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A Method of Model Validation for Chaotic Chemical Reaction Systems Based on Neural Network

Hwi Jin Kim and Kun Soo Chang†

Department of Chemical Engineering and Automation Research Center,
Pohang University of Science and Technology, San 31 Hyoja Dong, Pohang 790-784, Korea
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Abstract−A chaotic system with measurable state variables fewer than the degrees of freedom of the system is identified with the Artificial Neural Network (ANN) method combined with dynamic training. Instead of using the usual method of Sum of Square Errors (SSE), the identified models are validated with the return maps (embedded trajectories), the largest Lyapunov exponent, and the correlation dimension when there is no exogenous input, and bifurcation diagram when there is an exogenous input. This method is demonstrated for nonisothermal, irreversible, first-order, series reaction A→B →C in a CSTR.

Key words: Chaos, Neural Network, Dynamic Training, System Identification, Model Validation

INTRODUCTION

Complicated dynamic behavior occurs in many chemical processes involving chemical reactions, heat and mass transfer, separations and fluid flow because of their strong nonlinearity. Process engineers usually want to keep process conditions stable and under control to obtain a product with desired specifications of uniform properties. Very often in industrial processes, however, unexpected complex dynamic behavior is encountered even without external disturbances because of the inherent nonlinearity of the processes. In the past, a considerable number of studies have been carried out for processes showing multiple steady states, oscillatory behavior and chaos [Jorgensen and Aris, Coworkers, 1983, 1986; Doedel and Coworkers, 1986; Hudson and Coworkers, 1984, 1986, 1991; Lynch, 1992, 1993; Elnashaie et al., 1994, 1995; Ray and Coworkers, 1981, 1984, 1989, 1992, 1995, 1996]. Most of the studies are based on the mathematical models of systems derived from governing physical laws. In actual industrial processes, however, it is usually very difficult to obtain suitable physical models of processes because of both the complexity of the processes and the lack or inaccuracy of the system parameters. Even if obtained, the models derived from first principles are too mathematically involved and acquires too excessive computation to be performed online for many industrial applications such as in control and optimization. Another recourse is to use black box models determined by system identification techniques. Once models are obtained, they can be used as the surrogate models for prediction, control and optimization of the processes. Well-known stochastic difference equation models such as (N) ARMAX model, Artificial Neural Network (ANN) model and continuous-time model (i.e., set of ordinary differential equations) are used as basis models in this approach. Recently, ANN model has been widely used in process identification and control because of its ability to describe nonlinear systems. It generally shows better prediction than linear stochastic difference equation models. It can even describe steady state multiplicity and oscillatory behavior of the state variables of the system, and also provide the parameter ranges that lead to these types of behavior. This inherent capability of ANN is due mainly to the combination of nonlinear transfer functions used for each node. In many actual industrial processes, it is usually impossible to measure all state variables of the system. Reconstruction method [Packard et al., 1980; Takens, 1981; Sauer et al., 1991] can be applied to alleviate this physical limitation. From reconstructed state vectors of the system, we can reconstruct an attractor that is topologically equivalent to the attractor composed of the original state vectors of the system, and the reconstructed attractor will retain the dynamical invariants of the original attractor such as Lyapunov exponents, fractal dimension and entropy, if the embedding dimension is larger than twice the box-counting dimension of the original attractor [Sauer et al., 1991]. When ANN is combined with the dynamic training method based on the historical database of available state variables, it can also serve as a powerful tool to describe and predict the original dynamic behavior of the system, even in the case that the number of measurable state variables is less than the degrees of freedom of the system.

In the black-box model approach, regardless of the structure of basis models and the identification method used to get model parameters, the validation of an estimated model is one of the most important steps. The validation criteria to be satisfied depend on the characteristics of the system and also on the final application objective of the model. A trivial way of validating an identified model is to compare the time series of the original system with the time series generated by the model and to calculate the mean square errors between them. However, this criterion is just a necessary condition for an identified model to capture the dynamical properties of the system; it is definitely not sufficient. In case of a chaotic system, although the initial prediction of an identified model can be very accurate, predicted values diverge from the original time series at much later prediction time no matter how good the model is. This is due to the inaccuracies in the model and the existence of positive Lyapunov exponents. Because nearby trajectories diverge locally in state-space for a chaotic system, the initial error due to the model-

