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Developments of Bilinear Models for Some Chemical Processes

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ABSTRACT. Bilinear models of some chemical processes were developed. The responses to various input changes were obtained with and without implementation of a recursive parameter estimation algorithm. Bilinear models are shown to be able to approximate the simulated processes more accurately than linear models. An approximation of a high order bilinear process by a first order bilinear model is also presented, and shown to be satisfactory.

1. Introduction

Nonlinear systems are described by complex nonlinear differential equations whose solution is difficult. Usually, linear approximation of a nonlinear system is possible only when the behavior of the system is confined in the region around some normal operating level.

The class of bilinear models has been introduced as a tool for examining many nonlinear phenomena[1]. As an approximation to general nonlinear plant, the bilinear model can provide a more accurate representation than the linear one[2]. Many successful applications results can be found in the literature[1,3] which illustrate the effectiveness of the use of bilinear models as approximations for nonlinear systems. It has been reported[4] that for a general plant in which the control appears linearly, a dynamically equivalent bilinear model can be found.

In this paper, approximations of some nonlinear and bilinear chemical processes by first order bilinear models are introduced. Comparison between linear and bilinear approximations with and without parameter estimation is also presented.

2. Continuous Stirred Tank Reactor (CSTR)

The simulated continuous stirred-tank reactor (CSTR) process consists of an irreversible, exothermic reaction $A \rightarrow B$, in a constant reactor cooled by a single coolant

stream which can be modeled by the following equations:

$$C_A(t) = a_1(C_{A0} - C_A(t)] - k_0 C_A(t)\exp(a_3 / T(t)] \tag{1}$$

$$T(t) = a_1[T_0 - T(t)] + a_2 C_A(t)\exp[a_3 / T(t)] + a_4 C_A(t) q_c(T_{c0} - T(t)] - a_4 q_c \exp[a_5 / q_c(t)](T_{c0} - T(t)) \tag{2}$$

where,

$$a_1 = (q/V); a_2 = [(-\Delta H\, k_0)/(\rho\, C_p)]; a_3 = -E/R;$$
$$a_4 = [(\rho_c\, c_{pc})/(\rho c_p V)]; a_5 = [(-hA)/(\rho_c\, c_{pc})]$$

The nominal CSTR parameters used in the simulation are as follows[5]:

C_A	Measured product concentration = 0.1 mol/l
T	Reactor temperature = 441 K
q_c	Coolant flow rate = 100 l/min
C_{A0}	Feed concentration = 1 mol/l
T_0	Feed temperature = 350 K
T_{c0}	Inlet coolant temperature = 350 K
V	CSTR volume = 100 l
hA	heat transfer term = 7×10^5 cal min^{-1} K^{-1}
k_0	Reaction rate constant = 7.2×10^{10} min^{-1}
E/R	Activation energy term = 1×10^4 K
ΔH	Heat of reaction = -2×10^5 cal/mol
ρ, ρ_c	Liquid densities = 1×10^3 g/l
C_p, C_{pc}	Specific heats = 1 cal g^{-1} K^{-1}

Linearization around the steady state values of reactor temperature (T_{ss}) and coolant flow rate (q_{cs}) is carried out for the exponential terms: $\exp[a_3/T(t)]$ and $q_c(t)\exp[a_5/q_c(t)]$. Using Taylor's series expansion yields:

$$\exp[a_3/T(t)] = \exp[a_3/T_{ss}] - [T(t) - T_{ss}](a_3/T_{ss}^2)\exp[a_3/T_{ss}] \tag{3}$$

$$q_c(t)\exp[a_5/q_c(t)] = q_{cs}\exp[a_5/q_{cs}] + a_6[q_c(t) - q_{cs}] \tag{4}$$

where $a_6 = [1 - (a_5/q_{cs})]\exp(a_5/q_{cs})$

Substitution of equations (3) and (4) into equations (1) and (2) and rearranging will yield the following bilinear model for CSTR:

$$T(t) = b_1 T(t) + b_2 C_A(t) + b_3 C_A(t)T(t) + b_4 q_c(t)T(t) + b_5 q_c(t) + b_6 \tag{5}$$

