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Low Order Empirical Modeling for Nonlinear Systems

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Abstract. A simple, low order, empirical model structure is presented for approximating the dynamic behavior of single-input, single-output *nonlinear* systems. The continuous-time polynomial structure chosen for the model is a reasonable blend of the generality offered by nonlinear first principles models, and the simplicity typically associated with empirical *linear* models. The chosen model structure is first motivated, and its analytical characteristics discussed; three surprisingly straightforward techniques for estimating the model parameters — strictly from input/output data — are then presented. The modeling procedure is illustrated and evaluated with two examples.

Keywords. Nonlinear Model Identification, Nonlinear Dynamics, Polynomial Systems, Parameter Estimation, Least Squares.

1 INTRODUCTION

Model-based control strategies have become important in chemical process control, but their performance in practice depends on the fidelity of the models they employ. In this respect, first principles models are highly desirable, but they are generally difficult to develop. In contrast, empirical models are generally poorer, less informative approximations, but are much easier to develop. This is particularly true of simple linear models, explaining the popularity of the first order linear model, in spite of the inherent nonlinearities of many processes.

The development of *nonlinear* empirical models is more difficult and is an active area of research (cf. for example: Billings, 1980, 1984; Diaz and Desrochers, 1988; Haber and Unbehauen, 1990; Bhat and McAvoy, 1990; Pottmann and Seborg, 1992; Read and Ray, 1993). In particular, once we abandon linearity, the choice of a nonlinear model structure is by no means obvious. This paper is concerned with the development of a new, continuous-time nonlinear model structure which *deliberately* seeks a compromise between the generality offered by first principles models, and the structural simplicity of linear models.

Our starting point is the following model:

$$\begin{aligned} \frac{d\mathbf{x}}{dt} &= f_1(\mathbf{x}) + g_1(\mathbf{x})u \\ y &= h_1(\mathbf{x}) \end{aligned} \tag{1}$$

where $\mathbf{x}$ is an n-dimensional state vector, and y is the scalar output. As indicated in Kantor, 1987, a substantial number of first principles models for various chemical processes have this form. When $n = 1$ and $h_1(x) = x$ this equation reduces to:

$$\frac{dy}{dt} = f(y) + g(y)u \tag{2}$$

As a specific example, note that the isothermal reactor of Eaton and Rawlings, 1991, is of this form. Further note that when $f(y) = ay$ and $g(y) = b$ this equation reduces to the linear first order model. Consequently equation (2) can be expected to describe a wide range of *first order-like* nonlinear processes.

2 THE EMPIRICAL MODEL

The generality of the functions $f(y)$ and $g(y)$ prevents (2) from being directly useful for input/output identification. However, by taking Taylor series expansions of these functions around some point $y = y_0$, and retaining up to the *second order* terms, so that the domain of validity is extended beyond that for linear approximations, we obtain:

$$\frac{dy}{dt} = \left(\phi_0 + \phi_1 y + \phi_2 y^2\right) + \left(\gamma_0 + \gamma_1 y + \gamma_2 y^2\right) u \tag{3}$$

The model structure in (3) is what we propose for approximating the input/output behavior of SISO nonlinear systems. The identification problem therefore becomes that of finding appropriate values for the ϕ and γ parameters by fitting the model in (3) to input/output plant data. Observe that this model equation has the well known linear and bilinear model forms as special cases.

Analytical Characteristics. The fundamental characteristics of the proposed model in (3) are determined

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from the autonomous case ($u = 0$):

$$\frac{dy}{dt} = \left(\phi_0 + \phi_1 y + \phi_2 y^2\right) \tag{4}$$

and it can be shown that the fundamental behavior of the scalar family of quadratic systems represented in (4) is characterized by the behavior of the solutions to the equation:

$$\frac{dz}{dt} = \left(a_1 z + a_2 z^2\right) \tag{5}$$

Given the initial condition $z = z_0$ at $t = t_0$, the solution for $a_1 \neq 0$, is:

$$z(t) = \frac{a_1 z_0 \left[1 + \tanh\left\{\frac{a_1}{2}(t - t_0)\right\}\right]}{a_1 - (2a_2 z_0 + a_1)\tanh\left\{\frac{a_1}{2}(t - t_0)\right\}} \tag{6}$$

