MODELING OF A LYOPHILIZATION PLANT BY MEANS OF FUZZY-NEURAL VOLTERRA MODEL

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Abstract: *It is presented in this paper a design methodology for a truncated Volterra Fuzzy-Neural process model. The structure of the model is implemented by means of a simple fuzzy inference system with a learning procedure based on the minimization of an instant error. It is made simulation experiment in modeling of a nonlinear relation in a Lyophilization plant.*

МОДЕЛИРАНЕ НА ЛИОФИЛИЗАЦИОНЕН ПРОЦЕС ПОСРЕДСТВОМ НЕВРОННО-РАЗМИТ ВОЛТЕРА МОДЕЛ

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Резюме: *В този доклад е представена методология за проектиране на невронно-размит Волтера модел от ограничен ред. Структурата на модела се основава на опростена размита система с обучаващ алгоритъм базиран на минимизацията на моментната грешка. Направен е симулационен експеримент за апроксимиране на релация в лиофилизационен процес.*

1. INTRODUCTION

The identification of nonlinear systems has been an important area of research since Wiener published his work on nonlinear random theory [1]. Since then, many researchers have extended Wiener's work to the identification of polynomial and Volterra systems [2]. However, most of the research up to date is confined to the treatment of special cases, such as homogeneous Volterra systems [3] and finite order Volterra systems with Gaussian inputs [4].

The Volterra series have been widely applied as nonlinear system modeling technique with considerable success. However, at present, none general method exists to calculate the Volterra kernels for nonlinear systems, although they can be calculated for systems whose order is known and finite. When the nonlinear system order is unknown, adaptive methods and algorithms are widely used for the Volterra kernel estimation. The accuracy of the Volterra kernels will determine the accuracy of the system model and the accuracy of the system used for compensation. The speed of kernel estimation process is also important. A fast kernel estimation method may allow the user to construct a higher order model that gives an even better system representation.

The main criticism in using Volterra series as nonlinear models lies in its large number of parameters needed to represent the kernels [5], [6].

In this reason, in most practical solutions there are imposed some structural restrictions to Volterra type models in order to be attended a better model accuracy using a small number of parameters and to facilitate the identification procedures in notion to the computational effort.

Nevertheless, when a high order Volterra model even with a short memory is needed to solve an application, the main difficulty lies in the huge number of parameters that must be estimated. To eliminate this disadvantage a simple way is to reduce the number of parameters associated with the model.

Fuzzy-neural models have been proposed as an advantageous alternative to pure feed forward neural networks schemes for learning the nonlinear dynamics of a system from input-output data. It has been proved that many classes of fuzzy systems are excellent candidates for identification purposes as they hold the nonlinear universal approximation property and they are able to handle experimental data as well as a priori knowledge on the unknown system dynamics such knowledge is expressed by inferential linguistic information in the form of if/then rules the so-called fuzzy rules whose antecedents and consequents utilize fuzzy sets. The structure of the fuzzy identifier is somewhat determined by the rule antecedent and consequent variables by the number of their possible linguistic values or equivalently the number of membership functions and by the number of if/then rules [7].

This paper investigates the performance of a truncated Fuzzy-Neural Volterra estimator by considering nonlinear system identification for a Lyophilization plant. The model is based on so called “one step solutions” and when it is identified with the help of linguistic rules and data, gathered from the process, it has the potential to be transparent and easily interpretable [8]. A natural extension of the proposed approach is using the proposed model in a Model Predictive Control scheme.

2. VOLTERRA FUZZY-NEURAL MODEL

Various 'general' input/output model structures have been conceived to describe nonlinear systems. Among them, the Volterra series is the most widely used model structure. Theoretically, this model can represent a large class of nonlinear systems with arbitrary accuracy. But in practice, some structural restrictions must be imposed on this 'general' model due to the number of model parameters involved.

Therefore, in this approach it is considered the fuzzy-neural implementation of a second order Volterra model.

Using a simple fuzzy-neural approach the nonlinearity can be easily approximated as a set of functions. For this purpose it is used the Takagi-Sugeno fuzzy-neural technique and the model is taken in NARX type:

$$y(k) = f_y(x(k)) \tag{1}$$

where the elements of the considered regression vector *x(k)* are given by:

$$x(k) = [u(k-1), u(k-2), \dots, u(k-n_u), y(k-1), y(k-2), y(k-n_y)] \tag{2}$$

The unknown nonlinear functions f_y can be approximated by Takagi-Sugeno type fuzzy rules:

$$R^{(i)}: \text{if } x_1 \text{ is } \widetilde{A_1^{(i)}} \text{ and } x_p \text{ is } \widetilde{A_p^{(i)}} \text{ then } f_y^{(i)}(k) \tag{3}$$

$$f_y^{(i)}(k) = a_1^{(i)} y(k-1) + a_2^{(i)} y(k-2) + \cdots . + a_{ny}^{(i)} y(k-n_y) + y_o^{(i)} + b_1^{(i)} u(k-1) + b_2^{(i)} u(k-2) + \cdots + b_{nu}^{(i)} u(k-n_u) + v_{m_1}^{(i)}(k) + v_{m_2}^{(i)} \tag{4}$$

where

$$v_{m_i} = \sum_{j_1=1}^{n_u} \sum_{j_i=1}^{j_i-1} c(j_1, j_i) u(k - j_1)\, u(k - j_i) \tag{5}$$