†To whom correspondence should be addressed.
E-mail: kschang@postech.ac.kr

ing error, however small, is magnified. The model generated time series thus becomes completely different from the original time series in the long run. Consequently, for a chaotic system, mere comparison of time series and calculation of the mean square error does not necessarily give useful information for the validation of an identified model. Therefore, more sophisticated criteria are required. One of the criteria is to compare the reconstructed attractors. Because there exists a smooth invertible transformation between the original states and the reconstructed states with appropriately chosen delay time and embedding dimension, we can check if an identified model captures the original dynamic behavior of the system by comparing the reconstructed attractor from the time series of the original system with that from the model-generated by time series. In many cases, however, although the location and the overall shape of the reconstructed attractors look similar and thus the dynamic behavior of the system seems to have been reasonably captured, detailed characteristics such as the density of trajectories in some region of the attractor and the local divergence rate of nearby trajectories are somewhat different. Therefore, other criteria like Lyapunov exponent and correlation dimension that quantify numerically the matching between the dynamic behavior are also required. In nonlinear control systems, it is of primary importance to predict qualitative changes in the system behavior as a control parameter is varied. Because a bifurcation diagram is the plotting of steady state solutions of a system over a range of parameter values, it gives needed information on the systems nonlinear dynamical phenomena. Therefore, in case an identified model is used for control purposes, checking whether the model reproduces the bifurcation pattern of the original system or not can be a useful validation criterion. There are many related papers available in the literature (some of the papers are listed in Reference, from Abarbanel et al. to Wolf et al.).

In this paper, we identify a chaotic system with measurable state variable fewer than the degrees of freedom of the system and validate the identified models with the criteria used for nonlinear dynamics instead of SSE. We do this through the following example.

PROCESS MODEL

To show how the technique applies to real processes, and also to show the step-by-step procedure involved and the various computational techniques used, we consider the dynamic behavior occurring in a nonisothermal CSTR with two irreversible consecutive first-order reactions, A →B→C: the first exothermic, the second endothermic. We pick the reaction system described by the following dimensionless differential equations used by Kahlert et al. [1981]. Although we assume that these equations represent the system we study, we are not supposed to know these equations explicitly.

$$\frac{dx_1}{dt} = 1 - x_1 - Dax_1\exp\left[\frac{x_3}{1+\varepsilon x_3}\right]$$

$$\frac{dx_2}{dt} = -x_2 + Dax_1\exp\left[\frac{x_3}{1+\varepsilon x_3}\right] - DaSx_2\exp\left[\frac{\kappa x_3}{1+\varepsilon x_3}\right]$$

$$\frac{dx_3}{dt} = -x_3 + DaBx_1\exp\left[\frac{x_3}{1+\varepsilon x_3}\right] - DaB\alpha Sx_2\exp\left[\frac{\kappa x_3}{1+\varepsilon x_3}\right] - \beta(x_3 - u)$$

where the variables x_1 and x_2 denote the dimensionless concentrations of species A and B, x_3 is the dimensionless temperature in the reactor, Da is the Damköhler number, ε is the dimensionless activation energy, S is the ratio of the two rate constants, κ is the ratio of activation energies, B is the dimensionless adiabatic temperature rise, α is the ratio of heat effects, β is the dimensionless heat transfer coefficient, and u is the dimensionless coolant bath temperature and can be viewed as an externally manipulatable variable. The bifurcation analysis of the system equation is carried out by using numerical continuation techniques which are implemented in the software package AUTO [Doedel, 1986]. From the analysis, we can obtain the bifurcation diagram in Fig. 1 which classifies the parameter space into regions where qualitatively different dynamic behavior is observed.

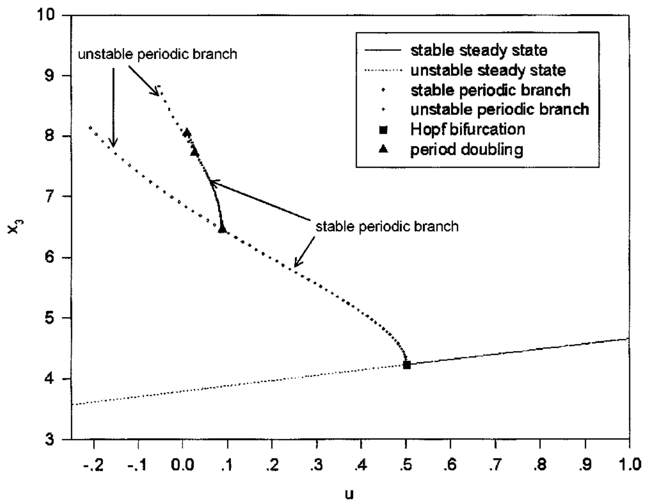

Fig. 1. Bifurcation diagram of the system.

