

## Development of Intelligent Models for the Prediction the Dynamics of Nonlinear Process

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The use of artificial intelligence (AI) techniques to address nonlinearity problems is gaining importance, mainly in context of industry 4.0. The present work was development of models based on artificial intelligence was performed to predict the concentration of cyclopentenol in a CSTR chemical reactor with the Van De Vusse kinetics. This reaction is known for its nonlinear behavior, which makes prediction difficult. Using simulations of this reactor in open and closed mesh combined with certain perturbations, a database was generated to train the models. The software MATLAB 2018a was used to implement the neural and the ANFIS systems. The input layer could be feed flow, feed temperature, heat provided by the thermal jacket, outlet temperature. The output were concentration of the component B and reactor temperature one step ahead. The models had good agreement, once presented remarkable performance reproducing the dynamics, obtaining  $R^2$  values near to 1 and error index near to 0.

### 1. Introduction

In recent years, the use of artificial intelligence techniques to deal with nonlinearity problems has been gaining importance, especially in the current competitive world, where cost reduction may be the differential. In the works Yang et al. (2018), Zhou et al. (2018) and Tsai (2011), artificial intelligence techniques were used to solve nonlinear problems. Predictive models involving process with chemical reaction can be difficult due to nonlinearity of chemical kinetics and the possibility of serial and parallel reactions. In this context, the CSTR chemical reactor with Van de Vusse kinetics is used as the standard nonlinear chemical process for the performance evaluation of controllers and predictive models. This reaction was studied in the Engell et al. (1993), Schäfer, et al. (2018) and Cassol et al. (2018).

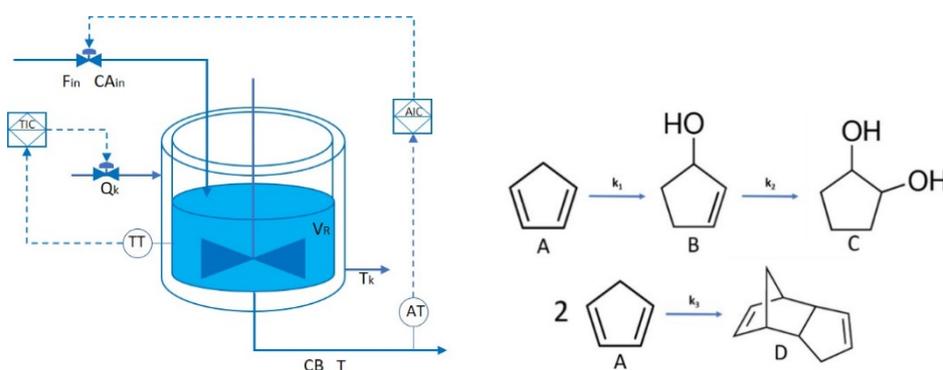


Figure 1: Van de Vusse CSTR reactor

## 1.2 Case Study - Van de Vusse Reactor

As described in more detail by Engell S.et al.,1993, the reaction occurs in a jacketed CSTR reactor, due to the exothermic nature of the reaction (Figure 1). In the Van de Vusse reaction, cyclopentenol (B) is produced from cyclopentadiene, with the formation of cyclopentanadiol (C) and dicyclopentadiene (D) as byproducts, according to the following reactions van de Vusse, J. G., 1964. Considering the constant density throughout the reactor and the ideal level control, for simplicity, the dynamics of the system is described by the following differential equations, resulting from the mass and energy balance of the reactor and the cooling jacket

Mass balance of component A:

$$\frac{dC_A}{dt} = \frac{F_{in}}{V_R} \cdot [C_{Ain} - C_A] - k_1(T) \cdot C_A - k_3(T) \cdot C_A^2 \quad (1)$$

Mass balance of component B:

$$\frac{dC_B}{dt} = -\frac{F_{in}}{V_R} \cdot C_B + k_1(T) \cdot C_A - k_2(T) \cdot C_B \quad (2)$$

CSTR reactor energy balance:

$$\begin{aligned} \frac{dT}{dt} = \frac{F_{in}}{V_R} \cdot [T^{in} - T] + \frac{k_w A_R}{\rho C_p V_R} \cdot [T_k - T] \\ - \frac{1}{\rho C_p} \cdot [k_1(T) \cdot C_A \cdot \Delta H_1 + k_2(T) \cdot C_B \cdot \Delta H_2 + k_3(T) \cdot C_A^2 \cdot \Delta H_3] \end{aligned} \quad (3)$$