$$C_A(t) = b_{c1} C_A(t) + b_{c2} C_A(t)T(t) + b_{c3} \tag{6}$$

where
$$b_1 = -a_1 + a_4 q_{cs} \exp(a_5 / q_{cs}) - a_5 a_6 q_{cs}$$
$$b_2 = a_2 \exp(a_3 / T_{ss}) + (a_2 a_3 / T_{ss}) \exp(a_3 / T_{ss})$$
$$b_3 = -(a_2 a_3 / T_{ss}^2) \exp(a_3 / T_{ss})$$
$$b_4 = -a_4 + a_5 a_6$$
$$b_5 = a_4 T_{c0} - a_5 a_6 T_{c0}$$
$$b_6 = a_1 T_0 - a_4 q_{cs} \exp(a_5 / q_{cs}) + a_5 a_6 q_{cs} T_{c0}$$
$$b_{c1} = -a_1 - k_0 \exp(a_3 / T_{ss}) - (k_0 a_3 / T_{ss}) \exp(a_3 / T_{ss})$$
$$b_{c2} = (k_0 a_3 / T_{ss}^2) \exp(a_3 / T_{ss})$$
$$b_{c3} = a_1 C_{A0}$$

The parameters of Equations (5) and (6) are estimated at each sampling period using a recursive least square method (RLS) with a variable forgetting factor[6]. The coolant flow rate was changed from an initial value of 100 l min^{-1} to 110, to 100, to 90, and back to 100, at 7 min intervals.

Figures 1 to 4 show the concentration and temperature responses to step changes in the coolant flow rate (q_c) with and without recursive parameters estimation. The figures show the results for the simulated CSTR, the bilinear models, and the linear models. It can be seen from the figures that bilinear models describe the dynamics of the CSTR more accurately than linear models which are included for the sake of comparison. Considerable improvement in the predictions of bilinear and linear models is observed when parameters estimation algorithm is implemented.

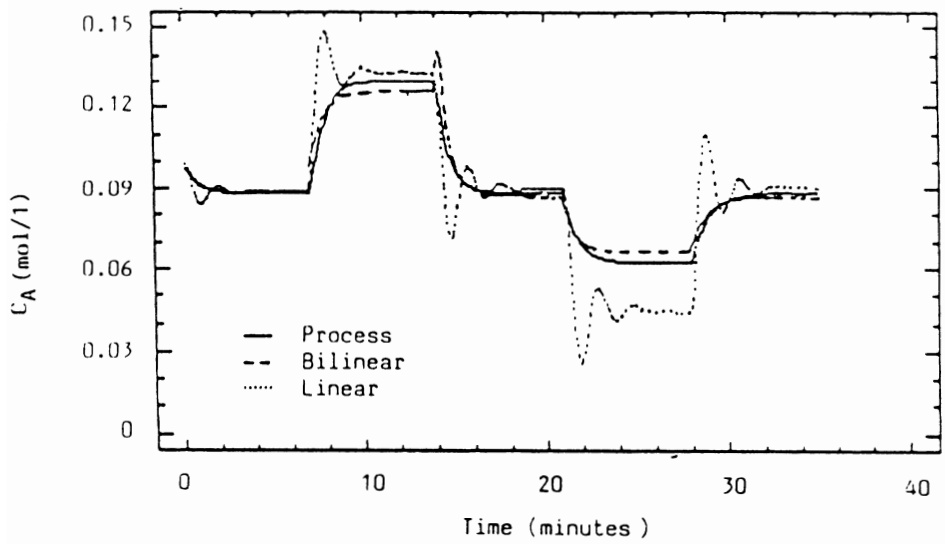

FIG. 1. Concentration response of CSTR without parameter estimation.