By inspection of (5), there are two steady states, $z_{1s} = 0$ and $z_{2s} = -a_1/a_2$ associated with this solution; furthermore, the flow in and out of these solutions depend on the signs associated with the coefficients a_1 and a_2. Observe that one of these solutions always escapes in the finite time, t_f, defined by:

$$t_f = t_0 + \frac{2}{a_1}\tanh^{-1}\left(\frac{a_1}{2a_2 z_0 + a_1}\right) \tag{7}$$

(The corresponding results for $a_1 = 0$ are easily obtained.) It is useful to illustrate the range of behavior of this model with a simple example. Consider the special case: $\phi_0 = 0$, $\phi_1 = -1$, $\phi_2 = 0$, $\gamma_0 = 1$, $\gamma_1 = 0$, $\gamma_2 = \alpha$; i.e. the model

$$\frac{dy}{dt} = -y + u + \alpha y^2 u \tag{8}$$

The special case $\alpha = 0$ corresponds to a linear system with a steady-state gain of 1 and a time constant of 1. For $\alpha \neq 0$, increasing the magnitude of α corresponds to increasing the severity of the nonlinearity.

For any α, the response of this system to an input step of magnitude u^* may be computed analytically. For $\alpha < 0$, this response is always stable, but as α becomes very large, the step response saturates at a value that is independent of the input step size. For $\alpha > 0$ the qualitative nature of the step response changes dramatically at the critical input amplitude $u_c = 1/2\sqrt{\alpha}$. For $|u^*| \leq u_c$, this response is stable and asymptotically approaches the value y^* given by:

$$y^* = 2u^*\left(\frac{1 - \sqrt{1 - \lambda^2}}{\lambda^2}\right) \tag{9}$$

where $\lambda = |u^*|/u_c$. Note that for $\lambda = 1$, $y^* = 2u^*$, so that one effect of the nonlinearity is to double the system steady-state gain. When $|u^*| > u_c$ (i.e. when $\lambda > 1$), the system exhibits a finite escape time that becomes shorter as λ increases.

The main point of this example is that the nonlinear model proposed in (3) exhibits a computable range of "qualitative validity." Since finite escape times represent an extreme form of instability not found in chemical processes, the specific model discussed above is only qualitatively valid (for any $\alpha > 0$) over its region of stability $-u_c \leq u^* \leq u_c$; outside this region the model exhibits non-physical behavior. Conversely if $|u| \ll u_c$, the step response is approximately linear and there is no advantage in considering the more complex nonlinear model. While this behavior has been described here for a special case of (3), it is generic and will be discussed further in a subsequent full paper.

3 IDENTIFICATION FROM INPUT/OUTPUT DATA

Continuous Time Least Squares. For any given value of the parameters in (3), the error $e(t)$ between the RHS and LHS of the equation may be written as:

$$\frac{dy}{dt} - \left(\phi_0 + \phi_1 y + \phi_2 y^2\right) - \left(\gamma_0 + \gamma_1 y + \gamma_2 y^2\right) u = e(t) \tag{10}$$

Representing the vector of model parameters as

$$\theta = \left[\begin{array}{cccccc} \phi_0 & \phi_1 & \phi_2 & \gamma_0 & \gamma_1 & \gamma_2 \end{array}\right]^T \tag{11}$$

then, a *least squares* estimation strategy involves minimizing the quadratic objective:

$$J = \frac{1}{2}\int_0^T e^2(t)dt \tag{12}$$

The necessary condition for the minimum is given by: $\frac{\partial J}{\partial \theta} = 0$ or, equivalently

$$\int_0^T \left(e(t)\frac{\partial e}{\partial \theta}\right) dt = 0 \tag{13}$$

And now because this model is linear in the parameters, this condition simplifies considerably, and allows us to solve for the unknown parameters analytically. By observing that:

$$\begin{aligned} \frac{\partial e}{\partial \theta} &= \left[\begin{array}{cccccc} \frac{\partial e}{\partial \phi_0} & \frac{\partial e}{\partial \phi_1} & \frac{\partial e}{\partial \phi_2} & \frac{\partial e}{\partial \gamma_0} & \frac{\partial e}{\partial \gamma_1} & \frac{\partial e}{\partial \gamma_2} \end{array}\right]^T \\ &= \left[-1, -y, -y^2, -u, -uy, -uy^2\right]^T \end{aligned} \tag{14}$$

we see that upon introducing (10) the condition in (13) gives rise to 6 "normal equations" in the form:

$$\mathbf{A}\theta = \mathbf{b} \tag{15}$$

which may be solved for θ, the vector of parameter values. The elements of the matrix A and the vector b are obtained by integrating input/output data (cf. Ogunnaike *et al.* 1994, for further details).

