Proceedings of the 19th World Congress
The International Federation of Automatic Control
Cape Town, South Africa. August 24-29, 2014

# A semi-batch reactor modeling based on PWARX systems

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**Abstract:** In this paper, we address the problem of identifying a semi-batch olive oil esterification reactor. In fact, this reactor can be considered as a PieceWise AutoRegressive eXogenous (PWARX) system. The Chiu's clustering procedure for the identification of PWARX systems is then applied. It consists in estimating both the parameter vector of each submodel and the coefficients of each partition. The results of the experimental validation illustrate the effectiveness of the proposed method. A comparative study with three existing approaches is also considered in this paper which shows that the proposed approach gives the best results in terms of precision.

*Keywords:* Hybrid systems, PWARX models, Identification, Chiu's clustering technique, Comparison study, Experimental validation.

## 1. INTRODUCTION

Batch reactors represent the cornerstone of several industrial plants such as chemical and pharmaceutical industries. In this paper, we consider a semi-batch reactor producing ester used in fine chemical industry like cosmetic products. This reactor prepares the ester by the reaction of a vegetable olive oil with free fatty acid and an alcohol at an equilibrium point with the elimination of water. Thus, the production of ester by this reactor includes three main steps which are heating, reacting and cooling. The first step allows to reach the equilibrium point which is obtained by increasing the temperature of the reaction products until a desired value. The purpose of the second step is to eliminate the resulting water of the reaction. This reactor uses a boiling technique to ensure this goal. Finally, the cooling step allows to decrease the temperature of the ester until a specified temperature. The optimization of the ester quality and the performance of the reactor can be guaranteed by an effective control system. The control of such reactor often requires that the dynamic behavior of the system must be represented by a mathematical model. This model can be built by the physical laws describing the heating and cooling phenomena that govern the behavior of the reactor. Consequently, it leads to a complicated nonlinear model. A solution to this problem consists in using the identification approach which allows to build a mathematical model from input-output data. The identification of the reactor is known to be a challenging identification problem due to the high nonlinearity, complexity, variability and uncertainty that such processes involve. Several approaches have been proposed in the literature for the identification of this reactor. These approaches can be classified in different ways depending on: the model structure, the solution type, the data processing strategy, etc.

The first approach is based on the linearization of the process around an operating point Mihoub et al. (2009a) Ben Abdennour et al. (2001). This approach allows the use of the linear systems identification and control methods which are highly developed in the literature. But, the obtained model is far from optimal. It is even quite surprising since it represents a nonlinear system by a single linear model describing the local behavior of the system around a single operating point.

To overcome this problem, the authors of Msahli et al. (2001) have suggested the use of the Volterra model. It is well known that the truncated Volterra model can represent any nonlinear system time invariant with fading memory Schetzen (1980) Mathews and Sicuranza (2000) Ogunfunmi (2007). Moreover, the parameters of this model are linearly related to the output, which allows the extension of some results of linear systems to nonlinear ones. However, it is important to note that the number of parameters of the Volterra model increases rapidly with the order and the memories. This is the main drawback of this model. Therefore, most of the researchers treat only the case where the order and memory are relatively small. This choice reduces the accuracy of the resulting model. The excitation signal which must be Gaussian represents also a fundamental problem for the identification of Volterra systems because in practical situations random signals may cause the wear of the actuators. Moreover, this method requires a very high number of measurements.

Another solution based on recurrent neural networks approach is proposed in Atig et al. (2010) Atig et al. (2012) to represent this reactor. The neural networks are capable of approximating any continuous nonlinear functions and have been applied to nonlinear process emulation. In fact, this approach consists in using a real time recurrent learning based on the gradient backpropagation learning algorithm. This algorithm is used for the adaptation of neural emulator parameters and weights. The major advantage of such method is that it doesn't depend on any preliminary knowledge about dynamics. But, it is well known that the gradient descent method is characterized by its slowness of convergence and it may converge to local minima.

Finally, we cite the approach proposed in Mihoub et al. (2009b)Ltaief et al. (2004). It consists in using the multimodel approach to represent this reactor. This approach is based on

the "divide to reign" strategy. It consists in decomposing the complex dynamic behavior of the system into a finite number of operating points. The set of local models is commonly known as the library of models. Each local model contributes partially to the global behavior of the system. Indeed, the output of the latter is obtained by aggregation of the contribution of each local model which is defined by a weighting function (also called validity). However, the construction of the library as well as the computation of validities is considered among the problems that are encountered in the multimodel approach.

