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INTELLIGENT APPROACHES IN ROBOTIC AND AUTOMATION & BIOINFORMATICS

INTELLIGENT CONTROL SYSTEMS

INTELLIGENT APPLICATIONS IN BIOMEDICAL ENGINEERING

Bio-Ethanol Production Optimization using ACD with ESN Critic

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Abstract—**In the present paper on-line action-dependent heuristic neuro-dynamic programming was applied for optimization of a complex nonlinear production process. The approach is based on recurrent neural network architecture – Echo state network (ESN) – as critic network within the frame of adaptive critic design (ACD) scheme. The subject for optimization is bio-ethanol fermentation. The aim was to increase process productivity defining optimal dilution rate profile. The obtained by simulations results are good basis for further experimental investigations.**

Keywords-adaptive critic design; action dependent heuristic dynamic programming; echo state network; bio-ethanol production process

I. INTRODUCTION

The environmental problems caused by the use of fossil feed stocks as energy source and the rapid increase of the oil-based fuels prices are the main reasons that have motivated the production of bio-fuels [1]. Bio-ethanol, as a clean, safe and renewable resource, has been considered as a potential alternative to the ever-reducing fossil fuels. Ethanol production has increased dramatically on the last years, because it is considered as a renewable and environmentally friendly alternative [2, 3]. However, the economical feasibility of the ethanol industry is still questioned and much effort should be done in order to improve the process, especially regarding to rapid fermentation and resistance to the main inhibition factors.

To eliminate inhibition caused by high concentration of substrate and product as well as to enhance ethanol productivity, cell immobilization approaches have been applied in ethanol production [3]. Immobilized cells fermentation has been shown to be more effective than the free yeast process, mainly due to the enhanced fermentation productivity, feasibility of continuous processing, cell stability and lower costs of recovery and recycling and downstream processing. Cell immobilization may also protect cells against shear force. However the industrial use of immobilized cells is still limited and further applications will depend on the development of immobilization procedures that can be readily scaled-up [4]. The main feature of immobilized-cell systems is the high attainable concentration of biocatalyst in a solid support, which, combined with a high reactor load, can lead to smaller reactor volumes as compared to suspended-cell processes [5].

In previous work [6] the influence of cells immobilization on the batch fermentation dynamics was investigated and several models were created to approximate the bio-ethanol production process. In the present paper one of the best obtained models is used for simulation optimization of the continuous bio-ethanol production. The main purpose was to obtain by simulations dilution rates that will increase ethanol productivity. This will allow spending of long and expensive experimental investigations. Only the reasonable optimization results will be subject of further experiments for process intensification.

Reinforcement learning (RL) is introduced as a method of artificial neural network training “by experience”, rather than “by examples”. Created initially to mimic animal behavior in an attempt to explain Pavlovian conditioning, RL is also recognized as an approximation of Bellman’s dynamic programming method [7] that is well known in the control community. During the last thirty years theoretical developments in this field (a very exhaustive retrospective can be found in [8]) have lead to methodologies known as neuro-dynamic programming [9] and adaptive critic designs (ACD) [10] also commonly known as Adaptive Dynamic Programming. The core of the methods is the approximation of Bellman’s equation or value function (which is the discounted sum of future rewards) using neural networks (also called “heuristic adaptive critic”). Usually the critic is trained off-line since it needs a collection of a variety of data from the beginning to the end of several process runs. Combination between off-line and on-line learning is also considered [11]. True on-line applications of ACD approaches, however, need very fast training algorithms [12]. In highly non-linear

environments the necessity for additional feedback connections arises, which further complicates the on-line training.

The recently proposed ESN structure [13, 14] incorporates a dynamic reservoir generated randomly and easily trainable output neurons. The less complex and much faster Recursive Least Square method (RLS) [14] can be applied for their on-line training. Moreover, the derivative calculation with respect to the ESN inputs (that is needed for gradient descent), requires much less computational effort, because of the ESN structure that naturally separates the reservoir from its input and output connections. In our previous investigations we applied this approach to a robot control task for obstacle avoidance [15] and for optimization of another biotechnological process – fed-batch production of a biopolymer [16].

Here the same approach is applied to continuous bio-ethanol production process optimization. The obtained dilution rates profiles are analyzed with respect to their technological significance and applicability. The presented simulation optimization results will be further subject of experimental investigation for confirmation and refinement.