Direct Integration. By direct integration, the model form in (3) becomes:

$$y(t_i) = y(t_0) + \int_{t_0}^{t_i} \left(\phi_0 + \phi_1 y + \phi_2 y^2\right) dt + \int_{t_0}^{t_i} \left(\gamma_0 + \gamma_1 y + \gamma_2 y^2\right) u(t) dt \quad (16)$$

and, without loss of generality, setting $t_0 = 0$, (16) reduces to

$$y(t_i) - y(0) = \phi_0 t_i + \phi_1 z_1(t_i) + \phi_2 z_2(t_i) + \gamma_0 w_0(t_i) + \gamma_1 w_1(t_i) + \gamma_2 w_2(t_i) \quad (17)$$

where

$$z_1(t_i) = \int_0^{t_i} y(t)dt; \qquad z_2(t_i) = \int_0^{t_i} y(t)^2 dt;$$
$$w_0(t_i) = \int_0^{t_i} u(t)dt; \qquad w_1(t_i) = \int_0^{t_i} y(t)u(t)dt;$$
$$w_2(t_i) = \int_0^{t_i} y(t)^2 u(t)dt$$

The model identification problem is now as follows: given input/output data $u(t_k), y(t_k); k = 1, 2, \ldots, N$, and $y(0)$, obtain estimates of the six model parameters using the equation:

$$y(t_i) - y(0) = \phi_0 t_i + \phi_1 z_1(t_i) + \phi_2 z_2(t_i) + \gamma_0 w_0(t_i) + \gamma_1 w_1(t_i) + \gamma_2 w_2(t_i) + \epsilon(t_i) \quad (18)$$

Here $\epsilon(t_i)$ represents the error associated with the model in this present form, and it consists of several components: *model structural error; observation error; other approximation errors.* (cf. Ogunnaike *et. al*, 1994). Observe that the system of N equations in (18) is of the standard linear regression model form:

$$\mathbf{y} = \mathbf{X}\theta + \epsilon \quad (19)$$

We may therefore employ *linear* parameter estimation techniques (such as *least squares*) to obtain optimal estimates of the six parameters in the original model equation.

The "Velocity" Form. Consider the situation in which the entire time interval (t_0, t_N) over which the data set has been collected is subdivided into several smaller time intervals, $T_1, T_2, \ldots, T_M$, where each T_i refers to the interval $t_{L_i} \leq t < t_{U_i}$, of length $\delta(T_i) = t_{U_i} - t_{L_i}$. Evaluating $y(t)$ at the boundaries of each interval using (16) yields:

$$y(t_{U_i}) - y(t_{L_i}) = \phi_0 \delta(T_i) + \phi_1 \tilde{z}_1(T_i) + \phi_2 \tilde{z}_2(T_i) + \gamma_0 \tilde{w}_0(T_i) + \gamma_1 \tilde{w}_1(T_i) + \gamma_2 \tilde{w}_2(T_i) \quad (20)$$

if we define

$$\tilde{z}_1(T_i) = \int_{t_{L_i}}^{t_{U_i}} y(t)dt; \qquad \tilde{z}_2(T_i) = \int_{t_{L_i}}^{t_{U_i}} y(t)^2 dt;$$
$$\tilde{w}_0(T_i) = \int_{t_{L_i}}^{t_{U_i}} u(t)dt; \qquad \tilde{w}_1(T_i) = \int_{t_{L_i}}^{t_{U_i}} y(t)u(t)dt$$
$$\tilde{w}_2(T_i) = \int_{t_{L_i}}^{t_{U_i}} y(t)^2 u(t)dt$$

i.e. an equation of the form:

$$\tilde{\mathbf{y}} = \tilde{\mathbf{X}}\theta + \tilde{\epsilon} \quad (21)$$

Equation (20) is a "velocity" (or differential) form of (17) in which, instead of integrals over the time interval $(0, t_i)$, of length t_i, and fixed origin $t = 0$, the integrals are taken over the intervals of length $\delta(T_i)$, and variable origin t_{L_i}. It is important to stress that despite appearances, it *does not* involve approximating a differential with a finite difference.

