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COMPUTATIONAL SOFT SENSOR FOR FUNGAL BIOFILTRATION PROCESS

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Abstract: Based on the data for the experimental measurements of the state on the fungal biofilter some process variables: the CO_2 concentration and the elimination capacity (CE) have been estimated using a differential neural observer scheme via the pressure difference data. This scheme is developed in two parts, the first is the dynamical neural network structure and the second is compound by the observer structure, this type of computational sensor is called soft sensor. The good performance for the estimate states is shown by the CE and CO_2 dynamical evolutions versus their estimate states on graphical way.

Keywords: Biofiltration, estimation, dynamical neural networks, neuro-observer.

1. INTRODUCTION

Treatment of off-gases from industries is an important measure to reduce atmospheric emissions of volatile organic carbon (VOC). These gases can be paraffinic (like methane), alcohols (methanol), hydrocarbons of petroleum of low weight molecular (benzene, toluene), halogen aromatics (for example, clorobencenes) and halogen aliphatic solvents (Rittman and McCarty 2001) (Roberge, Gravel et al. 2001; Ottengraf, Meeters et al. 1986; Rittman and McCarty 2001). Off-gases can be cleaned by various technologies such as incineration, adsorption, chemical scrubbing and biofiltration (Ottengraf 1987; Moretti and Mukhopadhyay 1993). Biofilters are beds packed with biologically active materials, such as compost, through which gases are ventilated. In the compost, contaminants are absorbed and subsequently biodegraded. Biofiltration was found to be cost-effective for off-gases with low concentrations of VOC ($<3 g/m^3$) (van Groenestijn and Hesselink 1993; van Groenestijn, van Heininge et al. 2001) and an odour reduction of 95 to 99% is possible (Hartung, Martinec et al. 2001). A biofilter system is typically composed of a blower, humidification system, biofilter unit, and in some cases, a granular activated-carbon backup. In addition to the humidification system, a method through a manually controlled spray is usually included (Eweis, Ergas et al. 1998). However, conventional biofilters, based on compost and bacterial activity, face problems with the elimination of hydrophobic compounds such as aromatic compounds, alkenes and alkanes. Because of the low solubility in water, the compounds are poorly absorbed by the bacterial biofilms. Besides that, biofilter operational stability is often hampered by acidification and drying out of the filter bed. To overcome these problems, biofilters with fungi on inert packing material have been developed (van Groenestijn, van Heininge et al. 2001). Fungi are more resistant to acid and dry conditions than bacteria, which is a helpful property when operating biofilters. Moreover, it is hypothesised that the aerial mycelia of fungi, which are in direct contact with the gas, can take up hydrophobic compounds faster than flat aqueous bacterial biofilm surfaces. However the main variables on this system can not be determined by direct measure, ones of these variables are the elimination capacities (CE), which describe the amount of pollutant eliminated by microbial activity; the CO_2 production and the ΔP, the pressure difference in a biofiltration system. In other side, the applications of the some dynamical systems used to described the unmeasured variables on a process using the measure variables, this have been implemented successfully and it is called observer (Luenberger 1964; Tsinias 1990). The immeasurable variables can be estimated without a physical sensor only based on the data reconstruction. Recently the

neural networks application on the identification and control process have developed into the biotechnology areas (Narendra and Parthasarathy 1995; Cabrera, Poznyac et al. 2002), the results have shown the possibility to design new class of sensor based on these methods.

The objective of this paper is to describe the observer system based on the dynamical neural networks to identify the elimination capacity (CE) in a *P. variotii* biofiltration system using the output data.

1.1 Dynamical neural networks.

During the evolution in a bioprocess all its states o variables are changed abruptly; the problem to identify these variables seems very complicate and probably unrealistic. That's why the observation (in this case, organics decomposition dynamics) is very important for an effective control design. Several approaches dealing with state estimation problem are widely used in practical applications. Among them there are the Lie-algebraic method (Knobloch, Isidori et al. 1993), Lyapunov-like observers (Slotine 1984), high gain observation (Giccarella, Mora et al. 1993; Michalska and Mayne 1995), optimization-based observer the reduced-order nonlinear observers (Garcia and D'Atellis 1995) and others.

There are two known types of ANN: static using back-propagation technique (Narendra and Parthasarathy 1995) and dynamic neural networks (DNN) (Poznyak, Sanchez et al. 2001). The first one deals with, the so-called, global optimization problem trying to adjust the weights of such NN in order to minimize an identification error. The second approach, exploiting the feedback properties of the applied DNN (see Fig.1), permits to avoid many problems related to global search extremum converting the learning (training) process to an adequate feedback design. If a mathematical model is incomplete or partially known, this DNN-approach provides an effective instrument to attack a wide spectrum of problems such as identification, state estimation, trajectories tracking an etc.

