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Nonlinear dynamic model reduction via quasilinearization /

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NONLINEAR DYNAMIC MODEL REDUCTION

VIA

QUASILINEARIZATION

by

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A B S T R A C T

The existing algorithms for nonlinear model reduction are very complicated. In this work a simple approach is presented which requires no extensive amount of computational effort and appears promising. The use of an identification technique (quasilinearization) along with a pseudosteady-state hypothesis is demonstrated to have successful application in nonlinear dynamic model reduction.

The proposed approach was applied to a twelve-equation model of a low-density polyethylene chemical reactor and resulted in a two-equation model which is in excellent agreement with the original system and exhibits significantly improved performance over a previously developed low-order model. Furthermore, quasilinearization was able to find a low-order model which approximated more than one dynamic response of the large scale system.

Although, no claims for a rigorous approach are made, this work supports the contention that quasilinearization can contribute to nonlinear model reduction. Its application in practical situations, can provide simple and accurate approximants suitable for off- and on-line control use.

Nomenclature

Notation

C_P	=	specific heat (0.57 kcal/kg. K)
E_I, E_P, E_T	=	activation energy (cal/mol)
f	=	initiator efficiency factor
$(-\Delta H)$	=	heat of polymerization (21.4 kcal/mol)
I^*	=	initiator concentration (mol/LT)
k_I, k_P, k_T	=	rate constants
M^*	=	monomer concentration (mol/LT)
P	=	pressure (atm)
Q	=	flow rate (LT/s)
Q_r	=	recirculating flow rate (LT/s)
t^*	=	time (sec)
T^*	=	temperature (K)
V	=	volume (LT)
λ^*	=	radicals concentration (mol/LT)
τ	=	residence time (s)

Subscripts

0	=	input conditions
1	=	volume 1

2	=	volume 2
3	=	volume 3
I	=	initiation
P	=	propagation
T	=	termination
R	=	reference condition

Superscripts

1	=	feed 1
2	=	feed 2
*	=	dimensional variable

Dimensionless Variables

ξ_i	=	$\frac{V_i}{V}$
ϵ	=	$\frac{Q_r}{Q_1+Q_2}$
α	=	$\frac{Q_1}{Q_1+Q_2}$
I	=	I^*/I_R^*
I_0	=	I_0^*/I_R^*
λ	=	λ^*/I_R^*
M	=	M^*/M_0^*

$$T = T^*/T_R^*$$

$$t = t^*/\tau$$

$$\gamma_I = E_I/RT_R^*$$

$$\gamma_P = E_P/RT_R^*$$

$$\gamma_T = E_T/RT_R^*$$

$$Da_I = k_I \exp(-\gamma_I)\tau I_R^*$$

$$Da_P = k_P \exp(-\gamma_P)\tau I_R^*$$

$$Da_T = k_T \exp(-\gamma_T)\tau I_R^*$$

$$\beta = \frac{(-\Delta H)\ M_O^*}{p\ C_P\ T_R^*}$$

I N T R O D U C T I O N

Engineering problems often deal with physical systems represented by models which are much more complex than the capabilities of a given computing facility would allow the model to be. In these cases some degree of reduction becomes necessary if modern control techniques are to be employed. The reduced models designed for this purpose have applications in both on-line and off-line studies. In off-line applications it is desirable to have the minimum number of computations per second. On the other side, in on-line applications, especially in industrial processes, the tasks to be solved are more difficult since the computations must be very fast while the available machines are relatively small. In reality, in closed loop controllers, real-time data must be processed fast enough to drive the actuators that control the process. Therefore, an accurate low-order model is of great importance.

The problem of determining reduced-order representations for large linear systems, which are able to describe the static and dynamic behavior of the system within defined bounds of accuracy, has been explored in numerous papers in the last two decades. Analysis to measure the performance of these techniques in order to decide which method is best is generally inconclusive, and the usual recommendation is to choose a technique which seems suitable for the particular circumstances prevailing.

Many of these methods use a dominant eigenvalue approach (Davison, 1966), a continued fraction expansion (Chen and Shieh, 1968), moment matching (Lal and Mitra, 1974), Pade-approximations (Slamash, 1974), a mixed Cauer form expansion (Shieh and Goldman, 1974), Routh approximations (Hutton and Friedland, 1975), approximations using orthogonal functions (Bistritz and Langholz, 1979) or some direct approximation to the frequency response of the system transfer function (Hsia, 1972).

While an extensive body of literature is available for reduction schemes for linear systems, few results are available in the literature regarding methods suitable for use with nonlinear dynamic systems. Quite often to find an accurate approximant that has only a few ot the states and terms of the original model, one is forced to design and test all possible approximants to find the optimal one. This exhaustive approach involves the consideration of an enormous number of models. In other cases, control of large scale nonlinear systems is achieved by linearizing the original model, performing a model reduction and then designing a controller for the reduced order,linear system. However, retaining the dominant nonlinearities in the reduced model and then linearizing may lead to improved performance.

A. A. Desrochers has published a number of papers [1,2] proposing an algorithm based on conjugate direction ideas and projection matrices which leads to simplification and/or reduction of the original model. Each model structure is represented as a node in

a tree and costs are assigned along the branches of the tree relating the importance of each model term. Although the method has experienced some success, it requires a large amount of computational effort and it may not lead to reduction but only simplification of the model.

Another reduction technique was proposed by Masri, Miller, Sassi and Caughey for discrete multidegree-of-freedom dynamic systems that possess arbitrary nonlinear characteristics. The method uses conventional condensation techniques for linear systems along with nonparametric identification developments and may be used in the field of applied mechanics.

In this work, an identification algorithm (quasilinearization by Bellman and Kalaba [4,5]), along with a pseudosteady-state hypothesis for some of the system states, is employed for nonlinear dynamic model reduction. The motivation for the approach presented is that many problems of current interest have essential nonlinearities, so linearization is an unacceptable approximation. Furthermore, controllers based on models (model-based controllers) must complete their calculations quickly if control is to be effective. Therefore, nonlinear model reduction is often important. On the other side, quasilinearization is of limited usefulness in system identification because of its generally small region of convergence and susceptibility to noise. However, in its favor are quadratic convergence properties, its reliance on the powerful general-purpose ODE solvers available and its easy implementation. Therefore, this

work demonstrates that quasilinearization is an effective model reduction tool in whose application the mentioned disadvantages are less limiting.

The first section describes the quasilinearization algorithm with its various simplifications, followed by an example where some difficulties (i.e. small region of convergence) of the method are discussed. The next section presents the original model, a twelve-order system of a low-density polyethylene reactor, and the development of the reduced model, a two-equation model. In the third section, the quasilinearization technique is employed for the parameter identification of the reduced model. Finally, the dynamic responses of the original, a previously developed low-order model and the proposed model are compared for several step input changes .

CHAPTER ONE

QUASILINEARIZATION

1.1 General Description

Parameter estimation in systems described by a set of ordinary differential equations is of great importance in process modelling, simulation and optimization. A very powerful technique is the quasilinearization approach first introduced by Bellman and Kalaba [3,4] for solving boundary value problems arising in nonlinear differential equations. Its application to the identification of parameters of nonlinear systems is due to Kumar and Shridar [5], Sage and Eisenberg [6], and Detchmendy and Shridar [7].

By quasilinearization the nonlinear problem is regarded as the limit of a sequence of linear problems. It may be applied to continuous or discrete systems [8]. The form of the nonlinear equations must be known a-priori and the parameters to be identified are assumed stationary. The method is of particular importance because measurements on all of the states are not required. Given a sufficient number of measurements of some states, the present approach may yield estimates of both the parameters and the initial values of the other states simultaneously.

Starting from an initial trial solution, convergence occurs rapidly if the initial guess is "close enough" to the true solution.

Small region of convergence is a problem for the method and several attempts have been made to overcome it [9,10,11,12].

1.2 Problem Statement

Consider a nonlinear system given by:

$$\dot{\underset{\sim}{x}} = \underset{\sim}{f} (\underset{\sim}{x}, \underset{\sim}{p}, \underset{\sim}{u}) \qquad (1.1)$$

where: $\underset{\sim}{f}$: n-dimensional nonlinear function,

$\underset{\sim}{x}$: n-dimensional state vector,

$\underset{\sim}{p}$: r-dimensional parameter vector,

$\underset{\sim}{u}$: q-dimensional input vector.

The output vector $\underset{\sim}{y}(t)$ is related to the state vector by a linear relationship:

$$\underset{\sim}{y}(t) = \underset{\sim}{C}\ \underset{\sim}{x}(t) \qquad (1.2)$$

where $\underset{\sim}{C}$ is the (mxn) observation matrix, which is assumed to be constant, since this is the case for most situations. The reader should consult Kalogerakis and Luus [13] for a nonlinear relationship between output and state vector.

The problem is to estimate the unknown parameter vector $\underset{\sim}{p}$, which minimizes the sum of the squared errors:

$$S = \sum_{i=1}^{N} [\ \underset{\sim}{y}(t_i) - \tilde{\underset{\sim}{y}}(t_i)\ ]^T\ \underset{\sim}{Q}(t_i)\ [\ \underset{\sim}{y}(t_i) - \tilde{\underset{\sim}{y}}(t_i)\ ] \qquad (1.3)$$

where: $\underset{\sim}{y}(t_i)$: given measurements of the output vector,

$\tilde{\underset{\sim}{y}}(t_i)$: estimated output vector,

$\underset{\sim}{Q}(t_i)$: (mxm) positive definite, symmetric weighting matrix.

1.3 Quasilinearization Method

First, the elements of $\underset{\sim}{p}$ are assumed stationary and then an augmented state vector is defined by:

$$\underset{\sim}{z} = \begin{vmatrix} \underset{\sim}{x} \\ \underset{\sim}{p} \end{vmatrix} , \qquad \text{where} \quad \dot{\underset{\sim}{z}} = \begin{vmatrix} \dot{\underset{\sim}{x}} \\ \underset{\sim}{0} \end{vmatrix}$$

Therefore, equation (1.1) becomes:

$$\dot{\underset{\sim}{z}} = \underset{\sim}{\psi} (\underset{\sim}{z}, \underset{\sim}{u}) \tag{1.4}$$

Employing a first order Taylor-series expansion, we derive the (j+1)th estimate for $\dot{\underset{\sim}{z}}$ from the jth estimate as follows:

$$\dot{\underset{\sim}{z}}^{j+1} = \underset{\sim}{\psi}(\underset{\sim}{z}^{j+1}, \underset{\sim}{u}) = \underset{\sim}{\psi}(\underset{\sim}{z}^{j}, \underset{\sim}{u}) + \frac{\partial \underset{\sim}{\psi}}{\partial \underset{\sim}{z}}\Big|_{\underset{\sim}{z}^j} (z^{j+1} - z^{j}) \tag{1.5}$$

Note that equation (1.5) is linear in $\underset{\sim}{z}^{j+1}$ and may be expressed as:

$$\dot{\underset{\sim}{z}}^{j+1} = \underset{\sim}{A}^{j} \underset{\sim}{z}^{j+1} + \underset{\sim}{b}^{j} \tag{1.6}$$

where:

$$\underset{\sim}{A}^{j} = \frac{\partial \underset{\sim}{\psi}}{\partial \underset{\sim}{z}}\Big|_{\underset{\sim}{z}^j}$$

$$\underset{\sim}{b}^j = \underset{\sim}{g}\,(\underset{\sim}{z}^j, \underset{\sim}{u}\,) - \underset{\sim}{A}^j \underset{\sim}{z}^j$$