Modulating Functions. It is possible to unify — and extend — the preceding identification methods by employing the theory of modulating functions (cf. Co and Ydstie, 1990). By presenting each method in terms of modulating functions, we are able, among other things, to convert the parameter estimation problem to that of choosing the appropriate modulating function. These issues are discussed further in the subsequent full paper.

4 EXAMPLES

The Isothermal Reactor

The process (cf. Eaton and Rawlings, 1991) is an isothermal continuous stirred tank reactor in which a second order reaction is taking place; it is modelled by:

$$\frac{dy}{dt} = -ky^2 + \left(\frac{d}{V} - \frac{1}{V}y\right) u \quad (22)$$

where: y is the reactant concentration (mols/liter); u is the inlet flow rate (liters/hr); d is the inlet concentration of the reactant; k is the reactor rate constant, and V is the reactor volume. It is important to note that the model is precisely of the form in (3) with: $\phi_0 = 0; \phi_1 = 0; \phi_2 = -k$; $\gamma_0 = d/V; \gamma_1 = -1/V; \gamma_2 = 0$.

The actual plant parameters are $V = 10.51$ liters; $d = 3.5$ mol/liter; $kV = 15.8\ l^2$ mol/hour. The reactor is operated at the nominal conditions: $y = 0.5; u = 1.3$, with u constrained to lie between 1.0 and 3.0 liters/hr.

Results. The input shown in Figure 1 is a sequence of random steps with switching probability $P_s = 0.05$; the value at each transition is drawn from a gaussian distribution centered around the nominal condition $u = 1.3$ with variance $\sigma^2 = 1$.

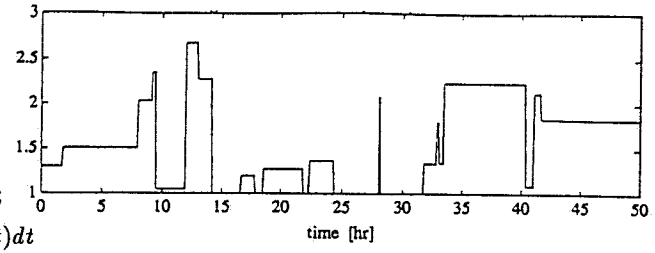

Fig. 1. Isothermal reactor input sequence

The "true" (continuous) process response to this input signal (obtained from (22)) is represented by the solid line in Figure 2; when this output is "sampled" with

$\Delta t = 0.1$ hrs, with 5% noise superimposed, the data is represented by the dots in Figure 2.

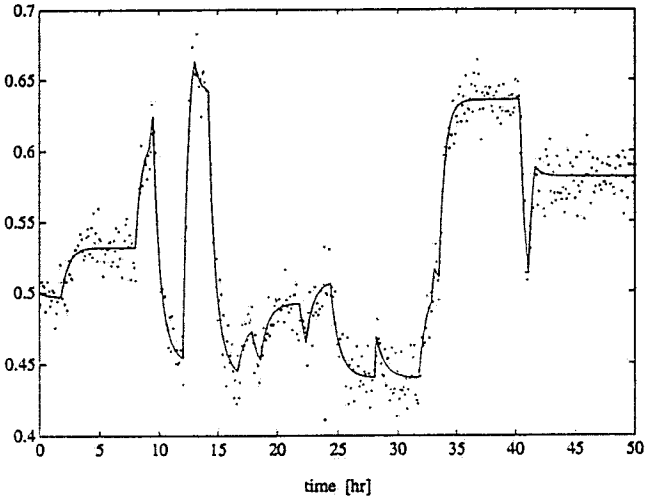

Fig. 2. Isothermal reactor output with 5% noise

In identifying the model in (3) from this input/output data set, we investigate first the situation in which the parameters ϕ_0, ϕ_1, γ_2 are pre-specified to be zero, and only the non-zero parameters are identified. The estimates returned for these parameters by the three identification schemes are summarized in Table 1 below:(*idct* refers to the continuous time least squares method; *dint* refers to the direct integration method; and *vint* refers to the "velocity" form).