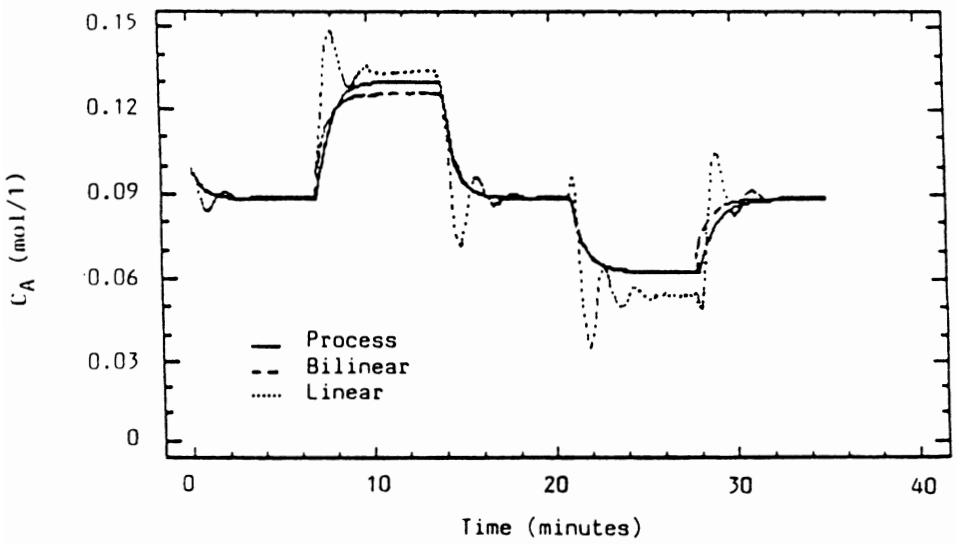

FIG. 2. Concentration response of CSTR with parameter estimation.

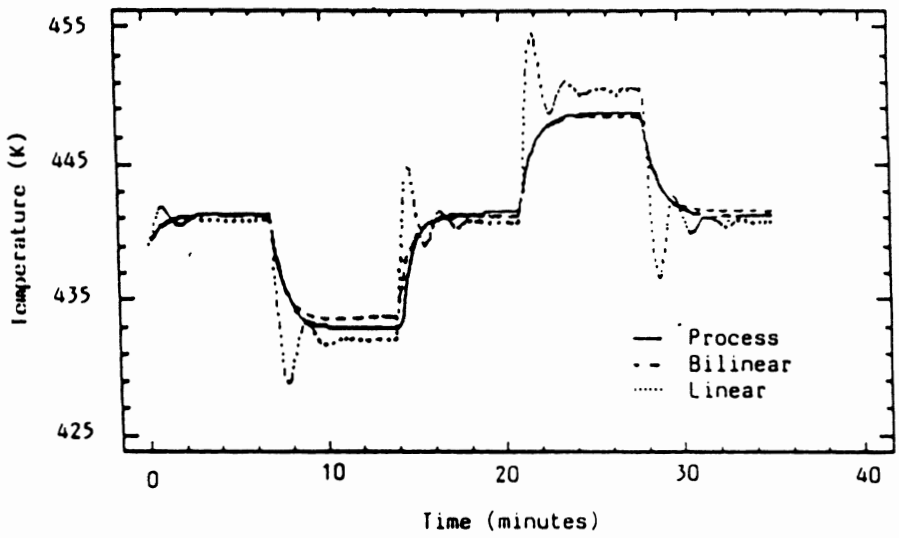

FIG. 3. Temperature response of CSTR without parameter estimation.

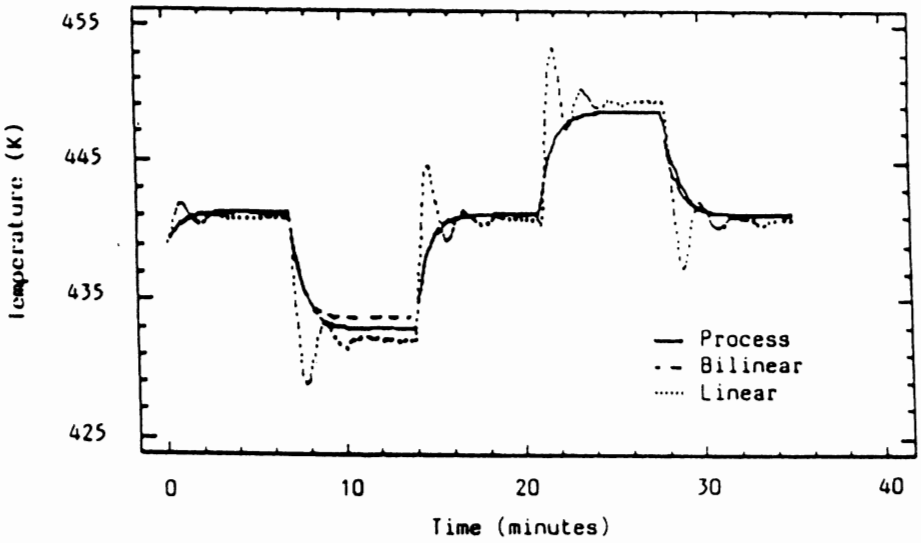

FIG. 4. Temperature response of CSTR with parameter estimation.