Equation (1.6) has the general solution:

$$\underset{\sim}{z}^{j+1}(t) = \underset{\sim}{\Phi}^{j+1}(t)\ \underset{\sim}{z}^{j+1}(0) + \underset{\sim}{g}^{j+1}(t) \qquad (1.7)$$

where $\underset{\sim}{\Phi}^{j+1}(t)$ is the (n+r)x(n+r) dimensional homogeneous solution matrix given by:

$$\dot{\underset{\sim}{\Phi}}^{j+1}(t) = \underset{\sim}{A}^j\ \underset{\sim}{\Phi}^{j+1}(t)\ , \qquad \underset{\sim}{\Phi}^j\ (0) = \underset{\sim}{I} \qquad (1.8)$$

and $\underset{\sim}{g}^{j+1}(t)$ is the particular solution which satisfies the following equation:

$$\dot{\underset{\sim}{g}}^{j+1}(t) = \underset{\sim}{g}^j(t) - \underset{\sim}{A}^j[\underset{\sim}{z}^j(t) - \underset{\sim}{g}^{j+1}(t)]\ , \quad \underset{\sim}{g}^j(0) = \underset{\sim}{0} \qquad (1.9)$$

The estimated output may be expressed as:

$$\tilde{\underset{\sim}{y}}(t_i) = [\ \underset{\sim}{C},\ \underset{\sim}{0}\ ]\ \underset{\sim}{z}(t_i) = \tilde{\underset{\sim}{C}}\ \underset{\sim}{z}(t_i) \qquad (1.10)$$

Substitution of (1.10) into (1.7) yields:

$$\tilde{\underset{\sim}{y}}(t_i) = \tilde{\underset{\sim}{C}}\ \ \underset{\sim}{\Phi}^{j+1}(t_i)\underset{\sim}{z}^{j+1}(0) + \tilde{\underset{\sim}{C}}\ \underset{\sim}{g}^{j+1}(t_i) \qquad (1.11)$$

The optimal $\underset{\sim}{z}^{j+1}(0)$ is the one which minimizes the squared error S in equation (1.3).

Substituting (1.11) into (1.3), we get :

$$S = \sum_{i=1}^{N} \{ \underset{\sim}{y}(t_i) - \tilde{\underset{\sim}{C}} [\underset{\sim}{\Phi}^{j+1}(t_i)\underset{\sim}{z}^{j+1}(0) + \underset{\sim}{g}^{j+1}(t_i)] \}^T \quad \underset{\sim}{Q}(t_i)$$

$$\{ \underset{\sim}{y}(t_i) - \tilde{\underset{\sim}{C}} [\underset{\sim}{\Phi}^{j+1}(t_i)\underset{\sim}{z}^{j+1}(0) + \underset{\sim}{g}^{j+1}(t_i)] \}$$

$\underset{\sim}{z}^{j+1}(0)$ is chosen by minimizing S by considering the condition

$\frac{\partial S}{\partial \underset{\sim}{z}^{j+1}} = 0$, which yields:

$$\underset{\sim}{W}\ \underset{\sim}{z}^{j+1}(0) = \underset{\sim}{d} \tag{1.12}$$

where:

$$\underset{\sim}{W} = \sum_{i=1}^{N} \{[\underset{\sim}{\Phi}^{j+1}(t_i)]^T\ [\tilde{\underset{\sim}{C}}\ (t_i)]^T\ \underset{\sim}{Q}(t_i)\ \tilde{\underset{\sim}{C}}\ (t_i)\ \underset{\sim}{\Phi}^{j+1}(t_i)\}$$

$$\underset{\sim}{d} = \sum_{i=1}^{N} \{[\underset{\sim}{\Phi}^{j+1}(t_i)]^T\ [\tilde{\underset{\sim}{C}}\ (t_i)]^T\ \underset{\sim}{Q}(t_i)\ [\underset{\sim}{y}(t_i) - \tilde{\underset{\sim}{C}}\ (t_i)\ \underset{\sim}{g}(t_i)]\}$$

Solving the system (1.12), $\underset{\sim}{z}^{j+1}(0)$ is obtained and with this value the above procedure is repeated to yield $\underset{\sim}{z}^{j+2}(0)$ and thus a sequence of parameter vectors is calculated. It is found that the sequence $\underset{\sim}{z}^{1}(0)$, $\underset{\sim}{z}^{2}(0)$,....., converges quickly to the optimum if the initial guess $\underset{\sim}{z}^{0}(0)$ is sufficiently good.

1.4 Algorithm

Therefore, the algorithm has the following steps:

Step 1 : Select an initial value $\underset{\sim}{z}^{j}(0)$ and set j=0.

Step 2 : Solve equations (1.6), (1.8) and (1.9) simultaneously to obtain $\underset{\sim}{z}^{j}(t_i)$, $\underset{\sim}{\Phi}^{j}(t_i)$ and $\underset{\sim}{g}^{j}(t_i)$, i=1,2,....,N.

Step 3 : Solve equation (1.12) for $\underset{\sim}{z}^{j+1}(0)$.

Step 4 : If

$$|| \underset{\sim}{z}^{j+1}(0) - \underset{\sim}{z}^{j}(0) || \leq \epsilon ,$$

where ϵ is a preset convergence criterion, stop;

otherwise set:

$$\underset{\sim}{z}^{j}(0) = \underset{\sim}{z}^{j+1}(0) ,$$

increase j by one and return to step (2).

The total number of differential equations that are integrated at each iteration is:

n - to generate $\underset{\sim}{z}^{j}(t)$,

n(n+r) - for the non-trivial components of the homogeneous solution matrix $\underset{\sim}{\Phi}(t)$,

n - for the non-trivial elements of the particular solution,

for a total of $n^2 + 2n + nr$. This represents a maximum number and may be reduced in individual cases.

1.5 Simplifications

1. The particular solution can be calculated at each iteration from Eqn. (1.7) and therefore the total number can be reduced to n^2+n+nr.
2. If the initial condition $\underset{\sim}{x}_0$ for the state vector is available, then using also Eqn. (1.7) instead of (1.9), the total number is reduced to $n(1+r)$ differential equations [11].

1.6 Example

Consider an unforced second order system which describes a nonlinear oscillator:

$$\ddot{x} + c_1\dot{x}^3 + c_2\dot{x} + c_3x^2 + x = 0 \qquad (1.13)$$

where c_1, c_2 and c_3 are constant parameters to be identified.

If we define:

$$x_1 = \dot{x}$$

$$x_2 = x$$

equation (1.13) can be expressed as a system of two first order ordinary differential equations:

$$\left.\begin{aligned} \dot{x}_1 &= -c_1x_1^3 - c_2x_1 - c_3x_2^2 - x_2 \\ \dot{x}_2 &= x_1 \end{aligned}\right\} \qquad (1.14)$$

or $\dot{\underset{\sim}{x}} = \underset{\sim}{f}(\underset{\sim}{x},\underset{\sim}{p})$, where $\underset{\sim}{p}^T = [\ c_1\ c_2\ c_3\ ]$

An augmented state vector $\underset{\sim}{z}$ is defined as:

$$\underset{\sim}{z}^T = [\ x_1\ x_2\ c_1\ c_2\ c_3\ ]$$

and (1.14) becomes:

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{c}_1 \\ \dot{c}_2 \\ \dot{c}_3 \end{bmatrix} = \begin{bmatrix} -c_1x_1^3 \ -c_2x_1 - c_3x_2^2 - x_2 \\ x_1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

or $$\dot{\underset{\sim}{z}}(t) = \underset{\sim}{\psi}(\underset{\sim}{z},t) \qquad (1.15)$$

The Jacobian matrix is given by:

$$\underset{\sim}{J} = \frac{\partial \underset{\sim}{\psi}}{\partial \underset{\sim}{z}} = \begin{bmatrix} R_1 & R_2 & R_3 & R_4 & R_5 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

where:

$$R_1 = -3c_1x_1^2 - c_2$$

$$R_2 = -2c_3x_2 - 1$$

$$R_3 = -x_1^3$$

$$R_4 = -x_1$$

$$R_5 = -x_2^2$$

The elements of the homogeneous solution matrix $\underset{\sim}{\Phi}(t)$ are generated by solving the following set of differential equations:

$$\left.\begin{aligned}
&\dot{\phi}_{11} = R_1\phi_{11} + R_2\phi_{21}, && \phi_{11}(0)=1\\
&\dot{\phi}_{12} = R_1\phi_{12} + R_2\phi_{22}, && \phi_{12}(0)=0\\
&\dot{\phi}_{13} = R_1\phi_{13} + R_2\phi_{23}, && \phi_{13}(0)=0\\
&\dot{\phi}_{14} = R_1\phi_{14} + R_2\phi_{24}, && \phi_{14}(0)=0\\
&\dot{\phi}_{15} = R_1\phi_{15} + R_2\phi_{25}, && \phi_{15}(0)=0\\
&\dot{\phi}_{21} = \phi_{11}, && \phi_{21}(0)=0\\
&\dot{\phi}_{22} = \phi_{12}, && \phi_{22}(0)=1\\
&\dot{\phi}_{23} = \phi_{13}, && \phi_{23}(0)=0\\
&\dot{\phi}_{24} = \phi_{14}, && \phi_{24}(0)=0\\
&\dot{\phi}_{25} = \phi_{15}, && \phi_{25}(0)=0
\end{aligned}\right\} \qquad (1.16)$$

The particular solution $\underset{\sim}{g}(t)$ is given by:

$$\left.\begin{aligned} \dot{q}_1 &= R_1(q_1-x_1) + R_2(q_2-x_2) - x_2 \quad , \qquad q_1(0)=0 \\ \dot{q}_2 &= q_1 \quad , \qquad\qquad\qquad\qquad\qquad\qquad q_2(0)=0 \end{aligned}\right\} \qquad (1.17)$$

Thus at each iteration :

- 14 differential equations are integrated:

  2 - to generate $\underset{\sim}{z}(t)$ [Eqn.(1.14)].

  10 - for the non-trivial components of $\underset{\sim}{\Phi}(t)$ [Eqn.(1.16)].

  2 - for the non-trivial elements of $\underset{\sim}{g}(t)$ [Eqn.(1.17)].

- the following system is solved for a new estimate of $\underset{\sim}{z}(0)$:

$$\sum_{i=1}^{N} \underset{\sim}{w}(t_i)\ \underset{\sim}{w}^T(t_i)\ \underset{\sim}{z}(0) = \sum_{i=1}^{N} \underset{\sim}{w}(t_i)[y(t_i)-q_2(t_i)] \qquad (1.18)$$

where : $\underset{\sim}{w}^T(t_i) = [f_{21}(t_i) \quad \phi_{22}(t_i) \quad \phi_{23}(t_i) \quad \phi_{24}(t_i) \quad \phi_{25}(t_i)]$

and $y(t_i)$ are noise-free measurements generated by integrating (1.14)

with: $\dot{x}(0) = 1.0$

$x(0) = 0.0$

$c_1 = 3.0$

$c_2 = -0.1$

$c_3 = 1.0$

The minimum number (N=5) of measurements, sampled every .2 seconds, is used along with the initial guess:

$$\underset{\sim}{z}^T(0) = [2.0 \quad 0.6 \quad 2.0 \quad 0.5 \quad 2.0]$$

It takes 1.44 CPU seconds on the LUCC CYBER 850 for the algorithm to converge to the exact solution with ϵ=.001:

$$\underset{\sim}{z}^T_{exact}(0) = [1.0 \quad 0.5 \quad 3.0 \quad -0.1 \quad 1.0]$$

1.7 Difficulties

Quasilinearization is a second-order iterative process and convergence, if it occurs at all, is quadratic and hence rapid. However, if the initial value $\underset{\sim}{z}^0(0)$ is not sufficiently close to the exact vector $\underset{\sim}{z}_{exact}(0)$, then convergence may not occur. The following difficulties have been noticed:

- small region of convergence,
- the region of convergence is significantly reduced when a large number of measurements is used.