TABLE 1: Estimates for the 3-Parameter Model

Parameter	Actual	idct	dint	vint
ϕ_2	-1.5033	-1.2692	-1.4573	-1.4114
γ_0	0.3333	0.2866	0.3413	0.3199
γ_1	-0.0951	-0.0899	-0.1271	-0.0975

These results demonstrate a dependence of the identified model parameters on the identification method. This dependence is not yet fully understood and is the subject of continuing investigation. Based on the preliminary results presented here however, it appears that the "velocity" form of the identification algorithm gives the best results. This is certainly true for the three parameter model identification results presented above.

As might be expected, the situation deteriorates when the entire set of of six parameters are identified from input/output data without constraining any of them to be zero. However the *prediction ability* of the identified models remains quite good. Another random step sequence (not shown, but different from the one used for the identification) is used to validate the identified models. The model responses to this validation sequence are shown in Figure 3, where the solid line represents the "true" process response. Observe that the reactor output predicted by the different models match the "true" output very well. *Relative prediction error variances* are shown in Table 2 below for both the 3-parameter model and the 6-parameter model.

TABLE 2: Relative prediction erorr variances

Model Type	idct	dint	vint
3-parameter	9.09E-05	3.18E-05	3.39E-05
6-parameter	2.11E-04	1.22E-04	1.81E-04

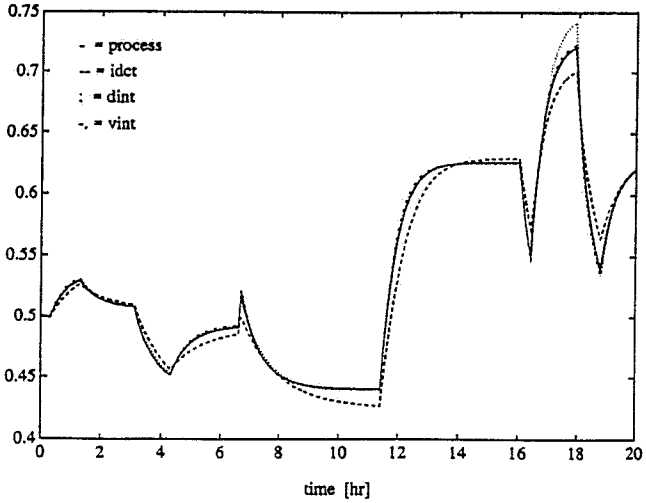

Fig. 3. Isothermal reactor model prediction

The Polymerization Reactor

The process in this case is the reactor used for the free-radical polymerization of methyl methacrylate with AIBN as initiator and toluene as solvent, discussed in detail in Congalidis *et al.*, 1989. The model employed in this example is as presented in Doyle *et al.*, 1992:

$$\begin{aligned} \dot{x}_1 &= 10(6 - x_1) - 2.4568 x_1 \sqrt{x_2} \\ \dot{x}_2 &= 1.342649(1 - u) - 10.1022 x_2 \\ \dot{x}_3 &= 0.0024121 x_1 \sqrt{x_2} + 0.112191 x_2 - 10 x_3 \\ \dot{x}_4 &= 245.978 x_1 \sqrt{x_2} - 10 x_4 \\ y &= \frac{x_4}{x_3} \end{aligned} \tag{23}$$

Here, the process input, u, is the initiator flow rate (m^3/hr), and the process output y is the number average molecular weight; the four state variables x_1, x_2, x_3, x_4 are respectively, the monomer concentration, the intiator concentration, the zeroth bulk moment, and the first bulk moment. The nominal operating conditions are given as: $u = 0.016783 m^3/hr$; $x_1 = 5.506774 kmol/m^3$; $x_2 = 0.132906$ kmol/m^3; $x_3 = 0.0019752$ kmol/m^3; $x_4 = 49.38182$ kg/m^3; $y = 25000.5 kg/kmol$. The initiator flow rate is constrained to lie between the values $0.0046 m^3/hr$ and $0.1164 m^3/hr$ in order to keep the number average molecular weight in the range 10000 to 40000 kg/kmol.

Observe that unlike the first example, this polymer reactor model is *not* of the form in (3). This allows us to investigate the ability of the proposed empirical model to approximate nonlinear systems of arbitrary form.