(i)=1,2,…N, where *N* is the number of the fuzzy rules, A_i is an activated fuzzy set defined in the universe of discourse of the input *x* and the crisp coefficients a_1, a_2,...a_{ny}, b_1, b_2,...b_{nu}, $c_{1,1}$, $c_{2,1}$, $c_{j1,ji}$ are the coefficients into the Sugeno function f_y.

Finally, the output of the designed Volterra Fuzzy-Neural model is computed as:

$$y(k) = \sum_{i=1}^{N} f_y^{(i)}(k) \bar{\mu}_y^{(i)}(k) \tag{6}$$

In general, the predictive form of the model is expressed as:

$$y(k + j) = \sum_{i=1}^{n_u} b_i u(k + j - i) + \sum_{i=1}^{n_y} a_i y(k + j - i) + y_o + \sum_{i=1}^{N} v_i(k + j) \tag{7}$$

In the VFN model it is needed to be determined the unknown parameters – the number of membership functions, their shape, the parameters of the function f_y in the consequent part of the rules. This is an identification procedure for which have been proposed numerous approaches. In this work it is applied a simplified fuzzy-neural approach, with a learning procedure described below.

2.1 LEARNING ALGORITHM FOR THE DESIGNED VOLTERRA FYZZU-NEURAL MODEL

It has been shown, that any time-invariant nonlinear system can be approximated by a finite Volterra series to an arbitrary precision. Volterra models have the property to be linear in their parameters, i.e. the coefficients of their kernels, so that standart parameter estimation methods can be used [9].

It is used two steps simplified gradient learning procedure as a learning algorithm. This procedure is based on minimization of the instant error between the process output and the model output. It is needed to be adjusted two groups of parameters in the fuzzy-neural architecture – premise and consequent parameters. The consequent parameters are the coefficients in the Sugeno function f_y and they are calculated by the following equations [10].

$$\beta_{ij}(k + 1) = \beta_{ij}(k) + \eta\varepsilon(k)\bar{\mu}_y^{(j)}(k)x_i(k)\,; \;\; \beta_{0j}(k + 1) = \beta_{0j}(k) + \eta\varepsilon(k)\bar{\mu}_y^{(j)}(k) \tag{8}$$

in which η is the learning rate and β_{ij} is an adjustable i^{th} coefficient in the Sugeno function f_y of the j^{th} activated rule.

The premise parameters are the centre c_{ij} and the deviation σ_{ij} of an activated Gaussian fuzzy set. They can be calculated using the following equations:

$$c_{ij}(k + 1) = c_{ij}(k) + \eta\varepsilon(k)\bar{\mu}_y^{(j)}(k)\left[f_y^{(i)}(k) - \hat{y}(k)\right] \frac{[x_i(k)-c_{ij}(k)]}{c_{ij}(k)^2} \tag{9}$$

$$\sigma_{ij}(k + 1) = \sigma_{ij}(k) + \eta\varepsilon(k)\bar{\mu}_y^{(j)}(k)\left[f_y^{(i)}(k) - \hat{y}(k)\right] \frac{[x_i(k)-c_{ij}(k)]^2}{\sigma_{ij}(k)^3} \tag{10}$$

3. SIMULATION EXPERIMENTS

3.1 PLANT DESCRIPTION

The assumed plant process in the following simulation experiments is a Lyophilization plant.

Lyophilization process (Sublimation drying) is widely used in pharmaceutical and food industries, preparing stable dried medications and foodstuffs for astronauts and alpinists. The main objective of the Lyophilization process is to remove the preliminary frozen water which takes part from the product structure by its sublimation. Using a Lyophilization plant the bound into the product water is removed by its transition from ice to vapor phase with no melting.

Referring to Fig.1 a simplified diagram of the main components of the Lyophilization plant is shown. The plant consists particularly of a drying chamber (1); temperature controlled shelves (2), a condenser (3) and vacuum pump (4). The major purposes of the shelves are to cool and freeze or to supply heat to the product. This is supported by the shelves heater and refrigeration system (5). On those shelves the product is placed (6). The chamber is isolated from the condenser by valve (7). The vacuum system is placed after condenser. After the process is completed the condenser will be heated in order to be removed the frozen ice from its wall [11], [12].