3. Plate Heat Exchanger (PHE)

In modeling PHE, the following assumptions were made[7]:

1. Heat losses to the surroundings are negligible.
2. Heat transfer within the fluid in any channel is by convection only.
3. The fluid will split equally between the parallel channels for each stream.
4. Thermal capacity of the plate wall is negligible.
5. The temperature distributions in all channels belonging to the same streams are identical.
6. The heat-transfer film coefficient depends mainly on the hot fluid velocity.
7. The physical properties of the fluid are constant over the range of temperature employed.
8. The rate of change of the cold-stream outlet temperature is identical to that of the hot stream.

3.1 Energy Balances

3.1.1 Cold Stream Side

$$V_c(dT_{co}/dt) = F_c T_{ci} - F_c T_{co} + [UA/(\rho c_p)]\Delta T_{lm} \tag{7}$$

where,

$$\Delta T_{lm} = [(T_{hi} - T_{co})] - (T_{ho} - T_{ci})]/\log[(T_{hi} - T_{co})/T_{ho} - T_{ci})] \tag{8}$$

3.1.2 Hot Stream Side

$$V_h(dT_{ho}/dt) = F_h T_{hi} - F_h T_{ho} - [UA/(\rho c_p)]\Delta T_{lm} \tag{9}$$

The nominal operating conditions used in this paper can be summarized as follows:

C_p specific heat = 1 cal g^{-1} $°C^{-1}$
F_c volumetric flow rate of cold stream = 3.5 l min^{-1}
F_h volumetric flow rate of hot stream = 2 l min^{-1}
T_{ci} inlet temperature of cold stream = 31°C
T_{co} outlet temperature of cold stream = 40°C
T_{hi} inlet temperature of hot stream = 60.5°C
T_{ho} outlet temperature of hot stream = 40.5°C
V_c volume of cold side channels = 1.0 l
V_h volume of hot side channels = 1.0 l
A heat transfer area = 1.0621 m^2
ρ liquid density = 1000 g/l

The overall heat-transfer coefficient (U) is a function of the hot stream mass flow rate (ρF_h) as follows[8]:

$$(1/U) = 1.2 \times 10^{-3} + \{7.06 \times 10^{-5} / [\rho F_h]^{0.95}\} \tag{10}$$

Experimental data reported by Al-Azahrani[7] indicates that T_{ho} is very close to T_{co}. Therefore, they can be substituted for each other without appreciable error. The following first-order discrete bilinear model can be obtained by incorporating the above assumptions into Equations (7) and (9):

$$\hat{T}_c(k) = (1 - (T_s F_c / 2V_c))T_c(k-1) + (T_s / 2V_h)F_h(k-1)T_c(k-1) + (T_s / 2V_h)T_{hi}F_h(k-1) \tag{11}$$

which can be rewritten as follows:

$$\hat{T}_c(k) = \hat{a}_1 T_c(k-1) + \hat{b}_1 F_h(k-1)T_c(k-1) + \hat{c}_1 F_h(k-1) \tag{12}$$

where $T_c = T_{co} - T_{ci}$ = process output; $\hat{T}_c$ = model output; $\hat{a}_1$, $\hat{b}_1$, $\hat{c}_1$ are mode parameters; F_h = manipulated variable; T_s = sampling time.

Similarly, second and higher order bilinear models can be constructed depending on the degree of approximation of the derivative terms in Equations (7) and (9).

Figure 5 shows the responses of the outlet temperature of the cold stream to step changes in the flow of the hot stream, which was changed from an initial value of 2 l min^{-1} to 3, to 2, to 1, and back to 2, at 5 min intervals. The figure shows the results of the simulated PHE, the bilinear model and the linear model when a parameter estimation algorithm is implemented. As it can be seen from Fig. 5, the bilinear model approximates the simulated PHE dynamics more accurately than the linear one. The response of the linear model shows large deviations from the simulated model for the negative step in the flow rate of the hot stream (1 l min^{-1}). For positive steps, small deviations are observed.