For this particular example, there is the additional practical issue of input and output variable scaling:

since the output variable is roughly 6 orders of magnitude larger than the input, it is essential to work in terms of variables scaled by respective nominal operating conditions. Thus, the model identification is carried out for this process using dimensionless variables $\bar{y} = y/25000.5$ and $\bar{u} = u/0.016783$.

Results. The issue of input selection is of particular importance for this process; but for the purpose of the current discussion, we merely state that an input sequence of the type shown in Figure 4 is essential in order to capture the true nonlinear essence of this process. Observe that this input sequence is a combination of a *low amplitude* sequence of random steps followed by a higher amplitude sequence. The first half of the specific sequence shown in Figure 4 is a sequence of random steps with switching probability $P_s = 0.05$, with the value at each transition drawn from a *uniform distribution* in the range $u = [0.0046, 0.016783]$; the random steps in the second half also have a switching probability of 0.05 but the values are drawn from a uniform distribution in the range $u = [0.016783, 0.1164]$.

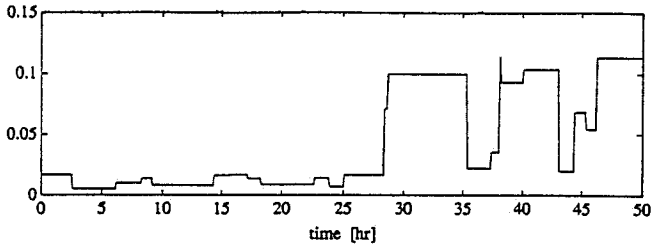

Fig. 4. Polymer reactor input sequence

As with the first example, the "true" continuous polymer reactor response to this input signal is obtained from (23); this is represented by the solid line in Figure 5. This output is "sampled" with $\Delta t = 0.1$ hrs, with 5% noise superimposed, and the resulting data is represented by the dots in Figure 5. The input/output data set thus generated (and made nondimensional as explained earlier) is used to identify the model in (3) by the three schemes. The resulting parameter estimates are summarized in Table 3 below.

TABLE 3: Estimated model parameters for the Polymer Reactor

Parameter	Actual	idct	dint	vint
ϕ_0	NA	0.4459	0.8200	-0.1640
ϕ_1	NA	0.7065	1.2282	2.8761
ϕ_2	NA	-0.4672	-0.6574	-1.2592
γ_0	NA	0.1261	-0.3070	-0.3707
γ_1	NA	-0.3625	1.2242	1.7379
γ_2	NA	-0.4353	-2.2757	-2.7817

As in the previous example, these results demonstrate a very strong dependence of the estimated parameters on the particular identification method used. Unlike the previous example, however, there are no "correct" parameter values, since the "true" model is not of the form (3). Consequently, in addition to the algorithm dependence of the estimated parameters discussed in the last example, we can expect additional variability in the estimated results due to the mismatch between the forms of the equations (3), and (23). Specifically, note that the question "what model of form (3) best approximates equation (23)?" will depend on how we define "best". This issue is an additional complication that is also under investigation. Nevertheless, the following results on the prediction ability of the three different models illustrate that, as in the previous example, the model predictions are good enough to warrant further consideration in spite of the observed variability in the estimated parameters.

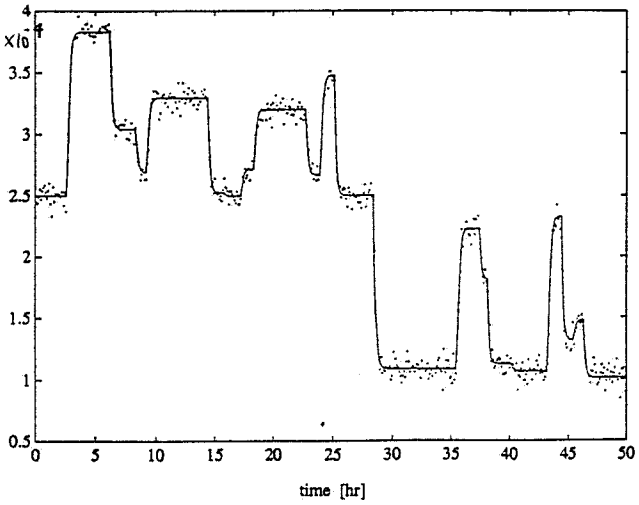

Fig. 5. Polymer reactor output with 5% noise

First, a validation sequence of random steps (not shown, but different from the one in Figure 4) is used as input to these identified models and the observed responses are compared with the corresponding "true" process response in Figure 6. The predictions obtained from the model identified by the direct integration method, and that from the model identified using the "velocity" form (the dotted line, and the dashed-dotted line respectively) match the actual response better than the prediction obtained using the results of the continuous time least squares method.