When the system parameter values are Da=0.26, ε=0.0, S=0.5, κ=1.0, B=57.77, α=0.42, and β=7.9999, the bifurcation diagram is obtained with control input *u* as the bifurcation parameter. The horizontal axis is the bifurcation parameter *u* and the vertical axis is state variable x_3 itself for stationary solutions and the maximum value of state variable x_3 for periodic solutions. There is a Hopf bifurcation point indicated by solid square at u=0.5027. It represents the possible onset of oscillatory behavior along a branch of solutions. At this point, the Jacobian matrix of the system equations has a pair of purely imaginary eigenvalues. Solid triangles denote period doubling bifurcation points. These points are characterized by a Floquet multiplier leaving or entering the unit circle at "−1." When the periodic branch is traced, it loses stability at this point, and a new periodic branch with double period emerges. This period doubling can occur repeatedly and lead to deterministic chaos. This is the period-doubling route to chaos and provides a possible scenario leading to chaos. In Fig. 1, only the first few members of the periodic doubling cascade are shown. Although AUTO based on numerical continuation techniques can locate period doubling bifurcation points, it cannot be used to detect the exact location of chaotic oscillation. It can still provide, however, useful bounds for the domain of existence of chaos. From Fig. 1, we can infer that chaos may emerge somewhere around u=0.0. To check this, we simulated the system equations when the system parameter values are Da=0.26, ε=0.0, S=0.5, κ=1.0, B=57.77, α=0.42, β=7.9999 as before, and u=0.0,

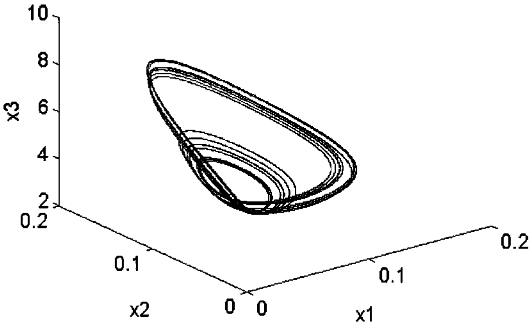

Fig. 2. 3-D phase portrait of the system.

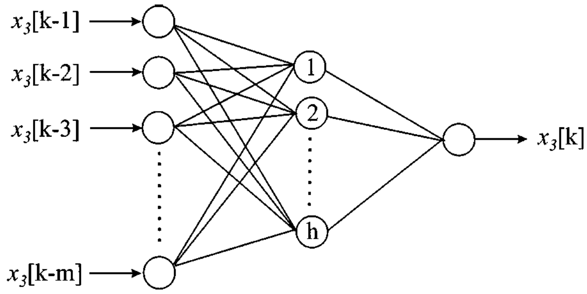

Fig. 3. Schematic representation of ANN in case of no exogenous input.

that is, when there is no control action. The simulation was carried out on IBM RS6000/370 using the IMSL subroutine ode_adams_gear. Fig. 2 shows the 3-D phase portrait of the system.

In Fig. 2, we see that the system demonstrates deterministic chaos. However, mere inspection of the attractor does not provide conclusive evidence on the existence of chaos since an orbit with large period can look similar in the phase plane. We can check the deterministic chaos by calculating the largest Lyapunov exponent and correlation dimension. The calculation was carried out for the time series data of the system using in-house implementations of the Wolf's algorithm [Wolf et al., 1985] for the largest Lyapunov exponent and the Grassberger and Procaccia algorithm [Grassberger and Procaccia, 1983] for correlation dimension. The obtained values are 0.00446 for the largest Lyapunov exponent and 1.535 for correlation dimension as summarized in Table 1.