There are known several effective approaches to the corresponding feedback design. One of them is Variable Structure Approach (VSA) (Utkin 1992). Under heavy uncertainty conditions it offers significant potential advantages comparing to other identification and control techniques: good transient behavior, global exponential stability of a small estimation error, unmodelled disturbance rejection capability, insensitivity to plant nonlinearities or parameter variations and remarkable stability and performance robustness. The corresponding procedures, treated within this theory, usually use so-called signum-type or switching (sliding mode) structures. Despite fruitful research in the variable structure control theory, few authors have considered the application of the main principles of sliding mode approach to the problem of observer design for dynamic system (Slotine 1984; Utkin 1992). In this study we suggest the DNN observer (DNNO), which incorporates switching type term to correct current state estimates using only available measurable output data.

The design, analysis and control of the concentrations on the biofilter have been the challenging tasks mostly, because of the inadequacy of on-line sensors with fast sampling rate and small time delay and the complex nonlinear interactive behavior of these concentrations. By these reasons, a robust identification technique seems to be attractive to avoid these limitations. On the other hand, there is not an adequate model for the biofilter which is driven with several variables like elimination capacity CE and CO_2 concentration. To solve the state estimation and parameter identification of these reactions without any model usage the following steps need to be applied: design a dynamical neural system with extra terms to observe the immeasurable variables.

Structure of DNNO with a sliding mode term. The DNN observer corresponding to the scheme given at Figure 1 is covered by the following ordinary differential equation:

$$\begin{aligned} &\frac{d\hat{x}_t}{dt} = A\hat{x}_t + W_1\sigma\left(\hat{x}_t\right) + W_2\varphi\left(\hat{x}_t\right)\gamma\left(u_t\right) \\ &+K_1\left(y_t - \hat{y}_t\right) + K_2 sign\left(y_t - \hat{y}_t\right) \\ &\hat{y}_t = C\hat{x}_t \end{aligned} \qquad (1)$$

Here $\hat{x}_t$ is the state vector of DNNO representing the current estimates of organics concentration, $\hat{y}_t$ is the output of DNN corresponding the estimates of the measurable CE concentration, A, K_1, K_2, are constant matrices adjusted during DNN training, $\sigma(.)$ and $\varphi(.)$ are standard sigmoid functions, h is a data delay constant, C is an output matrix, W_i ($i=1,2$) is the output weights tuning by a special on-line *learning* procedure (Poznyak, Sanchez et al. 2001). For the considered biofiltration process the state components are: x_1 is the CO_2 concentration variation in the biofilter; x_2 is the current difference pressure Δp and x_3 is the CE concentration.

The measurable data is the pressure difference in the biofilter output, that is $y_t = x_2$. So, in this case the output matrix is $C = (0,1,0)$. The gain matrix K_1 corresponds to a linear (Luenberger) correction term, K_2 is a sliding mode correction term matrix. The adequate learning of DNNO (2) provides a small enough upper bound (in an average sense) for the state estimation error $\Delta_t = \hat{x}_t - x_t$.

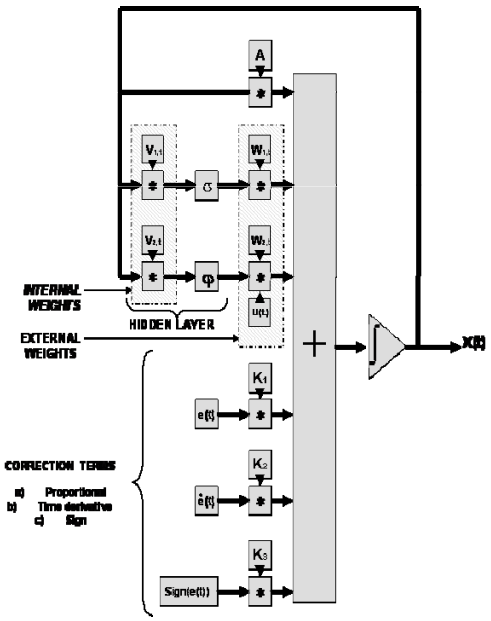

Fig. 1. Block diagram of the Neuro Observer added with the correction terms.