In this paper, we consider the special case of multimodel where the validities of sub-models is binary. In fact, we preconize the use of the PieceWise Auto-Regressive eXogenous (PWARX) model to represent the reactor. It consists in using the notion of hybrid system which can be used to represent complex nonlinear systems. In fact, we can decompose the domain range of the non linear system into a set of operating regions Lin and Unbehauen (1992). For each one, a linear or affine model is associated. So, the considered complex non linear system becomes by modeling an hybrid system switching between linear or affine submodels Roll et al. (2004) Nakada et al. (2005) Wen et al. (2007) Xu et al. (2012). The alternative of considering the semi-batch reactor as a PWARX system seems to be very interesting because the characteristic of the system can be considered as linear in each operating step (heating, reacting, cooling).
This paper is organized as follows. Section II recalls the description of the process. In section III, the proposed method for the identification of the reactor is detailed. In section IV, the performance of the proposed approach is evaluated and compared with three existing methods through the experimental results. Section V concludes the paper.

## 2. PROCESS DESCRIPTION

The semi-batch reactor studied in this paper is an olive oil esterification reactor producing ester with a very high added value which is used in fine chemical industry such as cosmetic products. The esterification reaction between vegetable olive oil with free fatty acid and alcohol, producing ester, is given by the following equation:

$$Acide + Alcohol \leftrightarrow Ester + Water. \quad (1)$$

The ratio of the alcohol to acid represents the main factor of this reaction because the esterification reaction is an equilibrium reaction i.e. the reaction products, water and ester, are formed when equilibrium is reached. In addition, the yield of ester may be increased if water is eliminated from the reaction. The removal of water is achieved by the vaporisation technique while avoiding the boiling of the alcohol. In fact, we have used an alcohol (1- butanol), characterized by a boiling temperature of 118° C which is greater than the boiling temperature of the water (close to 100° C) . In addition, the boiling temperatures of the fatty acid (oleic acid) and the ester are close to 300°C. Therefore, the boiling point of water may be provided by a temperature slightly greater than 100° C.
The reactor is constituted essentially of:

- A reactor with double-jackets: it has a cylindrical shape manufactured in stainless steel. It is equipped with a bottom valve for emptying the product, an agitator, an orifice introducing the reactants, a sensor of the reaction mixture temperature, a pressure sensor and an orifice for the condenser. The double-jackets ensure the circulation of a coolant fluid which is intended for heating or for cooling the reactor.
- A heat exchanger: It allows to heat or to cool the coolant fluid circulating through the reactor jacket. Heating is carried out by three electrical resistances controlled by a dimmer for varying the heating power. It is intended to achieve the required reaction temperature of the esterification. Cooling is provided by circulating cold water through the heat exchanger. It is used to cool the reactor when the reaction is completed.
- A condenser: It allows to condense the steam generated during the reaction. It plays an important role because it is also used to indicate the end of the reaction which can be deduced when no more water is dripping out of the condenser.
- A data acquisition card between the reactor and the calculator.

The block diagram of the process is shown in Fig.1.

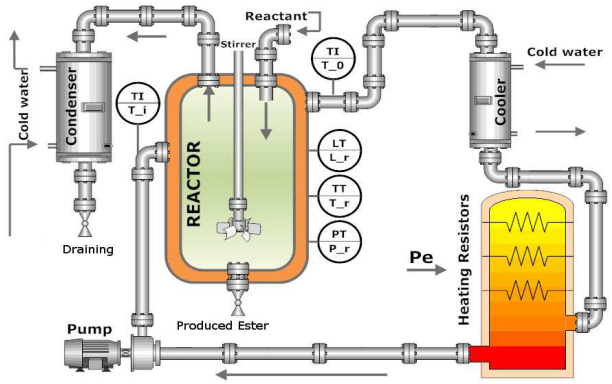


Fig. 1. Block diagram of the reactor.

The ester production by this reactor is based on three main steps as illustrated in Fig.2

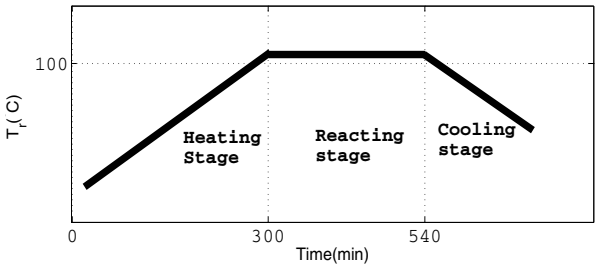


Fig. 2. Specific trajectory of the reactor temperature.

- Heating stage: The reactor's temperature $T_r$ is increased to 105° C.
- Reacting stage: The temperature should be kept constant at 105° C until the end of the reaction which can be detected by the absence of water at the condenser (when no more water is dripped out of the condenser).
- Cooling stage: The reactor's temperature is decreased.

An experimental study carried out on the reactor showed that the reactor can be considered as a Single-Input Single-Output (SISO) plant. The heating power $P_e$ and the reaction temperature $T_r$ represent respectively the input and the output of the