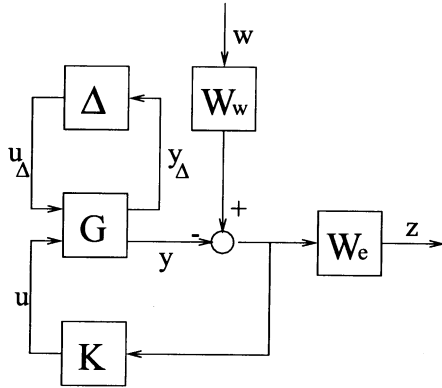


Fig. 3. Interconnection structure for the PMMA system ( $G$  = nominal linearized system).

$$W_e = \frac{s}{s + 10^{-4}} + 1, \quad W_w = 1. \quad (38)$$

The final interconnection structure is as shown in Fig. 3 is given by the interconnections of the  $G$ ,  $W_w$  and  $W_e$  blocks.  $G$  is the linearized nominal plant.

The dkit routine in the  $\mu$ -Analysis and Synthesis Toolbox [37] of MATLAB was used to design the stabilizing controller,  $K$ . Order reduction was performed using the sysbal and sresid routines. The resulting controller, is of the form

$$\begin{aligned} \dot{x}_K &= A_K \cdot x_K + B_K \cdot e \\ v &= C_K \cdot x_K + D_K e \end{aligned}$$

The following 4th-order controller results after model reduction.

$$A_K = \begin{bmatrix} -1.0 \times 10^{-4} & 1.7 \times 10^{-4} & 1.9 \times 10^{-1} & 1.4 \times 10^{-3} \\ -1.7 \times 10^{-4} & -1.7 \times 10^{-3} & -5.5 \times 10^2 & -2.9 \times 10^{-2} \\ 1.9 \times 10^{-1} & 5.5 \times 10^2 & -2.4 \times 10^3 & -3.3 \times 10^1 \\ 1.4 \times 10^{-3} & 2.9 \times 10^{-2} & -3.3 \times 10^1 & -8.9 \end{bmatrix}$$

$$B_K = \begin{bmatrix} -2.1 \\ -1.8 \\ 2.1 \times 10^3 \\ 1.5 \times 10^1 \end{bmatrix}$$

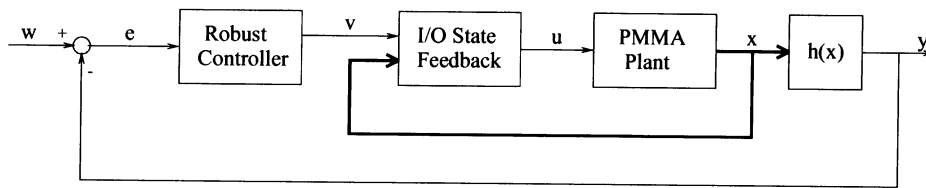


Fig. 4. Multi-loop structure for the implementation of the robust controller.

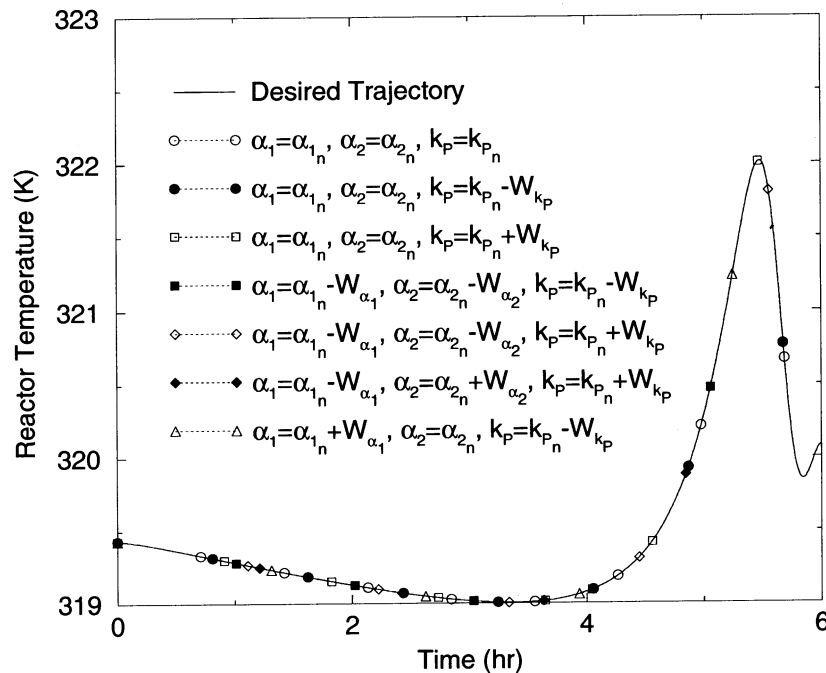


Fig. 5. Temperature profile obtained with robust controller for different values of the uncertain parameters.