Training DNNO. To guarantee a small enough state estimation error the adequate parameters of DNNO (2) should be selected. The stationary parameters *A, K_1, K_2* may be tuned during the so-called "*training*" process. The weights *Wi* (*i=1, 2*) are quickly adjusted on-line by the special differential learning law. In this section we consider in details the training procedure. It may be conducted using the data for the experimental measurements in order to serve for the correction of the parameters of DNNO as well as for adequate selection of the initial conditions in the applied learning procedure.
The weight matrices are updating with a special learning law is described by the equation

$$\dot{W}_t = \Phi\left(W_t, \hat{x}_t, u_t, t, y_t \middle| W^{(0)}\right) \qquad (2)$$

This statement is called the "learning law" (it is derived in the appendix section) in the DNN estimator and that is denoted by

$$\dot{W}_t^{(i,j)} = -k\,\mu_t\,S_t^{(i,j)} sign\left(\tilde{W}_t^{(i,j)}\right);\ i,j = 1,n \qquad (3)$$

where S_t is any matrix with the condition $tr\{S_t\} = 1$ and

$$\begin{aligned} &\mu_t := \left\| N_\delta P \tilde{W}_t^T \sigma(\hat{x}_t) \right\|_\Pi^2 + 2 e_t^T C N_\delta P \tilde{W}_t\, \sigma(\hat{x}_t) \\ &\Pi := C^T \Lambda_{\xi_2} C + \delta \Lambda_1, \quad \tilde{W}_t := W_t - W^{(0)*} \\ &e_t := y_t - C\hat{x}_t, \quad N_\delta := \left(C^T C + \delta I\right)^{-1}, \delta > 0 \end{aligned} \qquad (4)$$

and the matrix P is the positive solution for the algebraic Riccati equation given by

$$P\tilde{A}^{(0)*} + \left(\tilde{A}^{(0)*}\right)^T P + PRP + Q = 0 \qquad (5)$$

2. MATERIALS AND METHODS.

2.1 Experimental Considerations

The experimental data was obtained from the direct measures on the *P. variotii* biofiltration process (García-Peña, Hernández et al. 2001), during 60 days of operation; however the neuro observer was tested using the output data (in this case the current difference pressure) and obtained the other process variables: CE and CO_2 concentrations.

Biofilter. The biofilter was inoculated with the fungal strain *Paecilomyces variotii* CBS115145. The experiments were performed in a biofilter consisting of a 1 m high cylindrical glass column with an 8 cm inner diameter. The volume of the filter bed was 2.9 L. The reactor was filled with the inoculated packing material (vermiculite). The support was inoculated with a spore suspension an initial concentration of $2*10^7$ spores/g of initial dry mass. Air saturated with toluene was mixed with water-saturated air (70%) in order to obtain an initial toluene inlet concentration of 6 g/m^3. The gas stream was introduced at the top of the reactor. Airflow was regulated at 2.5 L/min by means of mass-flow controllers (60061; Cole Parmer, Vernon Hills, IL, USA). The empty bed residence time (EBRT) was 1.15 min. In some experiments, water or medium were added at the top intermittently. Elimination capacity (EC) of the toluene (S) is defined as EC (g/m^{3}h)=(S_{in} − S_{out})* Air Flow/ V reactor. Efficiency (%) is equal to 100* (S_{in} − S_{out})/S_{in}.

Analytical Methods. Toluene concentrations in the inlet and outlet stream of the biofilter were monitored with an FID gas chromatograph (GowMac, Series 580; Bridgewater, NJ, USA), equipped with a 1/8 in X 16 ft stainless steel column (Silar 10C, Grapac GC 80/100; Altech, Deerfield, IL, USA). The operation conditions were: injector, 190°C; oven, 180°C; detector, 200°C; carrier gas (N_2), 25 mL/min. Standard curves were obtained by injecting a known amount of toluene into a 500 mL calibrated glass bottle using a 10 mL liquid syringe. For the determination of the CO_2 concentration, an IR gas analyzer (1A-AA1, MIRAN A Foxboro, Bridgewater, MA, USA) at 4.3 mm with a 0.75 m path length was used. The same IR gas analyzer at 10.4 mm with a 20.25 m path length was also used to quantify NH3 concentration in the biofilter. Temperatures were measured by thermocouples T (CPSS-186G-12, Omega, Stamford, CT, USA) at the inlet, outlet and in the medium with a precision of ±0.1°C. A pressure transducer (7352-16, Cole Palmer, Chicago, IL, USA) was used to obtain the pressure drop through the bed. The air containing toluene vapour was supplied to the biofilter by a

compressor. The CO_2 concentration at the outlet of the biofilter was measured with an infrared analyzer (3400 Gas Analyzers; California Analytical Instruments, USA), the reported values correspond to the difference between the outlet and the inlet (ambient) CO_2 concentrations. The pressure drop was determined online by using a pressure transducer (22370,1E11-2; Omega Engineering, Stanford, CA, USA). Data acquisition device was used to monitor flows, temperature, CO_2 production, and pressure drop. The final biomass was determined by extracting the protein from the support. One gram of the packed material was mixed with 5 mL of phosphoric acid (0.5 M). The sample was boiled in a bath for 7 min and centrifuged at 5000 rpm for 15 min. The protein in the solution was quantified using the Bradford method.