SYSTEM IDENTIFICATION AND MODEL VALIDATION

In ANN, important steps are in the selection of appropriate number of layers and of neurons in each layer, and the choice of the transfer function used for each neuron and the training algorithm in order to obtain a good identified model. Usually, a trial and error procedure based on the criterion of minimization of sum of squares of ANN training errors is used for this purpose. For chaotic systems, however, this criterion may not provide useful information since identified models can show different dynamical behavior even though the training errors are roughly the same. Therefore, we validate identified models with the criteria such as return maps, the largest Lyapunov exponent, correlation dimension and bifurcation diagram instead of SSE. Then we determine the optimal ANN model describing the systems nonlinear dynamical behavior.

In this paper, we assume that not all state variables are measurable, which is often the case in many actual industrial processes. We assume only one state variable x_3 (temperature) is measurable. We try the three layer feed forward neural network combined with the dynamic training method based on the phase space reconstruction method to describe the chaotic system, and determine the optimal model by adapting only both the number of inputs to the ANN and the number of neurons in the hidden layer. The inputs to the ANN consist of historical database of the state variable x_3 when there is no exogenous input (u), and those of both the state variable x_3 and control input (u) in case exogenous input (u) exists. Each neuron in the hidden layer has the sigmoidal activation function, while the linear activation function is used for the output layer. The biases of the neurons in the input layer are assumed to be zero. The dynamic training method reviewed by Bhat and McAvoy [1990] with Levenberg-Marquardt optimization algorithm is used to train the network, and the training was carried out on DEC Alpha Server2100 using MATLAB.

1. In Case of No Exogenous Input

We now determine the optimal ANN model which best describes the chaotic behavior of the system itself at specified parameter values when there is no control action (u=0). Test ANN models used can be expressed as follows and the schematic representation of the models is shown in Fig. 3:

$$x_3[k]=f(x_3[k-1], x_3[k-2], \ldots, x_3[k-m])$$

where m is the number of delayed inputs, i.e., embedding dimension.

To train the test ANN models, a data set is generated from the system equation in section 2 with sampling period of 0.001 dimensionless time when only state variable x_3 (temperature) is measurable. This corresponds to the time delay between delayed inputs in the test ANN models. SSE is used to train the ANN models. First we check if the identified models capture the dynamic behavior of the original system by return maps. The time series data are assumed to lie on Poincaré section. Among an enormous number of candidates having roughly the same SSE, we found three candidates by trial and error which seem to describe the return maps of the original system closely. The number of delayed inputs(m) is 8 for all

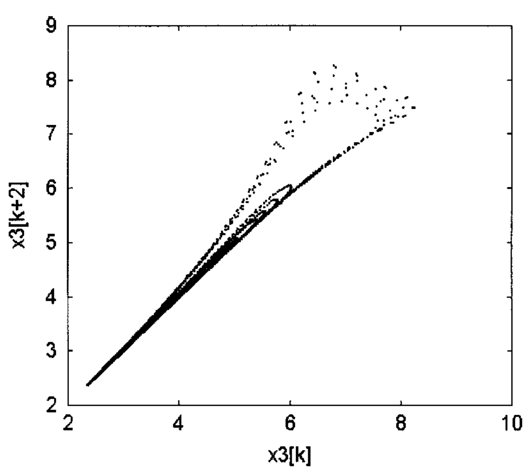

Fig. 4. Second return map of the original system.

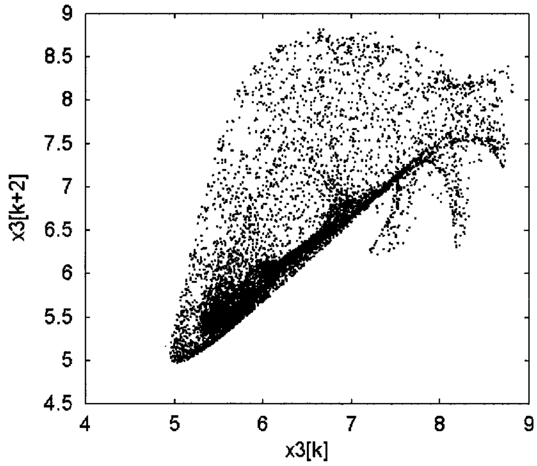

Fig. 5. Second return map of the ANN with h=3.