II. Problem Statement

A. ACD approach

The ACD approach also called neural dynamic programming or heuristic dynamic programming [9, 10] is an approximation of the classical dynamic programming in which the Bellman equation is approximated by a neural network that is then used to predict the future utility function to be minimized by adjusting control actions. Figure 1 shows the structure of ACD of the heuristic dynamic programming (HDP) type with action-dependent critic network, but without a model of the object under control [10, 17].

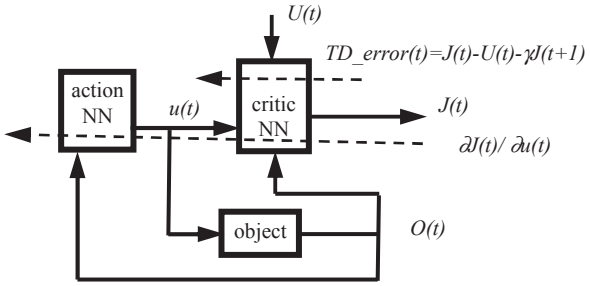

Figure 1. ACD scheme. Dashed lines represent the training cycle.

The vector *O(t)* represents the object state vector and *u(t)* is the control variable. The critic NN has to be trained to predict the utility function *U(t)* by approximating Bellman's equation as follows:

$$J(R(k),u(k)) = \sum_{t=0}^{k} \gamma^t U(O(t),u(t)) \qquad (1)$$

Dashed lines represent the information flow of parameter tuning algorithms for critic and action networks. The training of critic NN is aimed at minimization of the temporal difference error *TD_error(t)* while the action NN training aim is minimization or maximization of the sum of future rewards predicted by the critic. Thus the trained critic output must be $J(t)=U(t)+\gamma J(t+1)$ that is the accumulated sum of future rewards or the utility function *U(t)* that has to be minimized/maximized. Here γ is a discount factor that takes values from the interval *[0, 1]*. The main challenge for the on-line application of such a scheme is the training of the critic network because it has to be able to predict future reinforcements with good precision in order to allow adequate training of an actor network. In search of fast trainable NN structures and algorithms different approaches have been applied [11, 12]. The fast training algorithm of ESNs offers a good opportunity for ACD application [18].

B. Echo State Network Basics

ESNs are a kind of recurrent neural networks that arise from so called "reservoir computing approaches" [1]. The basic ESN structure is shown in Figure 2 below.

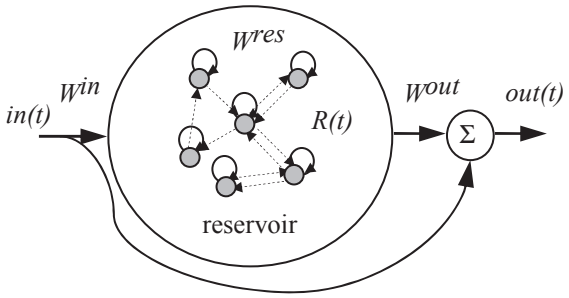

Figure 2. Echo state network structure.

The ESN output vector *out(t)* for the current time instance *k* is usually a linear function of its input and current state

$$out(t) = f^{out}\left(W^{out}[in(t),\ R(t)]\right) \qquad (2)$$

Here, *in(t)* is a vector of network inputs and *R(t)* a vector composed of the reservoir neuron states; f^{out} is a linear function (usually the identity), W^{out} is a trainable $n_{out} \times (n_{in} + n_R)$ matrix (here n_{out}, n_{in} and n_R are the sizes of the corresponding vectors *out*, *in* and *R*). The neurons in the reservoir have a simple sigmoid output function f^{res} (usually *tanh*) that depends on both the ESN input *in(t)* and the previous reservoir state *R(k-1)*:

$$R(t) = f^{res}\left(W^{in} in(t) + W^{res} R(t-1)\right) \qquad (3)$$

W^{in} and W^{res} are $n_{in} \times n_R$ and $n_R \times n_R$ matrices that are randomly generated and are not trainable. There are different approaches for reservoir parameter production [14]. A recent approach used in the present investigation is proposed in [19]. It is called intrinsic plasticity (IP) and suggests initial adjustment of these matrices, aiming at increasing the entropy of the reservoir neurons outputs.