2.2 Computational.

Based on the input-output data for the biofilter process dynamic variables, the numerical algorithm was implemented via personal computer. The DNNO was trained and tuned by the trial and test method the result variables were compared with the experimental data obtained by off line way in case of CE concentration and on line way for the CO_2 concentration, the last variable was used to compare the precision between the estimate an experimental states. Finally, the complete evolution for the CE and CO_2 concentrations was plotted for both states (estimate and measure).

3. RESULTS.

The DNNO was designed and trained to estimate the elimination capacity in the fungal biofilter treating toluene vapours as the figure 2 clearly shows. In this figure the CE estimate state is close to the experimental CE data, which denotes the DNNO good performance.

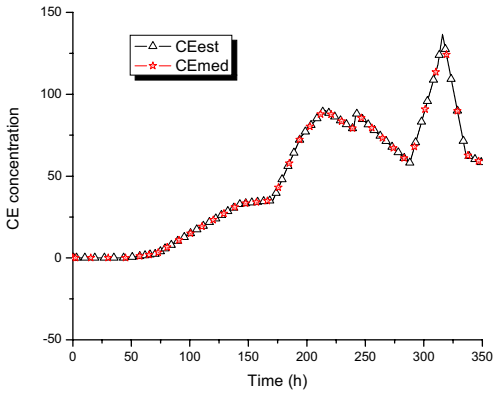

Fig. 2. Elimination capacity: estimate and measure states.

The evolution for the estimate state of CO_2 production and the experimental data are shown in the figure 3, the precision for the estimation is remarkable again because the trajectories follow the same pattern.

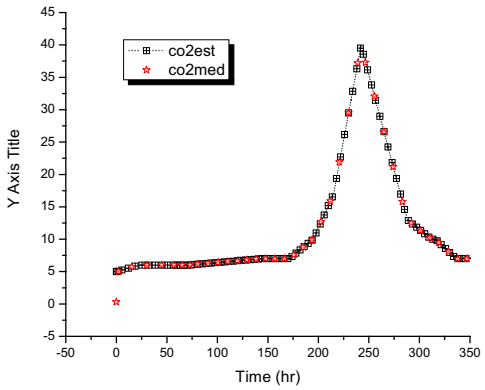

Fig. 3. CO_2 concentration: estimate and measure states.

4. CONCLUSIONS.

The results of the DNNO system shows that the use of this tool to measure the variables in this kind of processes is much simpler than is the performance were obtained of long and costly experiments.
This method could be use to develop soft sensor based on the DNNO structure and this could be a way to sense the other variables in a process when the instrumentation could be cost.

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APPENDIX

The proof for the Learning Law is described by
Proof Define the state estimation error as $\Delta_t = x_t - \hat{x}_t$ and the output error as

$$e_t = y_t - \hat{y}_t = Cx_t + \xi_{2,t} - C\hat{x}_t = C\Delta_t + \xi_{2,t}$$

for which the following identities hold

$$\Delta_t = N_\delta \left(C^T e_t - C^T \xi_{2,t} + \delta \Delta_t \right)$$

The dynamics of Δ_t is governed by the following ODE:

$$\dot{\Delta}_t = \dot{x}_t - \frac{d\hat{x}_t}{dt} = A^{(0)*}\Delta_t + \tilde{W}_t \sigma(\hat{x}_t) + W^{(0)*}\tilde{\sigma}_t + \tilde{f}_t + \xi_{1,t} - K_1(y_t - \hat{y}_t) - K_2 \mathbf{SIGN}(y_t - \hat{y}_t) \quad (6)$$

where $\tilde{\sigma}_t := \sigma(x_t) - \sigma(\hat{x}_t)$. Define the following Lyapunov function as:

$$V := V(x, \Delta, \tilde{W}) = \bar{V}(x) + \|\Delta\|_P^2 + k^{-1}\mathbf{tr}\{\operatorname{mod}\tilde{W}\}$$

$$\operatorname{mod}\tilde{W} := \left[|\tilde{W}^{(i,j)}| \right]_{i,j=\overline{1,n}}$$