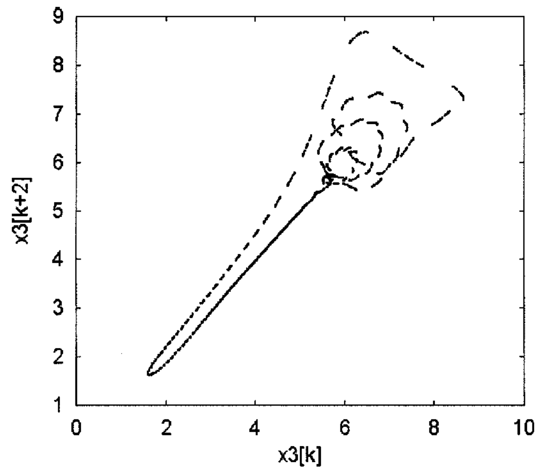

Fig. 6. Second return map of the ANN with h=4.

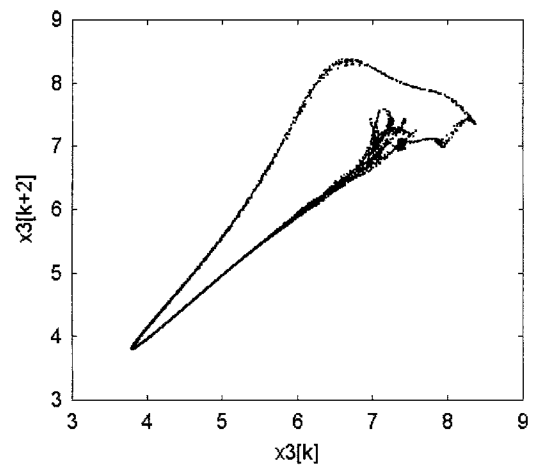

Fig. 7. Second return map of the ANN with h=5.

candidates, but the number of hidden nodes(h) is 3, 4 and 5, respectively. Fig. 4 denotes the second return map of the original system reconstructed from the time series of the state variable x_3, and Figs. 5-7 show the second return maps of the time series generated from the candidate models.

Table 1. Summary of the largest Lyapunov exponent and correlation dimension

	The largest Lyapunov exponent	Correlation dimension
Original system	0.00446	1.535
ANN with h=3	0.03824	2.127
ANN with h=4	0.002247	1.157
ANN with h=5	0.0197	1.078

In the figures, we find that the overall shape and the location of the return maps of the ANN with 4 and 5 hidden nodes are close to those of the return map of the original system. However, because the detailed characteristics of the return maps are somewhat different, we also calculate the largest Lyapunov exponent and correlation dimension to check the matching between the dynamics quantitatively. The calculations were carried out by using the previous method, and the obtained values are summarized in Table 1. From the results, we can conclude that the ANNs with 8 delayed inputs and 4 or 5 hidden nodes are the possible models to describe the chaotic behavior of the original system.

2. In Case of Exogenous Input

In this case, we validate identified models by checking if the models can predict the qualitative changes in the nonlinear behavior of the original system as the control input is varied. This can be done by bifurcation analysis. By checking where and how to bifurcate in bifurcation diagrams, we can determine the number of delayed inputs, delayed exogenous (control) inputs and hidden nodes of the optimal model which reproduces most faithfully the bifurcation pattern of the original system. Test ANN models can be expressed as follows and a schematic representation of the models is shown in Fig. 8.

$$x_3[k]=f(x_3[k-1], x_3[k-2], \ldots, x_3[k-m], u[k-1], u[k-2], \ldots, u[k-n])$$

where m is the number of delayed inputs, and n is the number of delayed exogenous inputs.

To identify the test ANN models, the input/output data set in Fig. 9 and 10 is generated from the system equation in section 2. The sampling time from the equation is 0.001 dimensionless time, corresponding to the time delay between two successive data points in

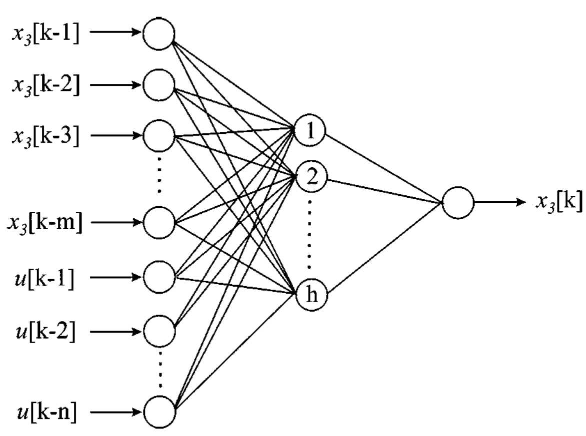

Fig. 8. Schematic representation of ANN in case of exogenous input.