ESN training can be done in an off-line or an on-line mode. For on-line training, the RLS algorithm [13] was proposed. It is claimed that it converges fast and it is less computationally expensive in comparison to BPTT-EKF methods [18].

C. Experimental Set-up

The used strain-producer is dry yeasts *Saccharomyces cerevisiae 46 EVD* provided by the company "*Martin Vialatte OEnologie*", France. They are kept at 4-6°C. Before utilization the yeasts were re-hydrated in 4% sugar solution at 30°C. The amount of that solution was 1:10 with respect to the dry biomass. The amount of inoculating material was 1% from the bio-reactor working volume because the aim was to achieve 10^7 CFU/ml. During the immobilization the amount of used biomass was determined such that we achieved 10^7 CFU/g preparations. Nutrition media composition is the following: glucose – 118,40; $(NH_4)_2SO_4$ – 2; KH_2PO_4 – 2,72; $MgSO_4x7H_2O$ – 0,5; yeasts extract – 1. The nutrient media was sterilized for 20 min at 121°C in autoclave. For yeasts cell immobilization 2% solution of Na-alginate was used. It was obtained by dissolution of alginate in distilled water via constant steering till obtaining of homogenous solution. After that the solution was sterilized for 20 min at 121°C. For jellification 2% solution of $CaCl_2$ also sterilized for 20 min at 121°C was applied.

The laboratory bioreactor is glass cylinder with geometrical volume of 2 dm^3 and working volume of 1.7 dm^3. It is equipped with six blade turbine stirrer and four baffles. On the top of its head plate orifices for feeding in of nutrition media and air, leading out of gases, inserting of heat-exchangers and sensors for pH, temperature and dissolved oxygen were mounted. The installation includes also measuring devices and controllers for the main process variables. The cultural media temperature is controlled via two channels: cold water of cooling and heater for heating. The active acidity (pH) was measured by combined glass-silver chloride electrode „Ingold, Switzerland".

The temperature and pH controllers are integrated into the control device type „Applikon, Holland" equipped with precise controllers. For maintaining of constant pH of the cultural media sterilized reagent – 20% KOH solution – was supplied via peristaltic pump. The temperature was maintained at 28°C±0.1. After reaching its desired value the pH controller was switched on in order to maintain the pH desired value. For both types of processes – with free and immobilized cells – pH was maintained at 4.5±0.05.

The bioreactor was sterilized in "cold" conditions using 0.3% solution of neomycin for 24 hours. After that it was washed out with sterile water. The suspension was inserted via peristaltic pump used also for pH control. The immobilized preparation was washed out with sterile physiological solution and than it was inserted into bioreactor at sterile conditions. After that the nutrition medium was inserted into apparatus. The amount of immobilized material was 10% from the nutrition medium volume. Samples for analysis of the main process variables – concentrations of glucose, biomass and product – were taken from the bioreactor every 2 hours.

D. Mathematical Model and Optimization Task

Since caring out of real experiments for process optimization is expensive and time consuming task, we need a simulation model of the process to replace the real object in the scheme form Figure 1. The mass-balance based ordinary equations mathematical model of the continuous ethanol fermentation with immobilized cells has the following form:

$$\begin{aligned} \frac{dX}{dt} &= \mu X \\ \frac{dP}{dt} &= qX - DP \\ \frac{dS}{dt} &= -\frac{1}{Y_{x/s}}\mu X - \frac{1}{Y_{p/s}}qX + D(S_{in} - S) \end{aligned} \tag{4}$$

It is based on the assumption that the substrate denoted by S is consumed with rate proportional to the increase rates of the cells X and product P concentrations. The constants $Y_{x/s}$ and $Y_{p/s}$ are called yield coefficients and μ and q denote the specific biomass growth and ethanol production rates respectively. The dilution rate D has influence only on product and substrate concentrations because biomass is immobilized in alginate pearls and hence it can't be taken out of the bioreactor by the out flow. Here S_{in} is concentration of substrate in feeding medium. Since in the literature there is big variety of mathematical dependences for the two main process kinetic rates μ and q, the choice of proper dependences is usually done by trail and error. In the [6] the Monod type dependences:

$$\mu = \mu_{\max}\frac{S}{K_{sx} + S},\ q = q_{p\max}\frac{S}{K_{sp} + S} \tag{5}$$

appeared to be the proper choice. Here μ_{max}, q_{max}, K_{sx} and K_{sp} are model parameters whose values were identified in [6].