Even though $\underset{\sim}{z}^0(0) = [1. \ , \ .5 \ , \ 4. \ , -.1 \ , \ 3.]$ seems a good guess, the algorithm was unable to identify c_1 and c_3. With initial guess $\underset{\sim}{z}^0(0) = [1. \ , \ .5 \ , \ 0. \ , -.1 \ , 0.]$ and the minimum number of measurements (N=5) convergence occurs, but if more measurements are taken (N=20), then the algorithm fails.

However, with N = j x (n+r) (where j is the iteration number) a significant increase in the size of the region of convergence is achieved.

Numerous approaches have been made to overcome this major problem of quasilinearization. Among them are, perturbed data by Donnelly and Quon [9], linear programming by Nieman and Fisher [10],shorter data length by Wang and Luus [11], and direct search optimization by Luus and Jaakola [14].

Finally, the solution of the system (1.18) proves to be quite an important portion of the algorithm [7]. In an ill-conditioned system the algorithm experiences difficulty in converging. Eventhough it is often difficult to distinguish between properties of the algorithm itself (small region of convergence) and properties of the particular problem (ill-conditioned system), a large condition number indicates the ill-conditioning of the system. An estimate of the standard condition number can be calculated by $|| W^{-1} || \, || W ||$ where:

$$|| W || = \max_{row} \Sigma \, |\text{elements in a row}|.$$

CHAPTER TWO

M O D E L

2.1 General Description

Commercially available polyethylene is manufactured either by a low-pressure process which yields a high-density product or by a high pressure process for low density polyethylene. The high-pressure process can be undertaken by any one of the four common polymerization techniques: bulk polymerization, solution polymerization, suspension polymerization and emulsion polymerization. The bulk technique, which is most commonly used, requires a highly purified ethylene stream and process pressure between 1000 and 3000 atm.

Two main commercial reactor designs have been developed: the tubular reactor and the stirred autoclave reactor. Reactor temperatures range between 100 and 300°C. Temperatures above 300°C are avoided because ethylene decomposition may occur. Successful operation of the reactor requires the proper selection of an initiator and the control of its injection rate, since this can significantly affect the polymerization rate and the temperature profile.

The development of a mathematical model which accurately predicts reactor performance is of practical importance and can contribute to the solution of many engineering problems. A number of researchers have made studies of polymerization reactor systems. Since 1970 it has been known (van der Molen and van Heerden) that the

operating conditions and the degree of mixing in the reactor affect the initiator productivity, but only in 1981 did van der Molen, Koenen and Donati [15,16] publish a number of experimental results from which this influence became obvious. Recently, in 1984, Marini and Georgakis [17] introduced two dynamic models for the low-density polymerization reactor; the first model assumes perfect mixture in the reactor and the second includes the mixing phenomena near the injection point.

2.2 Perfectly mixed model (model A)

Assuming that:

- any concentration or temperature gradient is negligible,
- the physical properties of the reacting medium do not change from input to output and
- the heat effect of the initiation and termination steps is not considerable,

then from mass and enthalpy balances the following set of equations can be derived:

$$\left.\begin{aligned}
\frac{dI}{dt} &= I_0 - I - Da_I I \exp(\gamma_I - \gamma_I/T) \\
\frac{d\lambda}{dt} &= -\lambda + 2f Da_I \lambda \exp(\gamma_I - \gamma_I/T) - Da_T \lambda^2 \exp(\gamma_T - \gamma_T/T) \\
\frac{dM}{dt} &= 1 - M - Da_P \lambda M \exp(\gamma_P - \gamma_P/T) \\
\frac{dT}{dt} &= T_0 - T + \beta Da_P \lambda M \exp(\gamma_P - \gamma_P/T)
\end{aligned}\right\} \quad (2.1)$$

where:

I = initiator concentration,

λ = radical concentration,

M = monomer concentration,

T = temperature.

The above system of equations was made dimensionless with respect to a reference temperature T_R^*, a reference feed initiator I_R^* and the input monomer concentration M_0^*. Model A predicts a continuous decrease in the initiator consumption when the polymerization temperature increases. However, experimental data show that this is true only for the region of low temperatures.

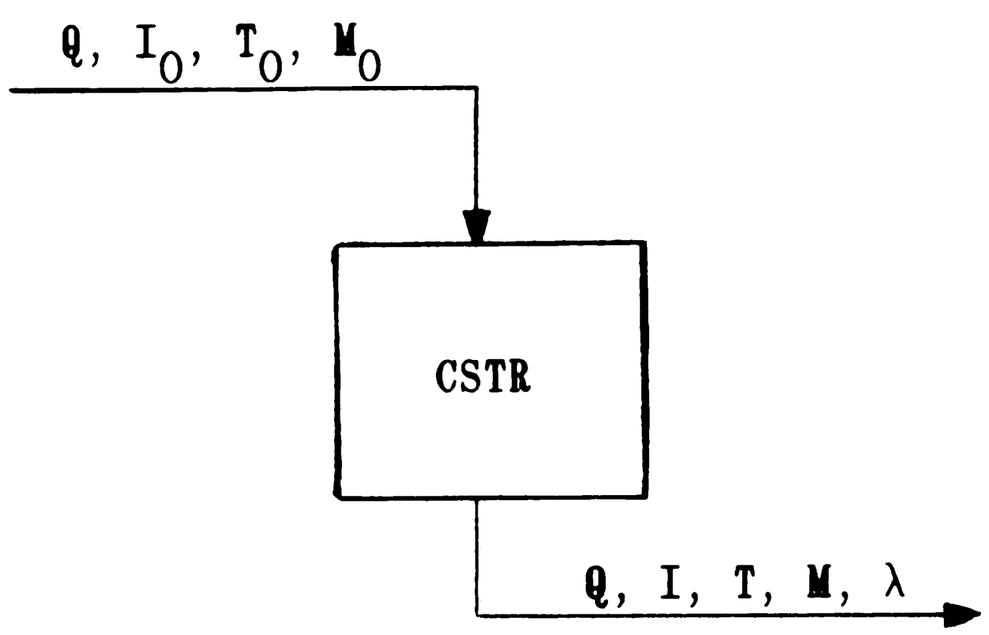

Figure 2.1 Schematic presentation of model A.

2.3 Imperfectly mixed model (model B)

In this model the entire reactor is divided into three CSTR's in series (Fig. 2.2). The first two units, which represent a small part of the total reactor ($V_1 = V_2 \simeq 5\%$), are employed to model the conditions at the injection point. V_3 is the remaining part of the reactor and in this unit the main polymerization takes place. Two external feeds are considered: Q^1 represents a cold stream of initiator and ethylene and Q^2 is a feed which comes from another reaction zone in a multiple zone reactor and contains a negligible amount of initiator.

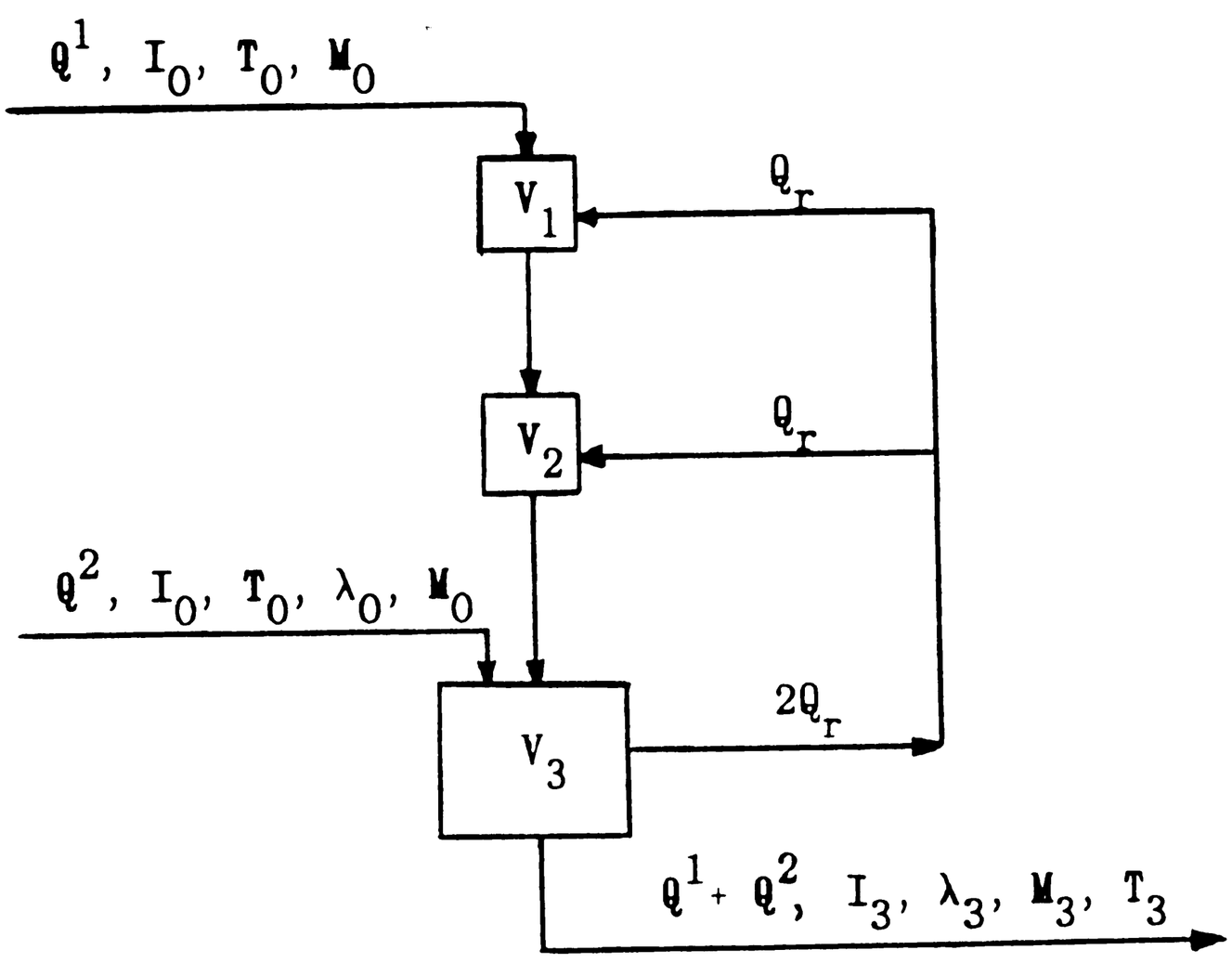

Figure 2.2 Schematic presentation of model B.