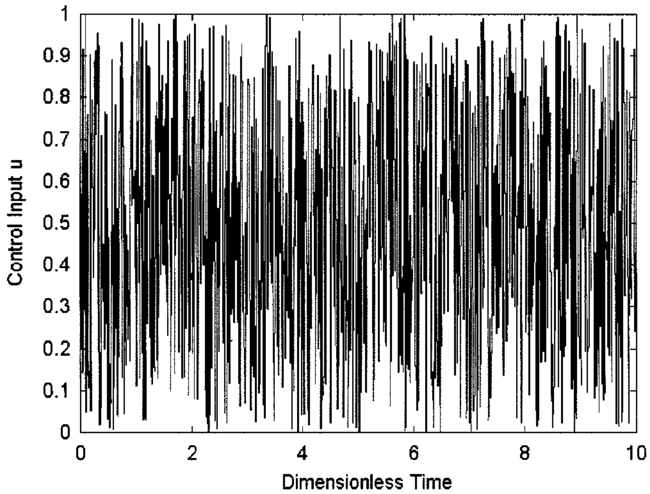

Fig. 9. Input data used in the identification in case of exogenous input.

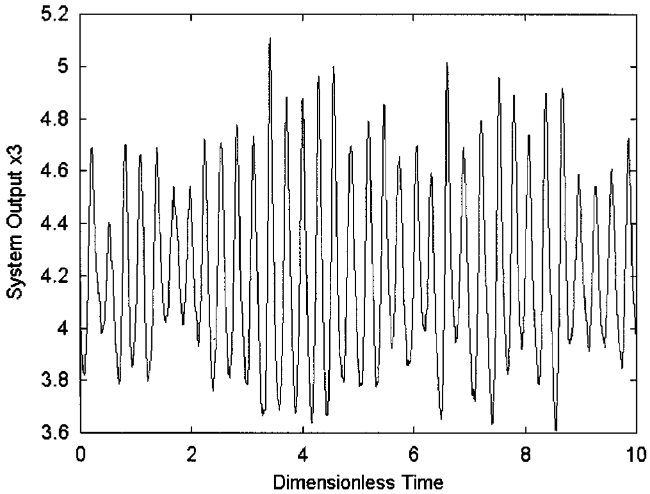

Fig. 10. Output data used in the identification in case of exogenous input.

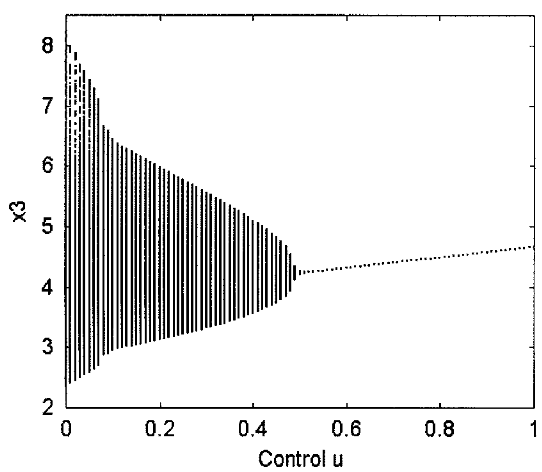

Fig. 11. Original system's bifurcation diagram.

the above test ANN models. The input used is composed of random numbers between 0 and 1 that are held constant for 0.01 dimensionless time.