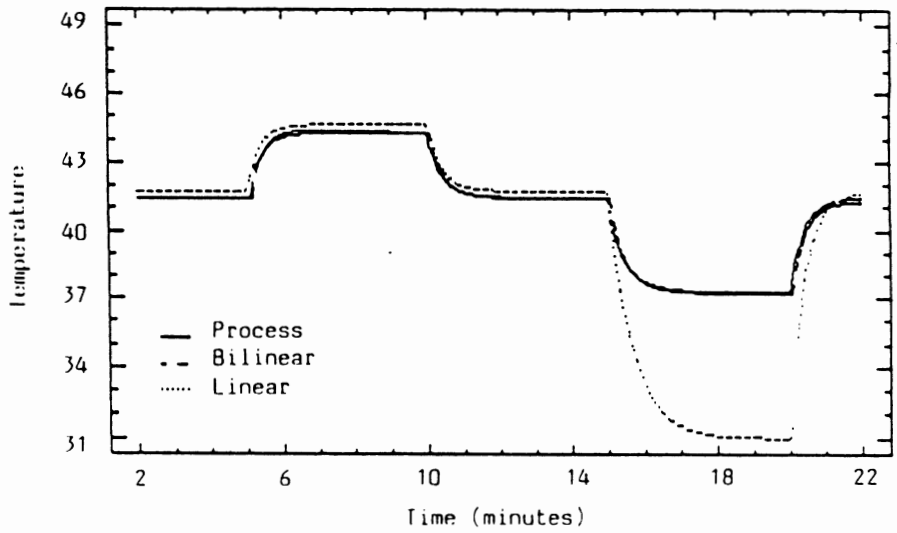

FIG. 5. Temperature response of PHE with parameter estimation.

4. Bilinear Processes

Bilinear models arise naturally in many chemical processes, where mass and energy balances contain products of flows and temperatures or concentrations. The order of those bilinear models may be high, which makes controller design complex. As an example of such processes, assume that a process can be described completely by a third order discrete, bilinear model of the form:

$$\begin{aligned} Y(k) = {} & 0.6Y(k-1) - 0.3Y(k-2) + 0.25Y(k-3) + 0.3Y(k-1)\,U(k-1) \\ & + 0.2Y(k-2)U(k-2) - 0.15Y(k1-3)U(k-3) + 0.5U(k-1) + \\ & 0.4U(k-2) + 0.3U(k-3) + d(k) \end{aligned} \tag{13}$$

where Y is the process output; U is the process input; and d is a step disturbance.

A first order bilinear model approximation of the process represented by Equation (13) gives:

$$Y_K^M = \hat{a}_1 Y_{k-1} + \hat{b}_1 Y_{k-1} U_{k-1} + c_1 \hat{U}_{k-1} \tag{14}$$

where Y^m is the model output.

The parameters of Equation (14) are estimated at each sampling instant using RLS with forgetting factor.

Figure 6 shows the responses of the process (Eq. 13) and the bilinear model (Eq. 14) to step changes in U which was changed from 0 to 1, to 0, to –1, and back to 1, at 5 min intervals. The figure shows that the response of the first bilinear model is very close to that of high order bilinear process (Eq. 13). The simulation was also conducted using a

second order bilinear model as an approximation for Equation (13), but no improvement in the approximation was observed over that of the first order one. Simulations were also conducted for higher order bilinear processes using bilinear model approximations with different orders whose parameters are estimated via RLS. The first order bilinear model approximation was found to be satisfactory.

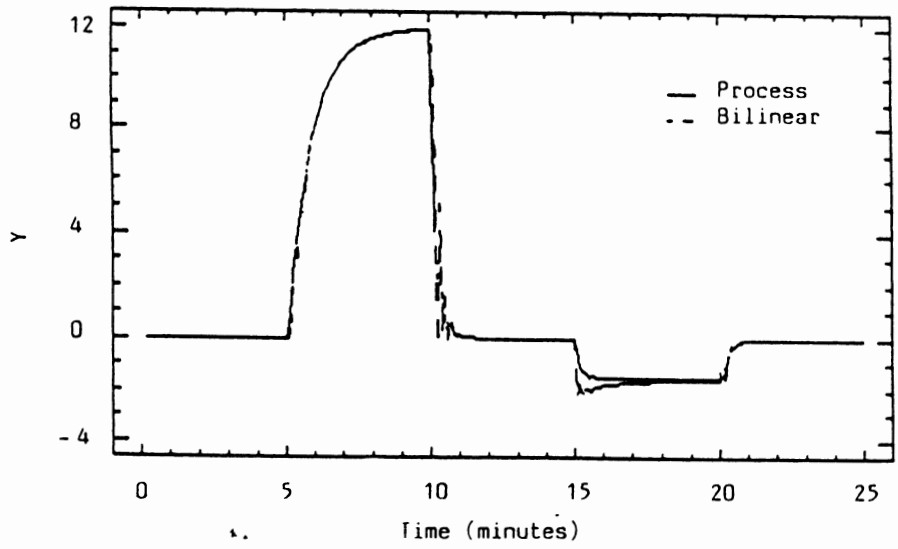

FIG. 6. Response of bilinear process with parameter estimation.