A set of twelve nonlinear differential equations is derived by applying mass and energy balances to each of the three units:

$$\xi_1 dI_1/dt = \alpha I_0 + \epsilon I_3 - (\alpha+\epsilon) I_1 - \xi Da_I I_1 \exp(\gamma_I - \gamma_I/T_1)$$

$$\xi_2 dI_2/dt = (\epsilon+\alpha) I_1 + \epsilon I_3 - (\alpha+2\epsilon) I_2 - \xi_2 Da_I I_2 \exp(\gamma_I - \gamma_I/T_2)$$

$$\xi_3 dI_3/dt = (\alpha+2\epsilon) I_2 + (1-\alpha) I_0 - (1+2\epsilon) I_3 - \xi_3 Da_I I_3 \exp(\gamma_I - \gamma_I/T_3)$$

$$\xi_1 d\lambda_1/dt = \epsilon\lambda_3 - (\alpha+\epsilon)\lambda_1 + 2f\xi_1 Da_I I_1 \exp(\gamma_I - \gamma_I/T_1) - \xi_1 Da_T \lambda_1^2 \exp(\gamma_T - \gamma_T/T_1)$$

$$\xi_2 d\lambda_2/dt = (\alpha+\epsilon)\lambda_1 + \epsilon\lambda_3 - (\alpha+2\epsilon)\lambda_2 + 2f\xi_2 Da_I I_2 \exp(\gamma_I - \gamma_I/T_2) + \\ - \xi_2 Da_T \lambda_2^2 \exp(\gamma_T - \gamma_T/T_2)$$

$$\xi_3 d\lambda_3/dt = (\alpha+2\epsilon)\lambda_2 + (1-\alpha)\lambda_0 - (1+2\epsilon)\lambda_3 + 2f\xi_3 Da_I I_3 \exp(\gamma_I - \gamma_I/T_3) + \\ - \xi_3 Da_T \lambda_3^2 \exp(\gamma_T - \gamma_T/T_3) \qquad (2.2)$$

$$\xi_1 dM_1/dt = \alpha + \epsilon M_3 - (\alpha+\epsilon) M_1 - \xi_1 Da_P M_1 \lambda_1 \exp(\gamma_P - \gamma_P/T_1)$$

$$\xi_2 dM_2/dt = (\alpha+\epsilon) M_1 + \epsilon M_3 - (\alpha+2\epsilon) M_2 - \xi_2 Da_P M_2 \lambda_2 \exp(\gamma_P - \gamma_P/T_2)$$

$$\xi_3 dM_3/dt = (\alpha+2\epsilon) M_2 + (1-\alpha) M_0 - (1+2\epsilon) M_3 - \xi_3 Da_P M_3 \lambda_3 \exp(\gamma_P - \gamma_P/T_3)$$

$$\xi_1 dT_1/dt = \alpha T_0 + \epsilon T_3 - (\alpha+\epsilon) T_1 + \beta\xi_1 Da_P M_1 \lambda_1 \exp(\gamma_P - \gamma_P/T_1)$$

$$\xi_2 dT_2/dt = (\alpha+\epsilon) T_1 + \epsilon T_3 - (\alpha+2\epsilon) T_2 + \beta\xi_2 Da_P M_2 \lambda_2 \exp(\gamma_P - \gamma_P/T_2)$$

$$\xi_3 dT_3/dt = (\alpha+2\epsilon) T_2 + (1-\alpha) T_0 - (1+2\epsilon) T_3 + \beta\xi_3 Da_P M_3 \lambda_3 \exp(\gamma_P - \gamma_P/T_3)$$

Model B gives the same steady-state prediction as model A for the low temperature region and at high temperatures it predicts correctly the increase of initiator consumption with temperature. The difference between the two models can be explained by the fact that the decomposition time of the initiator becomes smaller than the overall residence time and makes necessary the introduction of V_1 and V_2. In model B at high temperatures a great amount of produced radicals is wasted in V_1 and V_2 through the termination reaction and this leads to the observed increase in the initiator consumption. In Figure 2.3 a comparison between the two models is shown.

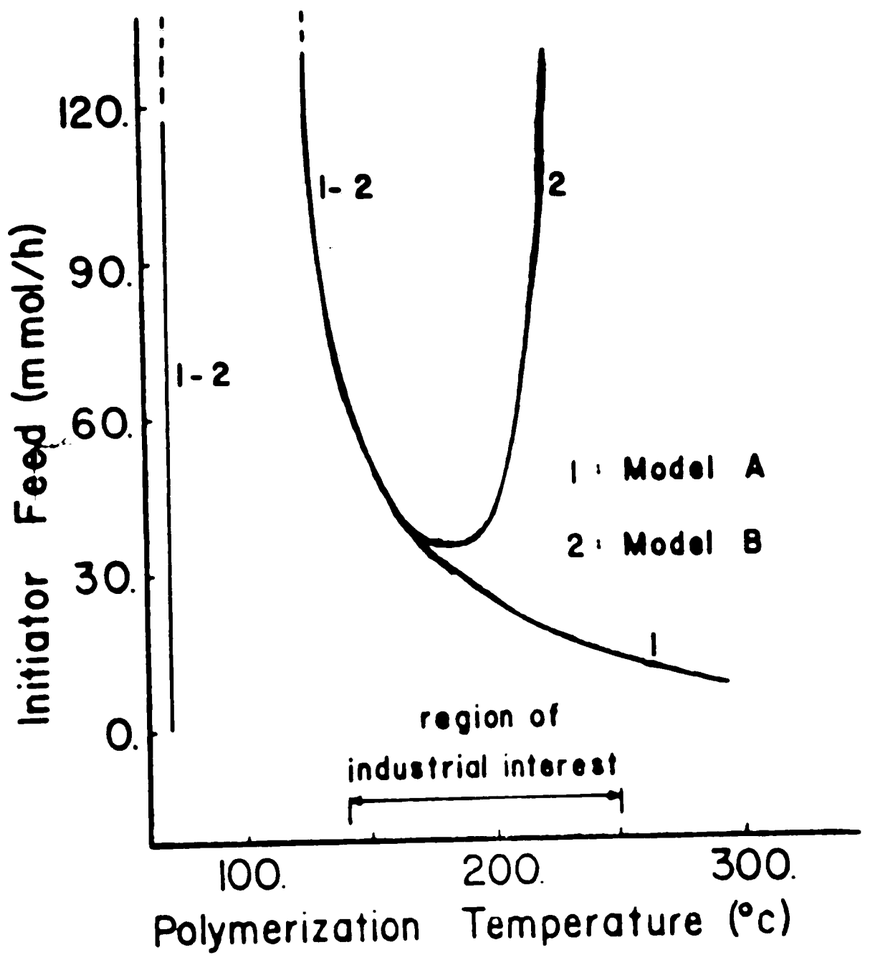

Figure 2.3: Change of initiator consumption with polymerization temperature for model A and model B. Initiator #10, Q=70[Kg/h], $Q^1=Q^2=Q/2$, Q_r=250[Kg/h], V=1[LT], $V_1=V_2$=0.015[LT], T_0=70[C], P=1570[atm].

2.4 Reduced Model

Generally, the development of an accurate mathematical model is of great importance but very often this model, due to its complexity, becomes unsuitable for on-line process control. Many researchers have studied model reduction and simplification and a large number of methods have been developed, so that the original model can be replaced by a simpler and to some extent accurate model. However, most of them are applicable to linear systems and only a few can be found for nonlinear cases [1,2].

For the low-density polymerization process, model B produces results very close to the experimental data but it is not suitable for on-line use because a large amount of computational time is required. On the other side, the simple model A is not acceptable due to its inaccurate predictions for the high temperature region. Here a new model is developed which is economical to evaluate and accurate, thus suitable for on-line purposes.

First consider the perfectly mixed model A, described by Eqns. (2.1). Of the four eigenvalues obtained from these equations, two are always very fast (-1000) compared to the dominant eigenvalues (-1,-3). In addition, the initiator and radical concentrations have very small residues corresponding to the dominant eigenvalues. Therefore, the pseudosteady-state hypothesis can be made for the initiator and radical concentrations and they can be expressed as functions of temperature and initiator feed:

$$\left.\begin{aligned} I &= \frac{I_0}{1 + Da_I \exp(\gamma_I - \gamma_I/T)} \\ \lambda &= \frac{1}{2}[-b + \sqrt{b^2 - 4c}\,] \end{aligned}\right\} \qquad (2.3)$$

where:

$$b = \frac{1}{Da_T \exp(\gamma_T - \gamma_T/T)} \qquad \text{and}$$

$$c = \frac{-\,2fI_0 Da_I \exp(\gamma_I - \gamma_I/T)}{Da_T \exp(\gamma_T - \gamma_T/T)\;[1 + Da_I \exp(\gamma_I - \gamma_I/T)]} \quad .$$

Because b is of order 10^{-8}, it can be neglected and then the second equation in (2.3) becomes:

$$\lambda = \sqrt{-c}$$

Substitution of initiator and radical concentration, I and λ, into (2.1) gives:

$$\left.\begin{aligned} \frac{dM}{dt} &= 1 - M + c_1 M\, R(T, I_0) \\ \frac{dT}{dt} &= T_0 - T + c_2 M\, R(T, I_0) \end{aligned}\right\} \qquad (2.4)$$

where:

$$c_1 = -\sqrt{2f/Da_T} \quad ,$$

$$c_2 = -\beta c_1 \qquad \text{and}$$

$$R(T, I_0) = \sqrt{I_0 Da_P \exp[(\gamma_P - \gamma_T/2)(1 - 1/T)]}\;\sqrt{[D_I/(1+D_I)]}$$

with $\qquad D_I = Da_I \exp(\gamma_I - \gamma_I/T)$.

At this point, we focus our attention only on the dynamic performance of the system and we will employ quasilinearization to identify c_1 and c_2, so that equations (2.4) represent the dynamic responses of the physical system (reactor) accurately.

In order to satisfy the original steady state of the system for every value of the parameters c_1 and c_2, equations (2.4) are rearranged as follows:

$$\left.\begin{aligned} \frac{dM}{dt} &= M_s - M - c_1[\, M\, R(T,I_0) - M_s R(T_s,I_{0s})] \\ \frac{dT}{dt} &= T_0 - T_{0s} - (T_s - T) + c_2[\, M\, R(T,I_0) - M_s R(T_s,I_{0s})] \end{aligned}\right\} \quad (2.5)$$

where:

T_0-T_{0s} is the change in input temperature,

I_0-I_{0s} is the change in initiator feed and

M_s, T_s are monomer concentration and polymerization temperature for T_{0s} and I_{0s}.

CHAPTER THREE

THE USE OF QUASILINEARIZATION FOR MODEL REDUCTION

3.1 Computational Algorithm

The computational algorithm that is used to solve the proposed problem is a modification of the usual quasilinearization procedure [11].

First consider the reduced model (2.6) which in matrix form is:

$$\dot{\underset{\sim}{x}} = \underset{\sim}{f}(\underset{\sim}{x}, \underset{\sim}{p}, \underset{\sim}{u})$$

where:

$$\underset{\sim}{x} = \begin{bmatrix} M \\ T \end{bmatrix} \qquad \text{and} \qquad \underset{\sim}{p} = \begin{bmatrix} c_1 \\ c_2 \end{bmatrix}$$

Therefore n=2 (# of equations) and r=2 (# of unknowns). The polymerization temperature is considered to be the output on which measurements will be taken, hence:

$$y = T = [0\ 1]\ \underset{\sim}{x}$$

Applying the quasilinearization procedure as outlined in chapter one, we derive six [n(r+1)] differential equations to be integrated and a linear system to be solved at each iteration step.