The main control variable of the process is dilution rate so it is subject of our optimization procedure. The preliminary experimental investigations [20] and technologists experience showed that the fermentation must be carried out in batch mode (with D=0) initially and to start feeding with nutrition media in continuous mode (D=const.>0) after some time. The main assessment criteria for the process are the obtained product (ethanol) concentration at the stationary phase of continuous fermentation and the process productivity calculated as PDg/(lh), i.e. the amount of ethanol at the output of the bioreactor every hour. Hence the utility function subject of our optimization procedure is:

$$U(P(t), D(t)) = P(t)D(t) \quad (6)$$

The moment of switching between batch and continuous regime is fixed to two reasonable times – 6th and 16th hour after fermentation start. The initial value of D was set small ($0.1h^{-1}$) and its upper bound is restricted to $0.725h^{-1}$ for technological reasons. The other variable subject to adjustment is concentration of feeding medium S_{in}. Hence we tried optimization with several different values of that variable too.

III. Results and Discussion

First we tried optimization procedure for different time of starting continuous fermentation – t_{feed}=6h and t_{feed}=16h. The concentration of the glucose in the feeding medium is S_{in}=11,8g/l in both cases. The results are shown on Figures 3 and 4. The optimization procedure took 132 and 148 iteration respectively evenly divided between critic and action training cycles.

In the case of t_{feed}=6h at the moment of feeding initiation yeast cells have to be in their exponential growth phase. After starting of continuous mode the product concentration decreases to about 3.97g/l. The biomass concentration increases with the starting of feeding with nutrition media. The obtained optimal dilution rate is again D=0.725h^{-1} that is in accordance with experimental results in [20]. The achieved process productivity is 4.21g/(lh) and ethanol outcome is 96% from the theoretically possible one.

In the second case (t_{feed}=16h) immediately after switching to the continuous regime the biomass started to grow fast trying to approach a new stationary state in accordance with the available substrate in the medium. At the same time we expect to maintain constant substrate concentration at about 5 to 6.5g/l. The product concentration at the system output starts to decrease form 39.38g/l to about 5.5g/l. This stationary concentration corresponds to outcome of 91% of theoretically possible one. The obtained optimal dilution rate is D=0,725h^{-1} that corresponds to the maximal productivity of 4.09g/(lh).

According to the simulation investigations switching to the continuous mode at 6-th hour leads to higher ethanol outcome with about 5% and a little bit higher productivity in comparison with the case of continuous mode starting at 16-th hour. This is due to faster adaptability of the cells to the changes in the medium during the exponential growth phase. Because both results are close to each other we can conclude that it is important to switch on the continuous regime of fermentation when the yeast cells are in the exponential growth phase.

The next investigations are aimed at revealing the influence of higher glucose concentrations in the feeding nutrition media. In both cases the continuous mode started after 16 hours of batch fermentation. Two concentrations of glucose in nutrition media are investigated: S_{in}=33.6g/l and S_{in}=118.4g/l. The results are presented on Figures 5 and 6. The optimization procedure took 94 and 260 iteration respectively.

In the first case (with S_{in}=33.6g/l) the achieved system productivity was 7.91g/(lh). However in contrast to the previous investigations here the product outcome is lower – about 60% from the theoretically possible one. The concentration of unfermented sugars at the system output is higher – about 12.72g/l. The biomass concentration increases.

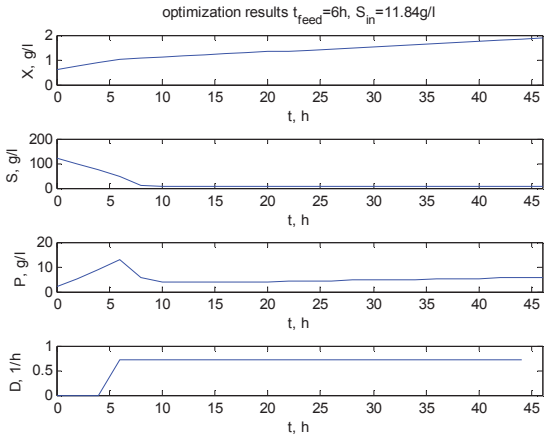

Figure 3. Optimization results for t_{feed}=6h and S_{in}=11.84g/l.