5. Conclusion

Approximations of CSTR and PHE by bilinear models have been described. The predictions of the bilinear models and the linear one for various input changes are obtained. The results are obtained with and without implementation of a parameter estimation algorithm (RLS). Simulations show that bilinear model approximates the process more accurately than the linear one. A considerable improvement in the responses is observed when a parameter estimation algorithm (RLS) is implemented. An approximation of a high order bilinear process with a first order bilinear model is also presented. The approximation was found to be satisfactory for various input changes.

References

[1] **Mohler, R.R.** and **Kolodiej, W.J.,** An overview of bilinear system theory and applications, *IEEE Trans. Sys. Man. Cybern,* SMC-10, **41:** 193 (1980).

[2] **Yeo, Y.K.** and **Williams, D.C.,** Bilinear model predictive control, *Ind. Eng. Chem. Res.,* **26:** 2257 (1987).

[3] **Mohler, R.R.,** *Bilinear Control Processes,* Academic Press, New York (1973).

[4] **Lo, J.T.H.,** Global bilinearization of systems with control appearing linearly, *SIAM J. Control,* **13:** 879 (1975).

[5] **Morningred, J.D., Paden, B.E., Seborg, D.E.** and **Mellichamp, D.A.,** An adaptive nonlinear predictive controller, *Chem. Eng. Scie.*,**47**(4): 755 (1992).

[6] **Ydstie, B.E.,** Adaptive process control, *Chem. Eng. Res. Des.*, **65:** 480 (1987).

[7] **Al-Zahrani, A.A.,** Adaptive bilinear model predictive control, *Proceedings of ASME Inter. Conf. on System Analysis & Design, London (UK), Sep.* **1**(2): 116-125 (1993).

[8] **Khan, A.R., Baker, N.S.** and **Wardle, A.P.,** The dynamic characteristics of a counter current plate heat exchanger, *Int. J. Heat & Mass Transfer*, **83:** 1269-1278 (1988).

Nomenclature

A	heat transfer area [m^2]
C_A	measured product concentration [mol/l]
C_{A0}	feed concentration [mol/l]
C_p	heat capacity [cal g^{-1} $^{\circ}C^{-1}$]
E/R	activation energy term [K]
F_c	volumetric flow rate of cold stream [l min^{-1}]
F_h	volumetric flow rate of hot stream [l min^{-1}]
h	heat transfer coefficient [cal m^{-2} min^{-1} K^{-1}]
ΔH	heat of reaction [cal/mol]
k_0	reaction rate constant [min^{-1}]
q_c	coolant flow rate [l/min]
T	reactor temperature [K]
T_0	feed temperature [K]
T_{c0}	inlet coolant temperature [K]
T_{ci}	inlet temperature of cold stream [°C]
T_{co}	outlet temperature of cold stream [°C]
T_{hi}	inlet temperature of hot stream [°C]
T_{ho}	outlet temperature of hot stream [°C]
V	CSTR volume [l]
V_c	volume of cold side channels [l]
V_h	volume of hot side channels [l]
ρ	liquid density [g/l]

تطـوير نمـــاذج شبـــه خطيـــة لبعض العمليـــات الكيميائيـــة

عبد الرحيم أحمد الزهراني

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جـــــدة - المملكة العربية السعودية

المستخلص . تم تطوير نماذج شبه خطية لبعض العمليات الكيميائية . كما تمت دراسة استجابة النماذج لعدة تأثيرات خارجية باستخدام معاملات للنماذج ثابتة أو تقديرها دوريًا . وقد بينت الدراسة أن للنماذج شبه الخطية قدرة ممتازة لتقريب العمليات الكيميائية بدقة أكثر من النماذج الخطية . كما تمت دراسة إمكانية تقريب العمليات الكيميائية شبه الخطية من ذوات الدرجة العالية بنماذج خطية من الدرجة الأولى ، وكانت النتائج مرضية .