Secondly let us define:

$$Q = \frac{\partial R}{\partial T} = \left[\gamma_p - \frac{\gamma_T}{2} + \frac{\gamma_I}{2[1+Da_I \exp(\gamma_I - \gamma_I/T)]}\right] \frac{R}{T^2}$$

where R is a function of T and I_o given by equation (2.5).

Thirdly define:

$$G = M\ R(T,I_o) - M_s\ R(T_s,I_{os})$$

where s is referring to the original steady state of the system.

Then the Jacobian matrix is given by:

$$\underset{\sim}{J} = \begin{bmatrix} c_1R - 1 & c_1M\ Q \\ c_2R & c_2M\ Q - 1 \end{bmatrix}$$

and the homogeneous solution matrix $\underset{\sim}{\phi}$ is generated by integrating the following set of differential equations:

$$\left.\begin{aligned}
\dot{\phi}_{11} &= (c_1R - 1)\phi_{11} + c_1M\ Q\phi_{21} + G\ , & \phi_{11}(0)=0 \\
\dot{\phi}_{12} &= (c_1R - 1)\phi_{12} + c_1M\ Q\phi_{22}\ , & \phi_{12}(0)=0 \\
\dot{\phi}_{21} &= c_2R\phi_{11} + (c_2M\ Q - 1)\phi_{21}\ , & \phi_{21}(0)=0 \\
\dot{\phi}_{22} &= c_2R\phi_{12} + (c_2M\ Q - 1)\phi_{22} + G\ , & \phi_{22}(0)=0
\end{aligned}\right\} \qquad (3.1)$$

In addition, the particular solution $\underset{\sim}{g}$ is obtained from:

$$\left.\begin{aligned}
q_1 &= x_1 - \phi_{11}c_1 - \phi_{12}c_2 \\
q_2 &= x_2 - \phi_{21}c_1 - \phi_{22}c_2
\end{aligned}\right\} \qquad (3.2)$$

Finally, the parameters c_1 and c_2 are calculated by solving the system (1.12) which in our case is:

$$\underset{\sim}{W}\ \underset{\sim}{p} = \underset{\sim}{d} \qquad (3.3)$$

where:

$$\underset{\sim}{W} = \sum_{i=1}^{N} \begin{bmatrix} \phi_{21}^2(t_i) & \phi_{21}(t_i)\phi_{22}(t_i) \\ \phi_{21}(t_i)\phi_{22}(t_i) & \phi_{22}^2(t_i) \end{bmatrix}$$

$$\underset{\sim}{d} = \sum_{i=1}^{N} \begin{bmatrix} \phi_{21}(t_i) \\ \phi_{22}(t_i) \end{bmatrix} \{ y(t_i) - q_2(t_i) \} .$$

The $y(t_i)$ are noise-free measurements generated by simulating the twelve-equation, imperfectly mixed model B (Eqn. 2.2) which represents the reactor in our case.

The following parameters are used for the integration:

<u>fluid-mechanic parameters</u>:

$$\alpha = 0.5 \quad , \qquad \xi_1 = \frac{V_1}{V} = \xi_2 = \frac{V_2}{V} = 0.015$$

$$\epsilon = \frac{Q_r}{Q^1} = 3.75 \quad , \qquad \xi_3 = \frac{V_3}{V} = 0.97$$

<u>kinetic parameters</u>:

initiator #10 : Da_I=97.468, γ_I=35.011, f=0.60

initiator #12 : Da_I=20.719, γ_I=35.90, f=0.98

propagation : Da_P=278.05, γ_P=8.084

termination : Da_T=1.22E7, γ_T=1.115

$\beta = 2.942$

reactor conditions:

residence time	τ = 26.9 sec
reference temperature	T_R^*= 180°C
reference initiator feed	I_R^*= 36.74 mmol/h
operating pressure	P = 1570 atm
input monomer concentration	M_o^*= 18.71 mmol/lt

Therefore at each iteration equations (2.6) and (3.1) are integrated simultaneously and then the particular solution is obtained from equation (3.2). Finally the system (3.3) is solved for the parameter vector.

The LUCC CYBER 850 is employed along with the IMSL subroutine DGEAR (a variable-step, variable-order Adams method) to integrate the twelve nonlinear equations of model B in order to generate the observations. The measurements are uniformly spaced on the time axis with a sampling period of 1.076 sec.

In general it has been observed that a trade-off is involved in selecting the length of the time interval corresponding to the first N measurements. From one point of view, a time interval as small as possible should be used at the beginning. The selection of parameter vector which will generate a trajectory close to the observed one becomes easier as shorter time intervals are considered. The other point of view is that the initial time interval has to be sufficiently

long so that the estimated parameters are close enough to the exact ones.

Detchmendy and Sridhar [7] have indicated, that a number of measurements (N) equal to approximately ten to fifteen times the minimum number of measurements produces satisfactory results (convergence occurs in 3 to 5 iterations). We start the algorithm with:

$$N_o = 5 \times r$$

and increase this number gradually

$$N = j \times N_o , \qquad j : \text{iteration number}$$

until the entire interval of interest has been used or until the estimates of the parameters change by a small percentage as additional measurements are added. An ϵ equal 0.0001 is taken in the convergence criterion.

3.2 Results

A number of computer experiments are performed in order to test the proposed algorithm on the problem under consideration.

Change of initiator feed rate. A step change of initiator feed I_o^* from 55.11 (mmol/h) to 91.85 (mmol/h) is applied to model B to produce the observations, while feed temperature is constant at 70°C. In table 1 the parameters are given along with the number of iterations and the required execution time for different time intervals.

Table 1.

Data Length (sec)	c_1	c_2	Iterations	cpu Time (sec)
5.38 [10]	-15.1628	1.6750	4	.129
10.76 [20]	-17.0088	1.7269	5	.205
26.90 [50]	-16.9286	1.7226	6	.339
37.66 [70]	-16.8364	1.7173	9	.604
53.80 [100]	-16.7671	1.7131	12	.998

The numbers in the brackets indicate the total number of measurements used. Obviously as N increases the number of iterations and the cpu time increase and the two-equation model exhibits closer dynamic performance. Figure 3.1 displays a comparison between the two models for various data lengths. For the 5.38 sec time interval (N=10) the reduced model approximates model B with an error of 1.1 degrees at steady state which is small compared to the polymerization temperature of 230°C. Furthermore, by employing 20, 50 or 100 measurements the above error becomes negligible and the two models exhibit almost identical transients. Consequently, the reduced model is in excellent agreement with model B and could be used for on-line control of polymerization temperature.

Change of feed temperature. A step change of feed temperature, T_o^*, from 70°C to 60°C is applied to model B with feed

initiator I_o constant at 1.95 (I_o^*=71.645 mmol/h). In Figure 3.2 model B and the two equation model with N=50 are shown to produce dynamic responses which are very similar.

Change of initiator type. At this time the type of initiator is changed from #10 to #12 with feed temperature at 70°C and feed initiator I_o at 1.95 (I_o^*=71.645 mmol/h). Even though polymerization temperature changes dramatically from 225°C to 265°C the reduced model is able to reproduce this transient as is shown in Figure 3.3.

Finally, the algorithm was employed to find a low-order model which could approximate more than one dynamic response of the original model. Data from two dynamic responses were considered:

- change of initiator feed from 55.11 to 91.85 (mmol/h),
- change of initiator feed from 73.48 to 110.22 (mmol/h).

The algorithm successfully converged. Obviously, the approximations are not as good as the previous ones (one dynamic response considered). However, using a weighting factor one of them can be improved while perhaps keeping the second within acceptable limits.

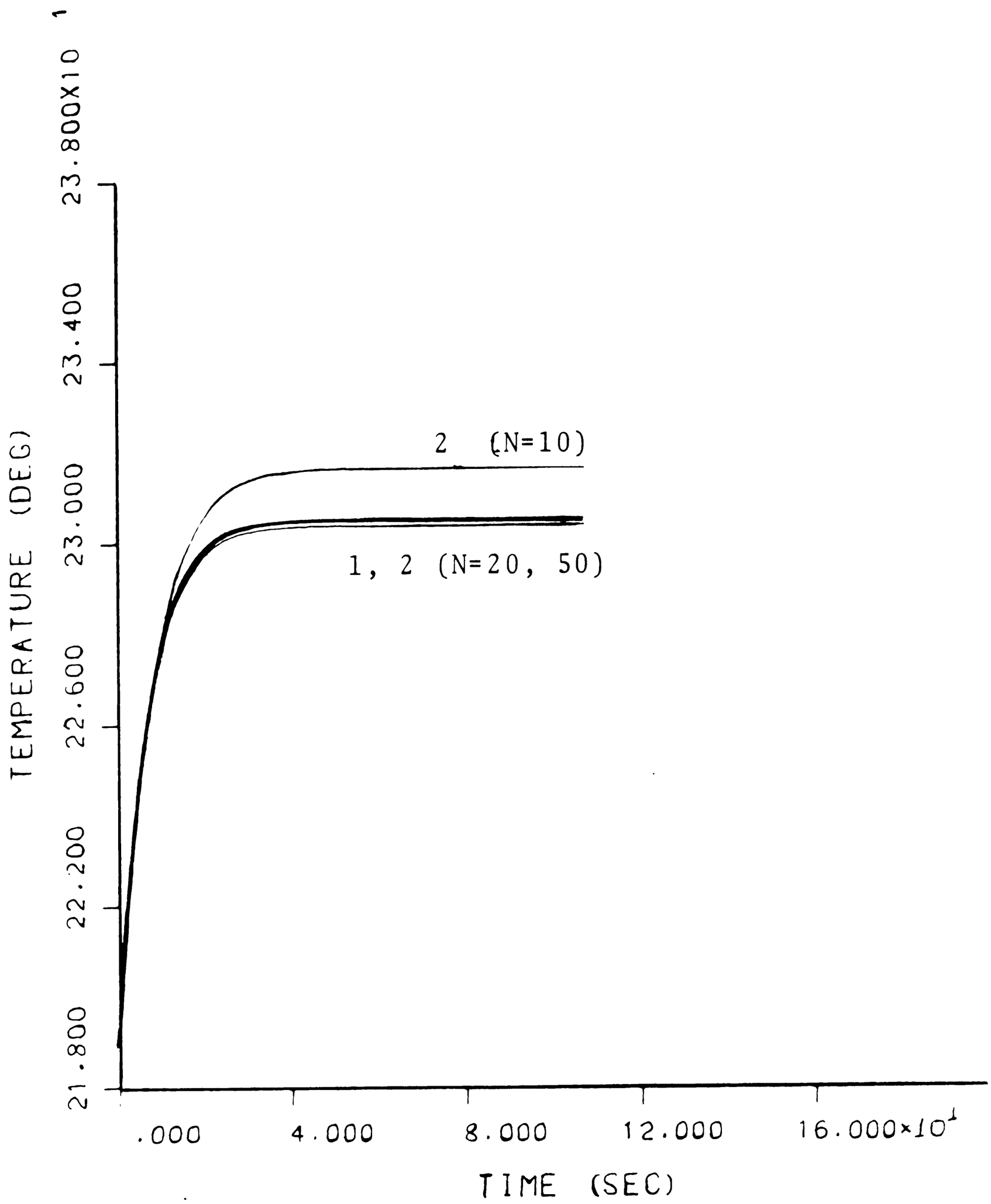

Figure 3.1 Comparison between model B (1) and reduced model (2) for a step change in feed initiator from 55.11 (mmol/h) to 91.85 (mmol/h) for various data lengths.