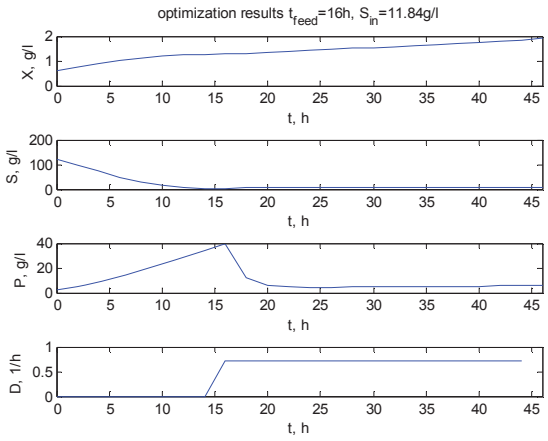

Figure 4. Optimization results for t_{feed}=16h and S_{in}=11.84g/l.

In the case of S_{in}=118.4g/l the productivity is 20.5g/(lh) and the ethanol outcome is 46% from the theoretically possible one. At the same time biomass increases considerably achieving at the end of simulation 9.59g/l that in real experiment will cause destruction of the alginate pearls of the cells carrier. After starting of the feeding the substrate concentration increases and the product starts decreases but at the end of simulation it still is not in stationary phase.

Although the substrate concentration increase leads to increase of the productivity at the same time the ethanol outcome decreases significantly. This is due to incomplete utilization of the sugars in the nutrition medium. Increased productivity is due to higher dilution rate and product concentration increase. However in real experiments due to restricted productivity we expect that increasing of dilution rate will not lead to such big productivity increase. The simulation optimization showed also that we have to search ways to prevent unlimited biomass growth in the alginate pearls. This can be done by reduction of nitrogen and phosphorus in the nutrition medium.

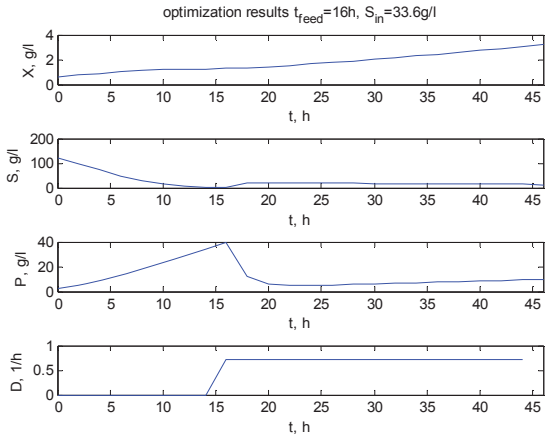

Figure 5. Optimization results for t_{feed}=16h and S_{in}=33.6g/l.

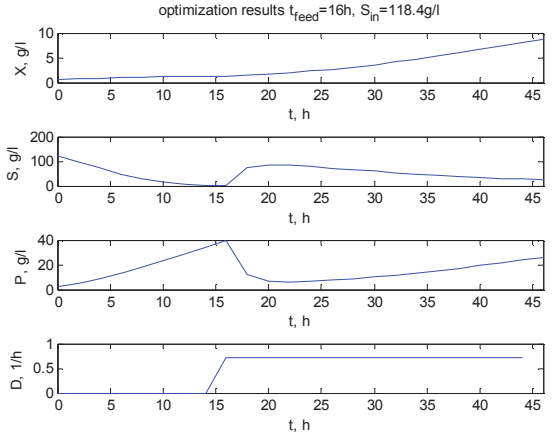

Figure 6. Optimization results for t_{feed}=16h and S_{in}=118.4g/l.

The simulation optimization showed also that we have to search ways to prevent unlimited biomass growth in the alginate pearls. This can be done by reduction of nitrogen and phosphorus in the nutrition medium.

IV. Conclusions

The investigated application of on-line ACD with ESN critic for optimization of bio-ethanol production showed technologically reasonable results achievement. In all investigated cases it took considerably small number of iterations. The obtained by simulations results are in agreement with preliminary experiments carried out and gave us a good basis for further experimental investigations towards process intensification.

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