After the product is entirely frozen, the chamber is evacuated in order to increase the partial vapor water pressure difference between the frozen ice zone and the chamber. The shelf heating system starts to provide enthalpy for the sublimation process. The sublimation takes place at a moving ice front, which proceeds from the top of the frozen material downwards. At the end of the primary drying, all the unconstrained water has been removed and what remains is the water which is constrained in the solution. At this point, the product can be removed, but in practice the water content is too high to guarantee biological stability. The stage in which the remaining water content is further reduced is called secondary drying, which takes place at higher temperature. In this contribution it is assumed only the first stage of the drying process called primary drying.

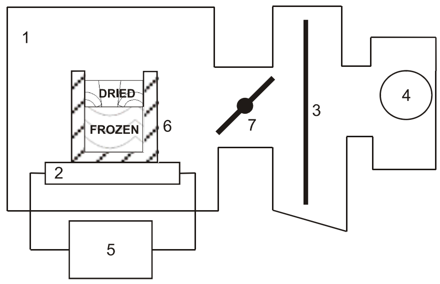

Fig.1. Simplified Lyophilization plant

3.2 SUBLIMATION IN A VIAL

The participating ice is the unconstrained water accumulated in the small cylindrical tubes. Throughout the primary drying the product, which consists of the dried layer on the top and the frozen core at the bottom, stays below a certain temperature to insure that no melting occurs.

In this contribution it is assumed a small scale Lyophilization plant, for drying of 50 vials filled with glycine in water adjusted to pH 3, with hydrochloric acid. The schematic diagram on Fig. 2 depicts the sublimation process occurring at the interface which is located at a distance *x* from the vial bottom. During sublimation the interface moves in a negative direction, while the product height remains constant. The sublimated water leaves product thought the already dried product layer.

Energy inside the frozen product layer is lost due to the sublimated water and the conducted heat to the dried product layer. The heat flux from the chamber to the condenser depends on the thickness of the crystallized water at the condenser wall.

The following initial conditions for simulation experiments are assumed:

- *Initial shelf temperature, before the start of the primary drying Ts_{in} = 228 K*
- *Initial thickness of the interface front x=0.0023m*
- *Thickness of the product L=0.003m*
- *Reference product temperature Tp=255 K*

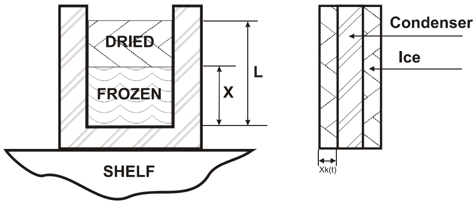

Fig.2. Sublimation in a vial

In the primary drying stage it is required to maintain the shelf temperature about 298 K, until the product will be dried.

3.2 SIMULATION EXPERIMENTS

The modeling process is made during a Lyophilization cycle and it is estimated the model error between output of the plant process and the artificial model.

It has to be mentioned, that the reference point for the end of simulation experiments was taken the final value of the interface front at value *x=0.0001* m. This is due to the nature of the Lyophilization process.

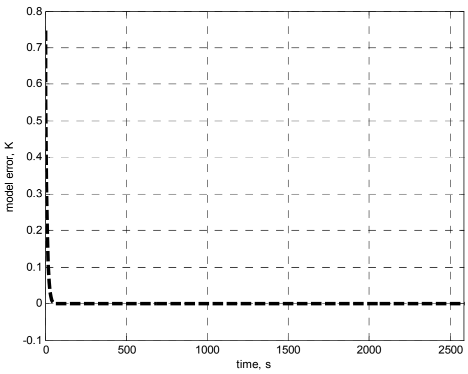

Fig.3. Model error during a lyophilizaition cycle

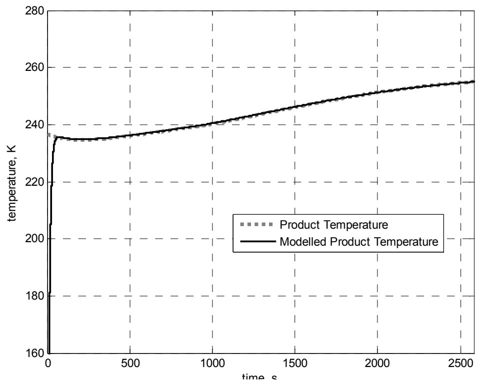

Fig.4. Modeling of relation in a Lyophilization cycle

4. CONCLUSIONS

It is presented in this paper a design methodology for a truncated Volterra Fuzzy-Neural process model. The model is approximated by means of a simple fuzzy inference system. The learning procedure for the designed model is based on the minimization of an instant error.

The simulation results show the efficiency of the proposed design approach. The predictive model follows the process output during the Lyophilization cycle and the model error between both is minimal.

The proposed modeling approach can be easily implemented in extension to Nonlinear Model Predictive Control.

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