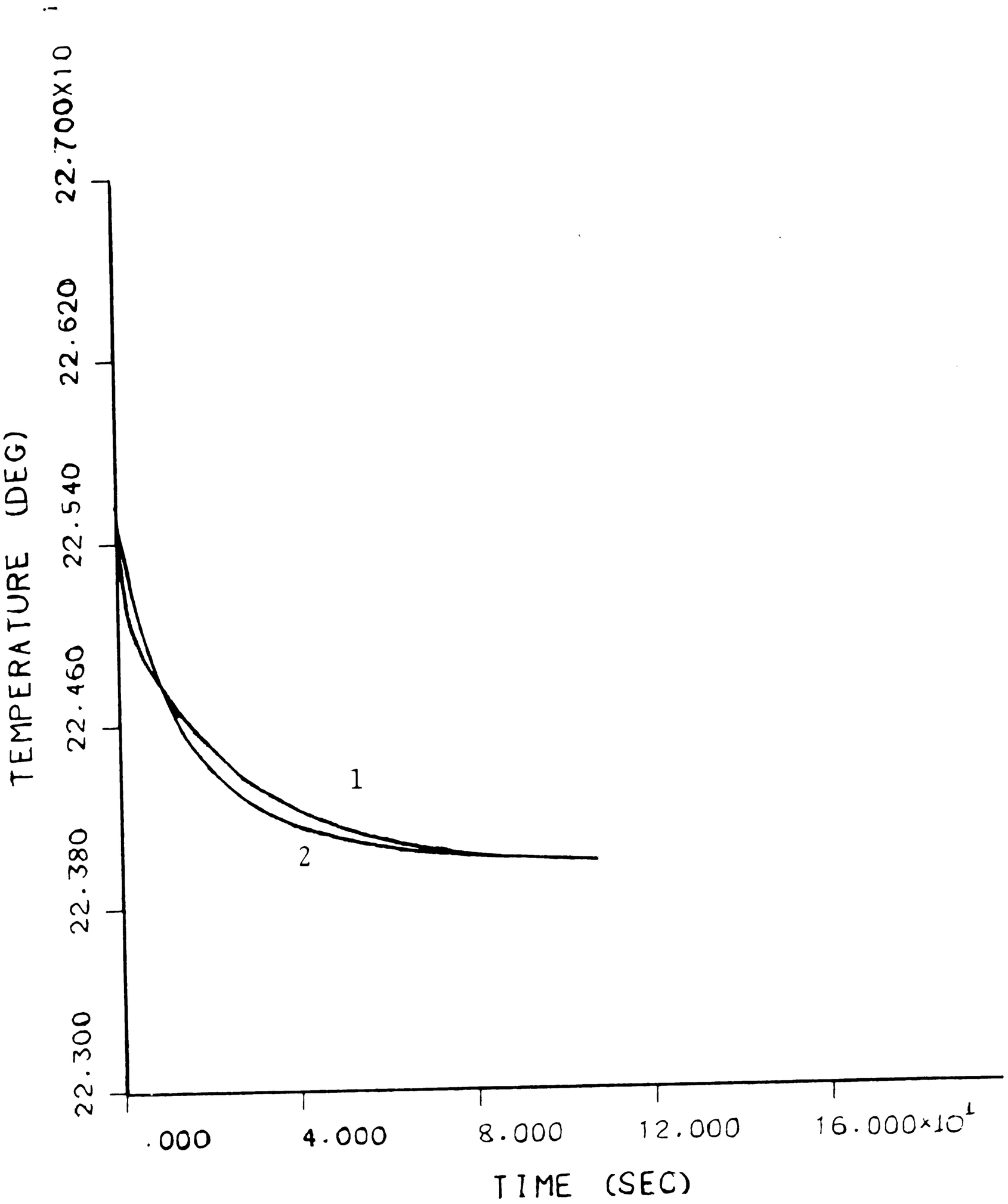

Figure 3.2 Comparison between model B (1) and reduced model (2) for a step change in feed temperature from 70°C to 60°C.

(c_1 = -1.8381, c_2 = -4.9173).

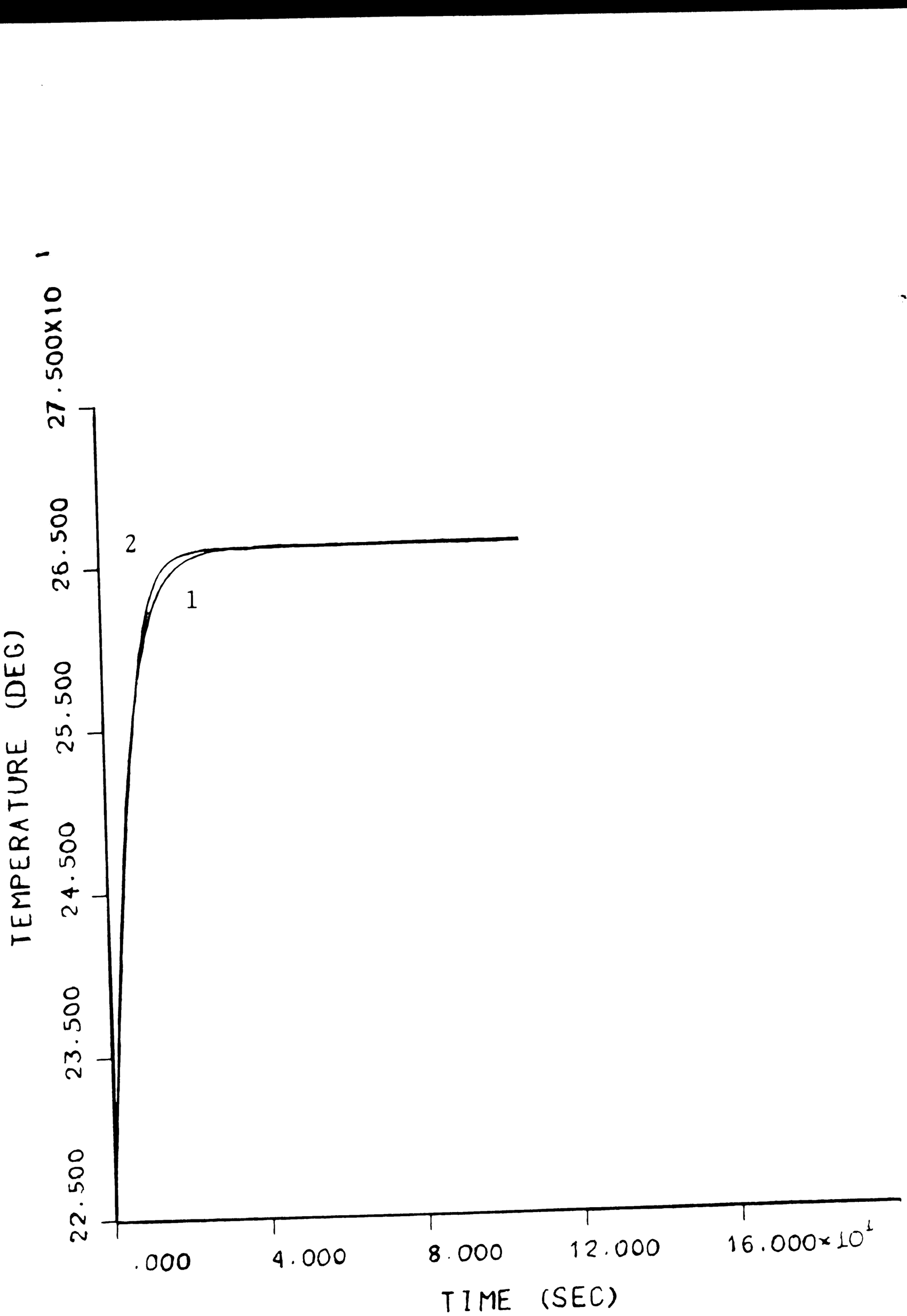

Figure 3.3 Dynamic responses of model B (1) and reduced model (2) to a change of initiator from #10 to #12.

(c_1 = -49.2157, c_2 = 9.7465).

3.3 Region of convergence.

Quasilinearization is known for its quadratic convergence to the optimum, but it appears to have a small region of convergence. The size of the region varies for different systems and becomes very small when strong nonlinearities are involved in the physical system. In addition, it has been observed that the data length affects the size of the region. With a large number of measurements a good initial guess is needed in order to secure convergence. Figures 3.4 and 3.5 display the region of convergence for our model for two cases:

1) the algorithm begins with ten measurements and gradually increases them to fifty,
2) the procedure employs fifty measurements from the beginning and keeps this number constant.

The enclosed area contains all the initial guesses for which the algorithm is able to identify parameters c_1 and c_2. However, this does not imply that outside that boundary divergence always occurs. In fact, the dots in Figures 3.4 and 3.5 indicate initial guesses for which successful runs occurred. Thus the limits of the region of convergence are not well defined, rather there is a transition area between the regions of convergence and divergence.

In the second case a reduction of the region is obtained which however is not significant. Moreover, there are points on the c_1, c_2 plane which are good initial guesses for this case but they cause