Thermal jacket energy balance:

$$\frac{dT_k}{dt} = \frac{Q_k}{m_k C_{p_k}} + \frac{k_w A_R}{m_k C_{p_k}} \cdot [T - T_k] \quad (4)$$

Tables 1 and 2 show the reaction kinetic parameters and reactor/jacket properties provided by Engell S.et al.,1993

Table 1: Parameters of the reactor

Parameters	Value
Solution density ( $\rho$ )	0,9342 kg.L <sup>-1</sup>
Heat capacity (Cp)	3,01 kJ.kg <sup>-1</sup> .K <sup>-1</sup>
Thermal conductivity ( $k_w$ )	4032 kJ.m <sup>-2</sup> .h <sup>-1</sup> K <sup>-1</sup>
Thermal exchange area ( $A_R$ )	0,215 m <sup>2</sup>
Reactor volume ( $V_R$ )	10 L
Thermal jacket mass ( $m_k$ )	5 kg
Heat capacity jacket (Cp <sub>k</sub> )	2,0 kJ.kg <sup>-1</sup> .K <sup>-1</sup>

Table 2: Kinetic Reaction Parameters

Reaction	$k_{i0}$	E <sub>ai</sub>	$\Delta H_{ri}$
$A \xrightarrow{k_1} B$	$1,287 \times 10^{12} \text{ h}^{-1}$	-9758,3 K	4,2 kJ.mol <sup>-1</sup>
$B \xrightarrow{k_2} C$	$1,287 \times 10^{12} \text{ h}^{-1}$	-9758,3 K	-11 kJ.mol <sup>-1</sup>
$2A \xrightarrow{k_3} D$	$9,043 \times 10^9 \text{ L.mol}^{-1}\text{h}^{-1}$	-8560 K	-41,85 kJ.mol <sup>-1</sup>

The behavior of the CSTR reactor with the van de Vusse kinetics at steady state is shown in Figure 2. The longitudinal and transverse profiles for certain temperatures and flow rates are shown in Figures 2.2 and 2.3, respectively.

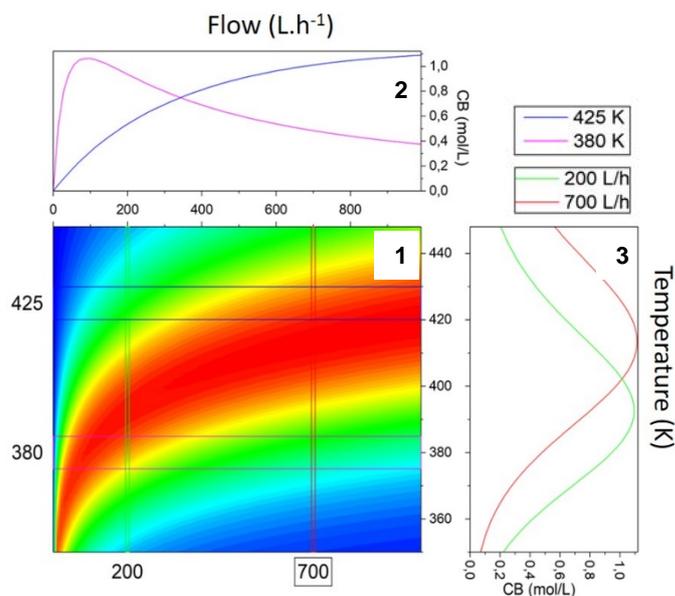


Figure 2: CB as a function of flow and temperature in the  $CA_{in}$  of  $5.1 \text{ mol.L}^{-1}$

## 2. Methodology

This process was studied by simulation, numerically integrating the nonlinear differential equations (equations 1 - 4). For the control system of CSTR reactor, two integrative proportional controllers (PI) were developed. One to control the concentration of component B and another to control reactor temperature, as shown in Table 3, where CB is the cyclopentenol concentration of the reactor outlet, T is the reactor temperature,  $F_{in}$  is feed flow and Qk is the heat removed from the reactor (Figure 1). These controllers were tuned according to the method of Ziegler-Nichols.

