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Development of real-time state estimators for reaction–separation processes: A continuous flash fermentation as a study case

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A B S T R A C T

The development of reliable on-line state estimators applicable to reaction–separation processes is addressed in this work. Artificial Neural Network-based software sensors (ANN-SS) are proposed to allow on-line measurement of key variables, with an estimation algorithm that uses secondary variables as inputs. A continuous laboratory-scale flash fermentation for bioethanol production is considered as a case study. The process consists of three interconnected units: fermentor, filter (tangential microfiltration for cell recycling) and vacuum flash vessel (for the continuous separation of ethanol from the broth). The concentrations of ethanol in the fermentor and of ethanol condensed from the flash are successfully monitored on-line using ANN-SS. The proposed model contributes to improve the understanding of the complex relationships between process variables in the reaction and separation units, which is of major importance to allow the operation of the ethanol production process near its optimum performance.

1. Introduction

The need to decrease residues generation and the pursuit of cost reduction in bioethanol production have motivated the investigation of more efficient processes to produce this biofuel. One of the proposed options is the use of reaction–separation systems, such as the continuous flash fermentation.

Alternative technologies designed to remove ethanol continuously from the fermentation broth have been investigated since the early 90s. Some examples of reaction–separation integration processes are: gas stripping, pervaporation, perstraction, liquid–liquid extraction, aqueous two-phase separation, among others. Cardona and Sanchez [1] point out that the reaction–separation integration is a particularly interesting choice for the intensification of ethanol production. When ethanol is removed from the culture broth, its inhibition effect on the growth rate is diminished or neutralized.

The continuous extractive fermentation has shown several advantages, such as low vinasse generation due to the possibility of feeding molasses at higher concentrations, which reduces costs in waste treatment, and the potentiality of eliminating one distillation column from the process. Further detail of technical features can be found elsewhere [2,3].

In the continuous flash fermentation, the performance of the whole process is significantly influenced by the relationships between process variables in the reaction and separation units. Thus, the availability of an accurate mathematical model is important to improve process performance and to define the most suitable operating conditions to achieve a particular objective. However, modeling of reaction–separation systems is extremely complicated. In the case of the flash fermentation the difficulty is the modeling of the vapor–liquid equilibrium for the fermented broth system, which is a complex multicomponent system with varying composition.

Another important application of an accurate mathematical model is the monitoring of the process states, which is an information source for the decision making in the production process. In general, monitoring of ethanol profiles in industrial plants is carried out as off-line analysis, often with a significant time delay between sampling and availability of the analysis results. An appropriate mathematical model can be used as a software sensor and allow real time monitoring of important variables.

As far as monitoring is concerned it is worthwhile mentioning the current limitation of more advanced analytical instruments (including near infrared spectrophotometers), and the challenges to be solved, such as insufficient accuracy, long dead-time, slow dynamics, large noise, low reproducibility, age deterioration, among others [4]. In industrial fermentation plants analytical instruments are difficult to calibrate, mainly due to the characteristics of industrial culture media, such as turbidity of the culture,

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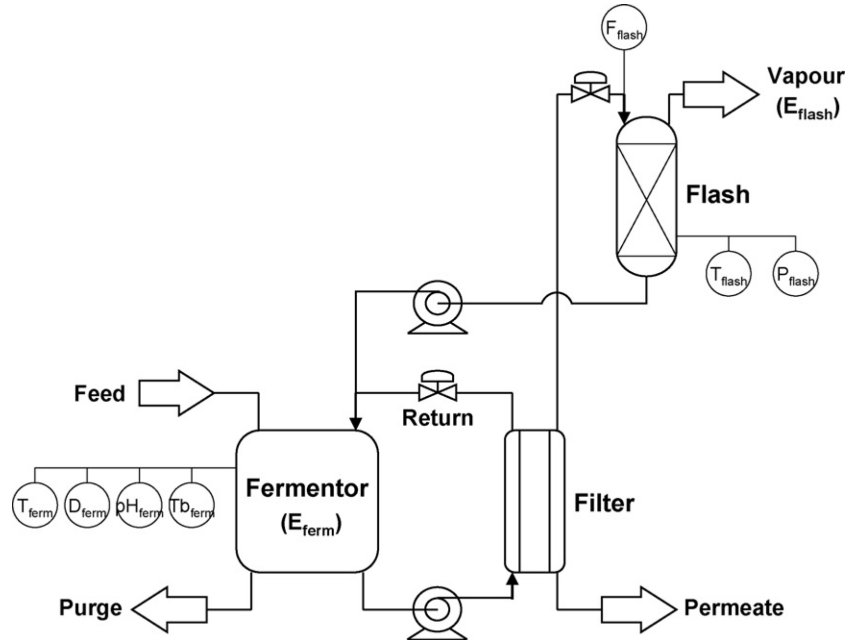

Fig. 1. Schematic diagram of the continuous flash fermentation process.

presence of dissolved CO_2, among others [5,6]. Nowadays the software sensor is the preferred alternative for monitoring state variables in biotechnological processes [7].