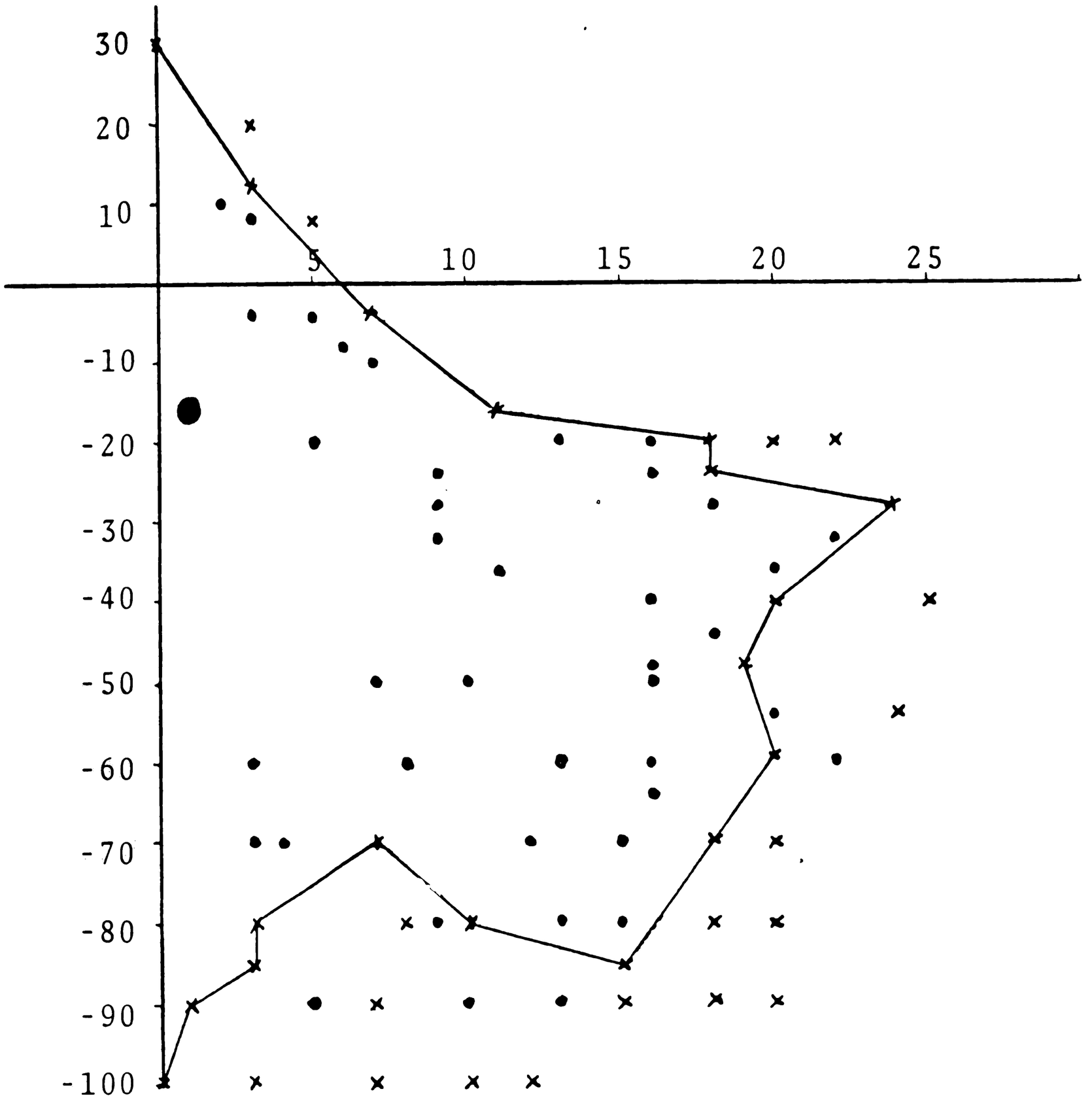

Figure 3.4 Region of convergence for the proposed model with N = j x 10 (j is the iteration number).

• successful run

* unsuccessful run

● exact values

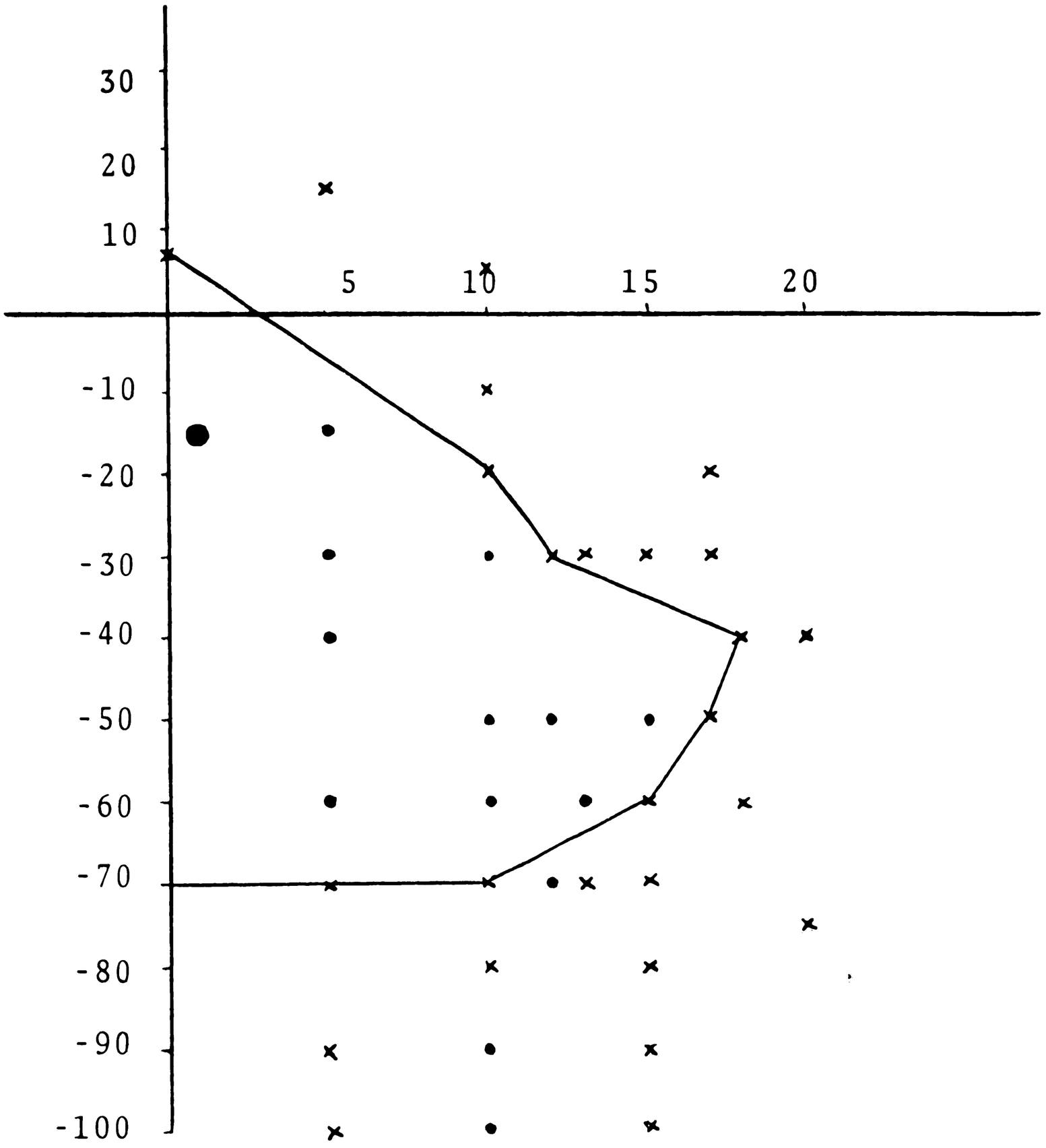

Figure 3.5 Region of convergence for the proposed model with N = 50.

• successful run

* unsuccessful run

● exact values

divergence in the first case (-100, 10). Consequently, we can say that an increased time interval may decrease the size of the region of convergence (closed area) but may not lessen the transition region.

The shape of the region could be explained by the fact that the output of the system, T, depends directly on c_2, since only c_2 is involved in the second equation of the model, and indirectly on the other parameter. Therefore a change in c_1 does not affect the output as much as a similar change in c_2 does. This can be seen also in the homogeneous solution matrix, which is the sensitivity matrix for outputs linearly related to the state [18], where ϕ_{22} is three orders larger than ϕ_{21}. For the above reason the region of convergence appears to be wider along the c_1 axis than along the c_2 axis.

3.4 State variables.

Of the two state variables of the reduced model, x_2 has been made to be the polymerization temperature, T, with excellent results, as we have seen in the previous sections of this chapter. Because on-line accurate measurements of the monomer concentration are not easy, only temperature T was considered in the output with the hope that x_1 will be close to the monomer concentration M, since the first equation came from the monomer equation of model A. However, this did not happen and x_1 has no physical meaning for the reactor. The fact

that we have changed significantly the equations from (2.4) to (2.5) when we forced them to satisfy the original steady state for every value of c_1 and c_2 can explain the above result. Thus our model represents the polymerization temperature T in the reactor with respect to feed temperature and feed initiator. Since x_1 is not the monomer concentration M, this can explain why the ratio c_2/c_1 is not equal to β in the proposed model.

3.5 Previous Reduced Model

Georgakis and Marini [18] have proposed a two equation model which, along with a "reaction rate controller", performs satisfactorily throughout the range of operating conditions of industrial interest. This model consists of two equations which basically come from a reduction of model A and have the following form:

$$\left.\begin{aligned} \dot{M} &= 1 - M - R \\ \dot{T} &= T_o - T + \beta R \end{aligned}\right\} \qquad (3.5)$$

where:

$$R = M\, F(T)\, \sqrt{I_o} \qquad \text{with}$$

$$F(T) = Da\, \exp[g(1-1/T)]\, \sqrt{r_i/(1+r_i+ar_ir_i)}.$$

$$Da = Da_P\, \sqrt{2f/Da_T}\ , \quad \gamma = \gamma_P - \gamma_T/2 \qquad \text{and}$$

$$r_i = Da_I \exp(\gamma_I - \gamma_I/T) .$$

Constant a takes into account the fluid dynamic characteristics of the reactor model and is given by:

$$a = 0.4 \frac{\text{mixing time}}{\text{residence time}} .$$

Figures 3.6, 3.7, 3.8 display a comparison between model B, reduced model by Georgakis-Marini and the proposed model.

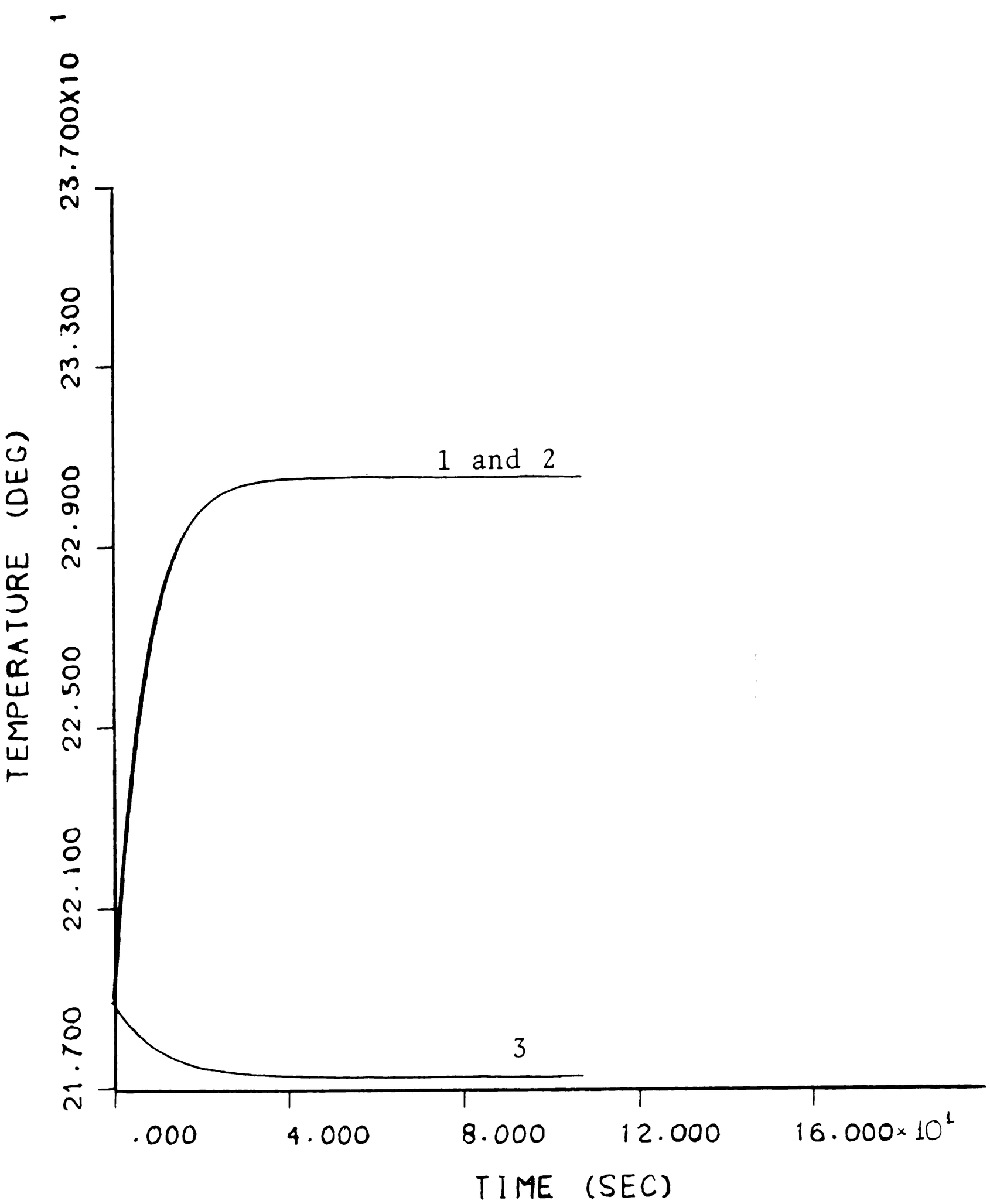

Figure 3.6 Comparison between model B (1), proposed model (2) and Georgakis-Marini reduced model (3) for a step change in feed initiator from 55.11 (mmol/h) to 91.85 (mmol/h).