Table 3: Control system developed

Control system	Controlled variable	Variable manipulated	Operating Range
Control system CB	CB	$F_{in}$	$100 - 1600 \text{ L.h}^{-1}$
Control system T	T	Qk	$0 - 85000 \text{ kJ.h}^{-1}$

This process was submitted to systematic disturbances under different control conditions. The process variables obtained in these simulations were stored in a database. For the development of the predictive models, the database, containing the process input variables and their respective outputs, was divided into 3 groups: (70% for training, 15% for validation, 15% for testing).

For the development of the hybrid system ANFIS (Adaptive-Network-Based Fuzzy Inference System) was used toolbox "Fuzzy Logic Designer" by Matlab® 2018b. The fuzzy groups were established through the sub clustering of the toolbox. This method automatically groups the data according to their degree of similarity. This algorithm has as parameters: influence radius, squash factor, acceptance rate and rejection rate. To create the neural network, the toolbox "Neural Fitting (nftool)" was used. This toolbox allows you to choose the training algorithm, activation function, the number of neurons in the hidden layer and other parameters.

## 3. Results and Discussion

A neural network model (RNA) predicting the concentration of compound B was developed for comparative purposes. This network is composed of 4 neurons in the hidden layer and with the same 6 inputs of the ANFIS system. The network topology and training parameters are shown in Figure 3.

This fuzzy inference system has 6 input variables (feed flow ( $F_{in}$ ), feed temperature ( $T_{in}$ ), concentration of cyclopentadiene in feed ( $CA_{in}$ ), heat withdrawn by the thermal jacket of the reactor (Qk), derived from the concentration of compost B at the instant ( $dCB / dt$ ) and the concentration of B in the previous instant ( $CB(t-1)$ ) and an output variable (the prediction of the cyclopentenol concentration at 3 instants ahead), according to Figure 4.

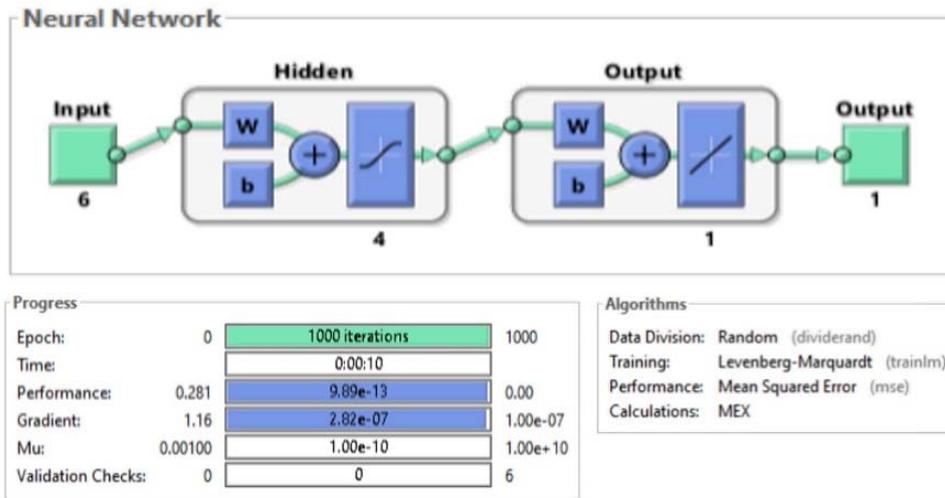


Figure 3: RNA topology and training parameters

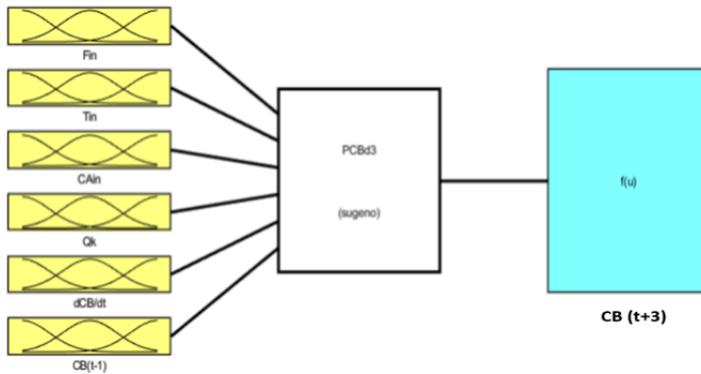


Figure 4: Fuzzy inference system for CB prediction

The number of Fuzzy groups per variable, the number of rules and consequently the topology of the neural network in the ANFIS system was determined by the sub. clustering of the toolbox. The parameters of this clustering are described in Table 4. Using the database obtained by previous simulations in closed meshes and others in open meshes, the network training of Figure 5 was performed. After a sequence of 15 training periods, the Fuzzy groups were presented in Figure 6. The data on training, testing and validation are given in Table 5.