Among an enormous number of candidates, we found three candidates by trial and error which seem to reproduce the bifurcation pattern of the original system closely. Fig. 11 shows the bifurcation

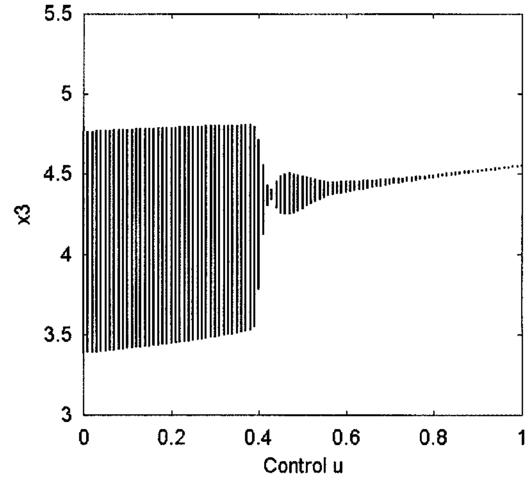

Fig. 12. Bifurcation diagram of the ANN with (m, n, h)=(8, 5, 7).

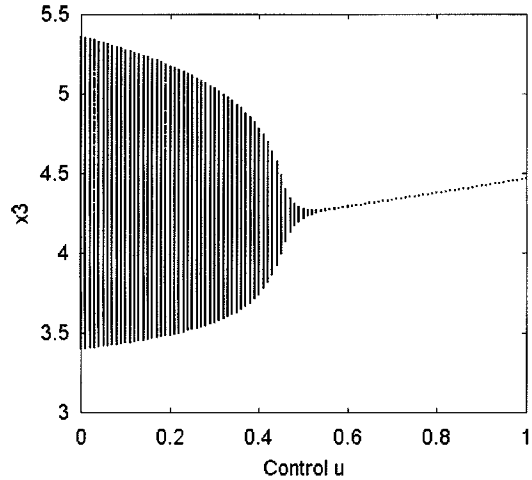

Fig. 13. Bifurcation diagram of the ANN with (m, n, h)=(8, 5, 8).

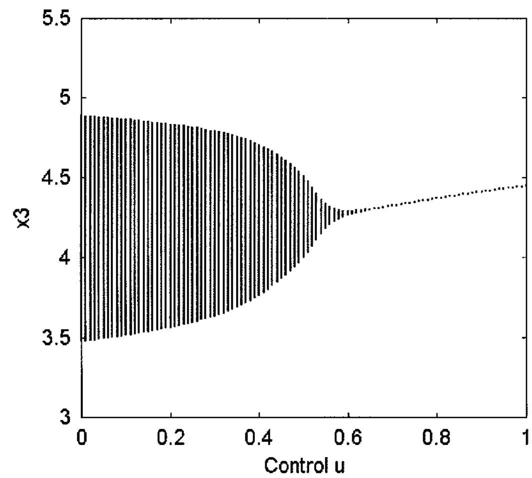

Fig. 14. Bifurcation diagram of the ANN with (m, n, h)=(8, 5, 9).

diagram of the original system and Figs. 12-14 denote the bifurcation diagrams generated from the time series of the candidate models when the number of delayed inputs (m) is 8 and the number of delayed exogenous inputs(n) is 5, but the number of hidden nodes(h) is 7, 8 and 9, respectively. We observe that the overall shape, the scale and the location of bifurcation of the ANN model with 8 hidden nodes are the closest to those of the original system. Note that the bifurcation diagrams show somewhat different behavior although the SSEs in ANN training are roughly 0.002 for all cases.

CONCLUSIONS

The identification and validation issues occurring in the chaotic system with observable state variable less than the degrees of freedom of the system are considered. ANN models are used as basis models. The technique is demonstrated through the nonisothermal, irreversible, first-order, series reaction A→B→C in a CSTR. In chaotic systems, because of the inaccuracies in models and the existence of positive Lyapunov exponents, the direct comparison of time series and calculation of SSE does not give much information for validation purposes. Therefore, more sophisticated criteria, such as return maps, Lyapunov exponents and correlation dimension in case of no exogenous input, and bifurcation diagram in case of exogenous input, should be used to validate the identified models. Then from the results, we can determine the optimal number of delayed (exogenous) inputs and hidden nodes, leading to the validation of the dynamic model.

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NOMENCLATURE

x_1 : dimensionless concentrations of species A
x_2 : dimensionless concentrations of species B
x_3 : dimensionless temperature in the reactor
Da : Damköhler number
ε : dimensionless activation energy
S : ratio of the two rate constants
κ : ratio of activation energies
B : dimensionless adiabatic temperature rise
α : ratio of heat effects
β : dimensionless heat transfer coefficient
u : dimensionless coolant bath temperature

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