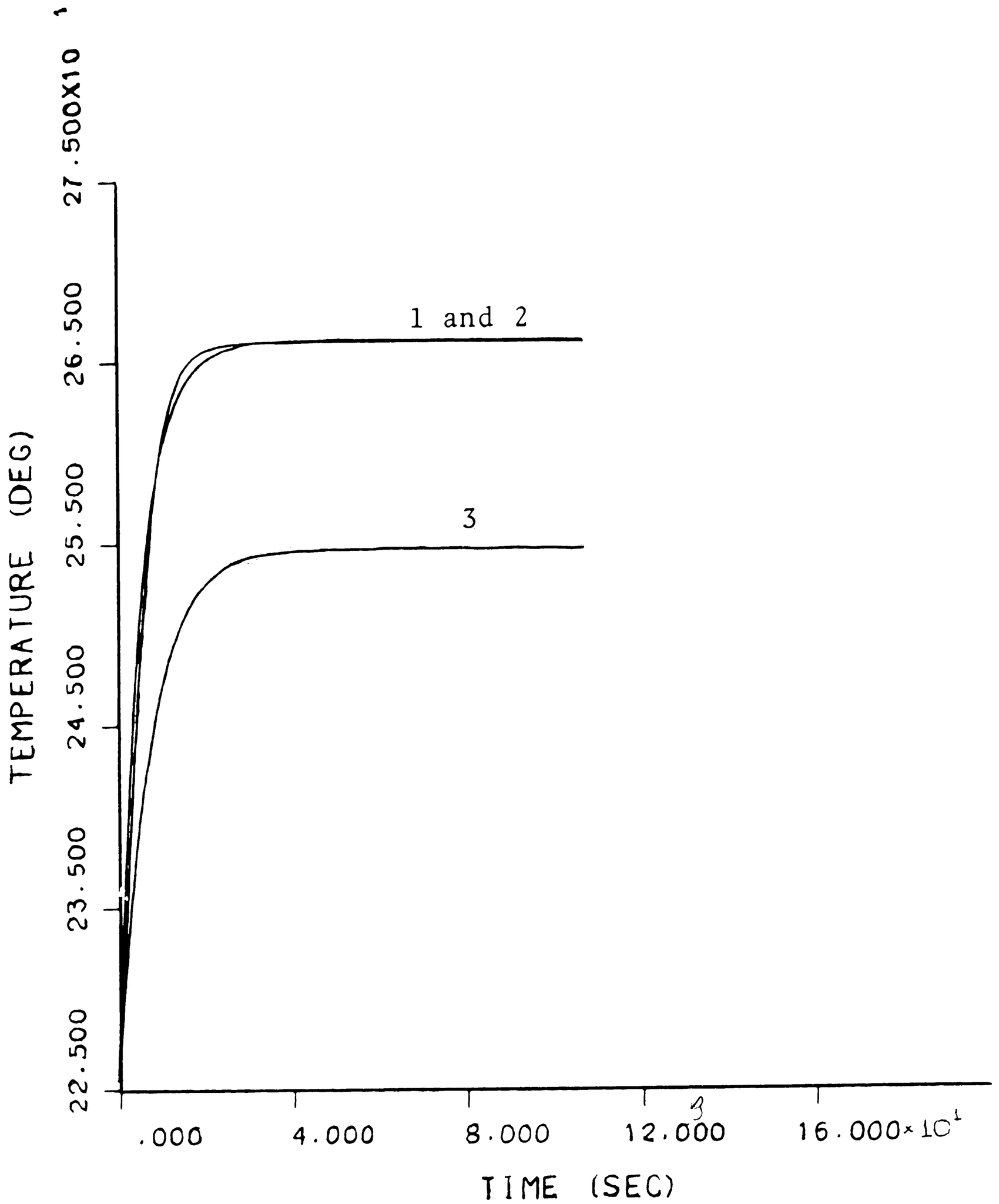

Figure 3.7 Dynamic responses of model B (1), proposed model (2) and Georgakis-Marini reduced model (3) and proposed model for a step change in feed temperature from 70°C to 60°C.

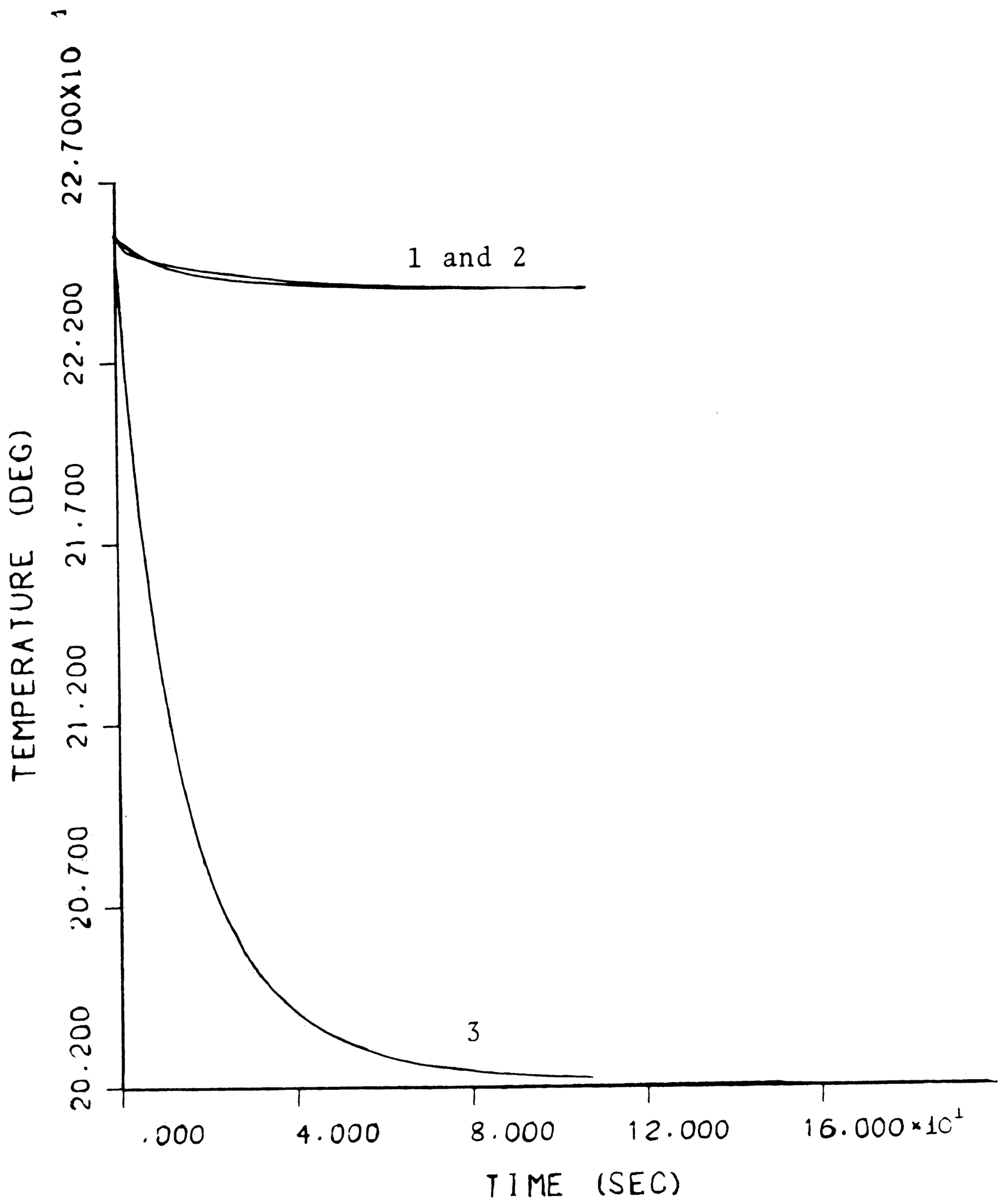

Figure 3.8 Dynamic responses of model B (1), proposed model (2) and Georgakis-Marini reduced model (3) and proposed model for a change of initiator from #10 to #12.

C O N C L U S I O N S

Employing a pseudosteady-state hypothesis for some of the system states, which is justified by the fact that these states have very small residues corresponding to the slow eigenvalues, a reduced model was obtained and then quasilinearization was used to identify the unknown parameters. The algorithm experienced no difficulty in converging when the initial guesses were close enough to the exact values. It was observed that the limits of the region of convergence are not well defined but there is a transition area between the regions of convergence and divergence.

The proposed model, a two-equation nonlinear model, accurately approximates the dynamic performance of a low-density polyethylene reactor for changes on type or quantity of initiator or feed temperature. In addition, it was found to exhibit significantly improved performance over a previously developed low-order model for the low-density polyethylene reactor by Marini and Georgakis.

Since measurements only from the reactor temperature were considered, one of the reduced model states represents the polymerization temperature but the other has no physical meaning for the reactor. However, this does not weaken the proposed model since in practice only temperature can be measured and thus used in control structures.

Attempts were also made to employ this approach in order to find a reduced model able to approximate more than one dynamic responses of the original system. Thus data from two dynamic responses were

considered and the parameters were successfully identified. Obviously, the approximations were not as good as in the case of one response considered. However, with a weighting factor one of the two approximations was improved while the second remained within acceptable limits of accuracy.

This work supports the fact that by combining quasilinearization and pseudosteady-state (where it is applicable) or sensitivity of the output to the several states for model reduction, simple and accurate low-order models can be obtained. This technique may be applied on practical situations where no need for the optimal reduced model exists. Its main advantages are those of quasilinearization: fast convergence and no need for measurements from all the system states. It seems promising even for on-line applications since with a small number of measurements it could be able to predict dynamic responses close to the real ones. Furthermore, if direct search optimization (14) or any other technique (9,11,12,13) is used along then the problem of small region of convergence could be overcome and successful runs are almost quaranteed.

Consequently, no claim of a rigorous method is made but some results are presented which support that quasilinearization is of great importance and can contribute to solving the problem of model reduction in practical situations and thus allowing the on-line use of control techniques on large scale dynamic nonlinear systems.

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RESUME

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Master of Science in Mechanical Engineering -- June, 1986.

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