Table 4: Sub clustering parameters

Parameters	Value
Influence	0.7
Squash factor	1.25
Acceptation	0.7
Rejection	0.15
Clusters	3 3 3 3 3 3

Table 5: Network training indices

Indexes	Value
Error training	$1.47 \times 10^{-7}$
Error validation	$4.95 \times 10^{-7}$
Error test	$1.48 \times 10^{-7}$

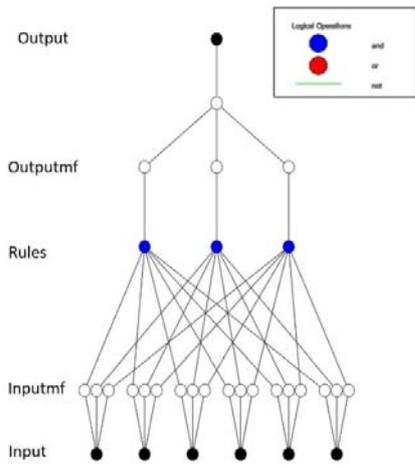


Figure 5: Neural network topology for the ANFIS system

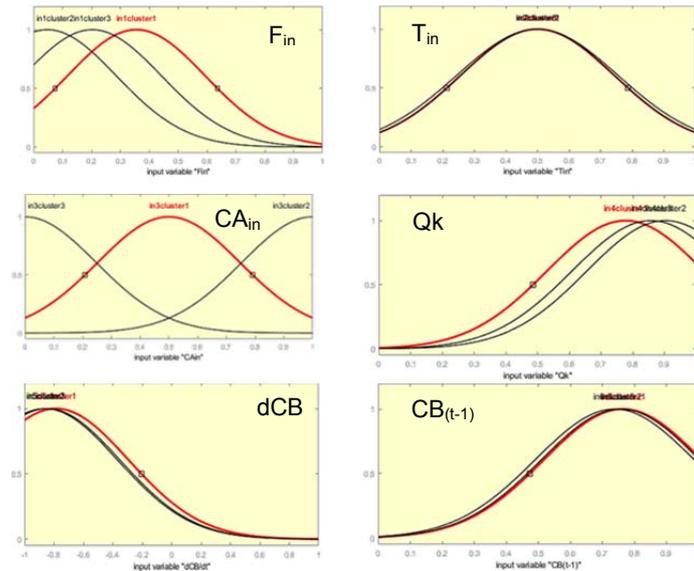


Figure 6: Fuzzy group obtained by sub clustering and training

The  $CA_{in}$  variable presented a symmetric division of the Fuzzy groups. The  $Fin$  and  $Qk$  entries were divided into shifted nearby sets. The variables  $dCB$ ,  $CB(t-1)$  and  $Tin$  presented three similar Fuzzy groups. Probably these groups were generated tow copies due to a need of the algorithm of toolbox or to increase the degree of freedom of the system. It can be observed the structure of the Fuzzy inference system in the neural network topology of Figure 5. Each input (the input variables) is connected to only three neurons of the next layer, responsible for the Fuzzy groups. The rules of inference are observed by the connection between the second (inputmf) and third layer (rules). Each blue neuron is connected only one of the neurons of the anterior layer cracks. The output of this network depends on the weighting of these three rules according to the activation of each Fuzzy groups, according to Figure 7.