The so-called software sensor is an algorithm where several measurements are processed together. The interaction of the signals from on-line instruments can be used for calculating or to estimate new quantities (e.g. state variables and model parameters) that cannot be measured in real-time. Software sensors can also be understood as an association of a sensor (a hardware), which allows on-line measurements of some process variables, with an estimation algorithm (a software), in order to provide on-line estimates of immeasurable variables, model parameters or to overcome measurement delays [8,9]. This approach is a promising research area with significant impact on industrial operation [4,9–11].

More recent works on software sensor for solving biotechnological complex problems are presented by Osorio et al. [6], Soons et al. [7], Arranz et al. [12], Yu et al. [13], Lee et al. [14], among others. The major purpose of using software sensors in bioprocesses is to assess the quality of the final product and to validate on-line analyzers, providing redundant measurements. Artificial Neural Networks (ANN) has been dominant in literature in the field of software sensor design.

Artificial Intelligence techniques such as ANNs have been widely applied for bioprocess modeling, monitoring and control. This technique is sought to efficiently combine all available knowledge and to direct the development toward an improved process operation strategy [15]. Besides, ANNs can be used to offer adaptive solutions, since the reestimation of their parameters is a straightforward procedure [16]. These characteristics are suitable for analyzing data from more complex processes such as the continuous flash fermentation, which have a large number of state variables.

In previous works [9,17], it was shown that multilayer perceptron (MLP) neural networks were easily implemented on a platform with direct interface to instruments, sensor and actuators in order to determine reliable performance prediction in dynamic systems. This procedure was possible due to its simple mathematical representation, as well as the low computational effort when compared with dynamical neural networks [18]. Although the major advantage of dynamic neural network is its inherent implementation of unknown time dependencies [18], some studies in dynamic system have shown that in certain situations MLP neural networks can present superior performance when compared to dynamic neural networks [19].

In this work a relatively simple ANN-based software sensors for monitoring a continuous flash fermentation process is proposed. On-line measurements, such as temperature, dilution rate, pH and turbidity in the fermentor, as well as temperature, pressure and feed flow rate in the flash vessel, are considered as inputs to the software sensor used to infer ethanol concentration in the fermentor and ethanol concentration in the condensed stream from the flash vessel. The ANN-SS is evaluated considering the accuracy with which it describes the experimental dataset. An approach based on Placket Burman design is used to evaluate the influence of the various considered inputs on the performance of the software sensor to predict the two responses.

2. Case study: continuous flash fermentation

Fig. 1 shows a schematic diagram of the continuous flash fermentation process investigated in this study. This process was developed in laboratory scale at the Laboratory of Bioprocess Engineering (State University of Campinas, Brazil) and consists of three interconnected units: fermentor, cell recycle system (tangential microfiltration) and vacuum flash vessel (ethanol-fermented broth separation unit). The total volume of the system is approximately 5 L. The following on-line variables are taken into consideration in this study: Pressure in the flash, P_{flash} (mmHg); Flash feed flow rate, F_{flash} (L/h); Temperature in the flash, T_{flash} (°C); Temperature in the fermentor, T_{ferm} (°C); Dilution rate in the fermentor, D_{ferm} (h^{-1}); pH in the fermentor, pH_{ferm}; Turbidity in the fermentor, Tb_{ferm} (%).

The process is started-up with the addition of the inoculum in a solution of sugar molasses from an industrial plant diluted to 180 g/L of total reducing sugars. It is operated in semi-batch mode until all the substrate is consumed, with addition of diluted molasses only to complete the volume of ethanol evaporated in the flash vessel. The objective is that biomass reaches a high concentration before the continuous fermentation begins. The end of the start-up stage is monitored by the stabilization of the turbidity as well as of the condensate volume readings. The continuous extrac-