$$C_K = [-2.1 \quad 1.8 \quad 2.1 \times 10^3 \quad 1.5 \times 10^1]$$

and

$$D_K = 1.5$$

This controller was implemented in a multi-loop control structure (Fig. 4) with an inner loop for the nominal I/O linearizing state feedback and an outer loop for the linear robust controller. Simulations were carried out for different values of uncertainties. It is clear from Fig. 5 that the robust controller provides excellent temperature tracking for a wide range of values of the uncertain parameters. Furthermore, the use of the robust controller resulted in a weight average molecular weight of 399,822 at the end of the batch which is very close to the desired value of 400,000.

## 5. Conclusions

In this paper, a robust multi-loop controller design technique has been developed for temperature tracking problems in jacketed batch reactors with parametric uncertainty. The inner loop *approximately* linearizes the system in an I/O sense. The outer loop is a robust controller which guarantees performance despite parametric uncertainty in the model. This methodology is illustrated in a simulation example of PMMA synthesis.

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## Appendix

$$A = \begin{bmatrix} -W_{\alpha_1} \delta_{\alpha_1} & 1 \\ \alpha_{2n} W_{\alpha_1} \delta_{\alpha_1} + \alpha_{1n} W_{\alpha_2} \delta_{\alpha_2} & \alpha_1 W_{k_p} \delta_{k_p} + \alpha_2 W_{\alpha_1} \delta_{\alpha_1} \end{bmatrix}$$

and

$$\alpha_1 = \frac{\alpha_0 C_m}{1 + \epsilon \frac{C_m}{C_{m_0}}} \frac{\partial}{\partial T} (\xi_0)$$

$$\alpha_2 = - \left( \frac{\alpha_0 C_m}{1 + \epsilon \frac{C_m}{C_{m_0}}} \frac{\partial}{\partial T} (k_{p_n} \xi_0) - \alpha_{1n} \right) \frac{1}{\alpha_{1n}} - 1$$

$$d_1 = \frac{\alpha_0 W_{k_p} \delta_{k_p} \xi_0 C_m}{1 + \epsilon \frac{C_m}{C_{m_0}}} + W_{\alpha_1} \delta_{\alpha_1} T_j$$

$$\begin{aligned} d_2 = & \left[ \left( 1 + \epsilon \frac{C_m}{C_{m_0}} \right) (-C_m W_{k_p} \delta_{k_p} \xi_0) \right] \alpha_0 \frac{\partial}{\partial C_m} \left( \frac{k_p \xi_0 C_m}{1 + \epsilon \frac{C_m}{C_{m_0}}} \right) \\ & + \left[ \left( 1 + \epsilon \frac{C_m}{C_{m_0}} \right) (-C_m k_{p_n} \xi_0) \right] \alpha_0 W_{k_p} \delta_{k_p} \frac{\partial}{\partial C_m} \left( \frac{\xi_0 C_m}{1 + \epsilon \frac{C_m}{C_{m_0}}} \right) \\ & + \left[ \frac{\alpha_0 W_{k_p} \delta_{k_p} \xi_0 C_m}{1 + \epsilon \frac{C_m}{C_{m_0}}} + W_{\alpha_1} \delta_{\alpha_1} (T_j - T) \right] \\ & \left[ \frac{\alpha_0 C_m}{1 + \epsilon \frac{C_m}{C_{m_0}}} \frac{\partial}{\partial T} (k_p \xi_0) - \alpha_1 \right] \\ & - \left( 1 + \epsilon \frac{C_m}{C_{m_0}} \right) (-C_m k_{p_n} \xi_0) \alpha_0 \frac{\partial}{\partial C_m} \left( \frac{k_{p_n} \xi_0 C_m}{1 + \epsilon \frac{C_m}{C_{m_0}}} \right) \frac{W_{\alpha_1} \delta_{\alpha_1}}{\alpha_{1n}} \\ & - W_{\alpha_2} \delta_{\alpha_2} T_j \alpha_1 + (-\alpha_{2n} T_j + \alpha_3 (T_\infty - T_j)) W_{\alpha_1} \delta_{\alpha_1} \\ & - (\alpha_{2n} (T - T_j) + \alpha_3 (T_\infty - T_j)) W_{\alpha_1} \delta_{\alpha_1}. \end{aligned}$$

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