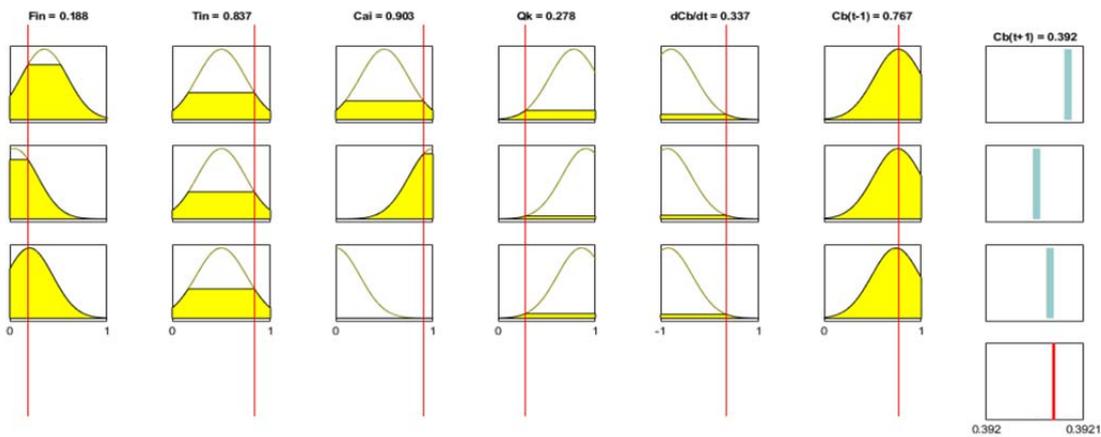


Figure 7: Example of activation of the ANFIS system

The real-time simulation with the predictions of the cyclopentenol concentration performed with the ANFIS system and with the artificial neural network is shown in Figure 8. The comparison between the concentration of component B at the time  $t$  and prediction of this concentration at time  $t+3$  in Figure 9.

Analyzing Figure 8, both models were able to predict the concentration of component B. In the initial overshoot, the model with neural networks obtained an oscillatory behavior with greater amplitude than the ANFIS system and the very concentration of B. For the purposes of application in control, this behavior may be interesting. These models intensify the error that would be generated by overshoot, making the performance of the controller more intense at this moment. The ANFIS predictive model obtained a correlation coefficient of 0.945 while the RNA model obtained a coefficient of 0.919.

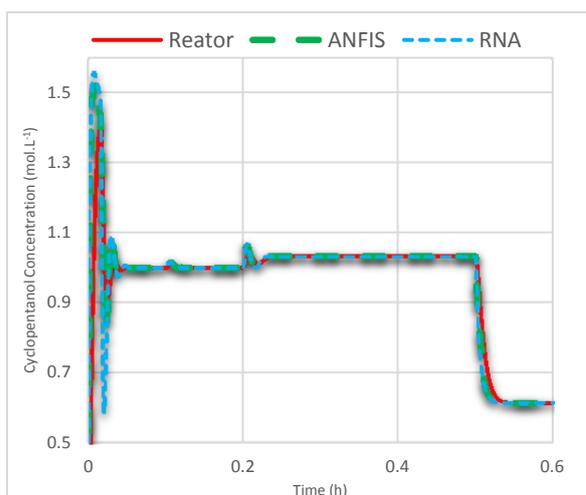


Figure 8: Simulation with CB predictions

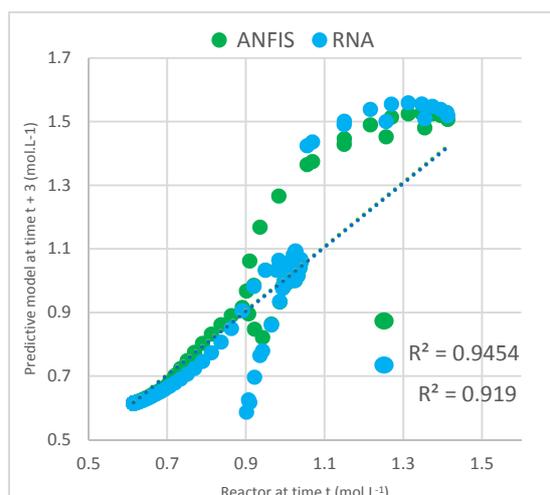


Figure 9: Evaluation graph of the predictive models

#### 4. Conclusions

In this work the performance of predictive models using artificial intelligence techniques was evaluated against a known chemical process benchmark, the CSTR reactor with Van de Vusse kinetics. The ANFIS and RNA models were able to predict the concentration of component B. The ANFIS system obtained a correlation coefficient of 0.945 while the RNA model obtained a coefficient of 0.919. These values allow the use of these models in predictive controllers and the development of virtual sensors.

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