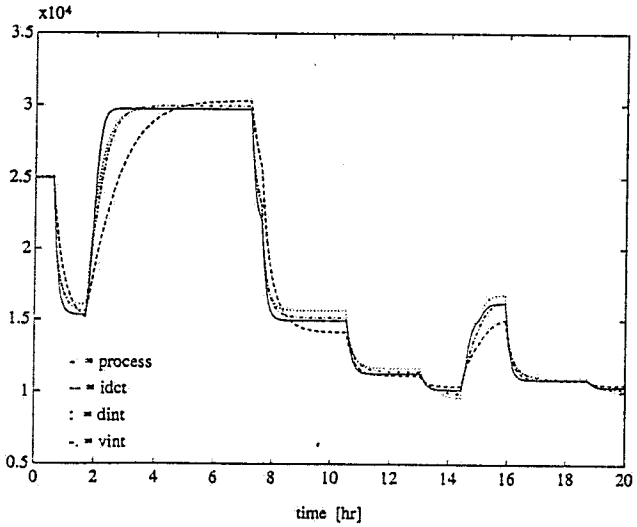

Fig. 6. Polymer reactor model prediction

Next, Figure 7 shows responses to a relatively *large* step-up (from 0.016783 to 0.1164) and a relatively *small* step-down (from 0.016783 to 0.0046) in initiator flow rate; the "true" process step responses are shown in the solid lines. Observe that in general, the model captures the asymmetric nonlinearity exhibited by the process quite well. Also, the models predict the *lowering* of the number average molecular weight in response to an initiator flow rate step-up remarkably well. The prediction of the step-down response (an increase in the molecular weight average) is not as precise dynamically, but the steady state gain is estimated with remarkable accuracy. It is important to keep in mind that these empirical models have been able to capture the dynamics of this polymer reactor, represented by the set of equations in (23), with a single differential equation and only *six* parameters.

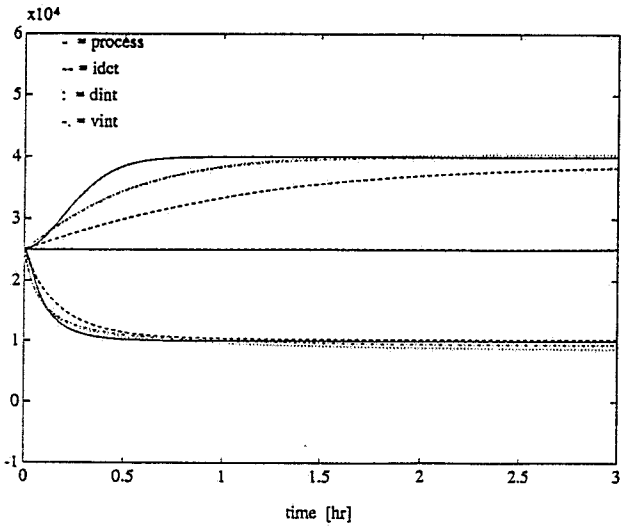

Fig. 7. Polymer reactor step responses

5 SUMMARY/CONCLUSIONS

We have presented a simple, low order, empirical model structure for input/output modeling of single input, single output systems. We have also presented three schemes by which this model can be identified from input/output data. Two process examples were used to illustrate and evaluate the applicability of the proposed model, and the model identification schemes.

The results we have presented here have implications for the practical application of nonlinear control theory: the proposed model form has been shown as capable of adequately approximating important nonlinear process behavior; the model parameters can be estimated by employing the same familiar linear regression methods used for *linear* model identifiction; and, the model's simple structure makes it easy to use as the basis for nonlinear control system design. (cf. for example Doyle, 1994).

Additional issues currently being explored include: (i) the extension of these empirical model identification concepts to higher order, as well as multivariable nonlinear systems; (ii) the development of specific controller design techniques based on this class of models.

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