It´s time derivative is

$$\dot{V} = \frac{\partial \bar{V}}{\partial x}\dot{x}_t + 2\Delta_t^T P\dot{\Delta}_t + k^{-1}\mathbf{tr}\left\{ \left(D\tilde{W}_t \right) \right\}$$

$$\left(D\tilde{W}_t \right) := \left[\mathbf{sign}\left(\tilde{W}_t^{(i,j)} \right) \dot{W}_t^{(i,j)} \right]_{i,j=\overline{1,n}}$$

Using (6) implies

$$\Delta_t^T P\dot{\Delta}_t = \Delta_t^T P\left[A^{(0)*}\Delta_t + \tilde{W}_t\sigma(\hat{x}_t) + W^{(0)*}\tilde{\sigma}_t \right] + \Delta_t^T P\left[\tilde{f}_t + \xi_{1,t} - K_1(y_t - \hat{y}_t) - K_2 \mathbf{SIGN}(y_t - \hat{y}_t) \right] \quad (7)$$

Notice that

$2\Delta_t^T PA^{(0)*}\Delta_t = \Delta_t^T \left[PA^{(0)*} + \left(A^{(0)*} \right)^T P \right]\Delta_t$. In (7) let use the matrix inequality

$$XY^T + YX^T \le X\Lambda X^T + Y\Lambda^{-1}Y^T$$

valid for any $X, Y \in R^{r\times s}$ and any $0 < \Lambda = \Lambda^T \in R^{S\times S}$

$$2\Delta_t^T P\tilde{W}_t\sigma(\hat{x}_t) + 2\Delta_t^T PW^{(0)*}\tilde{\sigma}_t + 2\Delta_t^T P\tilde{f}_t + 2\Delta_t^T P\xi_{1,t} \le 2e_t^T CN_\delta P\tilde{W}_t\sigma(\hat{x}_t) - 2\xi_{2,t}^T CN_\delta P\tilde{W}_t\sigma(\hat{x}_t) + 2\delta\Delta_t^T N_\delta P\tilde{W}_t\sigma(\hat{x}_t) + \tilde{f}_0 + \tilde{f}_1\|x_t\|^2_{\Lambda_{\tilde{f}}} + \Upsilon_1$$

$$\Delta_t^T \left[P\left(\bar{W}_{\Lambda_\sigma^{-1}} + \Lambda_{\tilde{f}}^{-1} + \Lambda_{\xi_1}^{-1} \right) P + l_\sigma \|\Lambda_\sigma\| I_{n\times n} \right]\Delta$$

$$2\Delta^T(t)PK_1(y_t - \hat{y}_t) = 2\Delta^?(t)PK_1\left[C\Delta(t) + \xi_{2,t} \right] \le \Delta^T(t)\left[PK_1C + C^TK_1^TP \right]\Delta(t) + \Delta^T(t)\left[PK_1\Lambda_{\xi_2}^{-1}K_1^TP \right]\Delta(t) + \Upsilon_2$$

and, in view of the selection $K_2 = \lambda P^{-1}C^T$ one gets

$$2\Delta_t^T PK_2\mathbf{SIGN}(y_t - \hat{y}_t) \le -2\lambda\textstyle\sum_{i=1}^n |C\Delta(t)|_i + 4\lambda\sqrt{n\Upsilon_2} \le 4\lambda\sqrt{n\Upsilon_2}$$

Substitution of all of these inequalities in (7) leads to the following inequality:

$$\dot{V}_t \le \Delta_t^T\left[P\tilde{A}^{(0)*} + \left(\tilde{A}^{(0)*} \right)^T P + PRP + Q \right]\Delta_t + \tilde{f}_1\|x_t\|^2_{\Lambda_{\tilde{f}}} + \tilde{f}_0 - n_1\|x_t\|^2 - \Delta_t^T Q_0\Delta + \Upsilon_1 + 2\Upsilon_2 + 4\lambda\sqrt{n\Upsilon_2} + \operatorname{tr}\left\{ k^{-1}\left(D\tilde{W}_t \right) + \mu S_t \right\}$$

Taking the learning laws as $k^{-1}\left(D\tilde{W}_t \right) + \mu S_t = 0$ and multiplying each component of this identity by $\mathbf{sign}\left(\tilde{W}_t^{(i,j)} \right)$ we obtain (3) and (4)

$$\dot{V}(t) \le -\alpha_Q\|\Delta(t)\|_P^2 + \rho_Q \ .$$

Integrating both sides and dividing by T , we get

$$\frac{1}{T}\int_{t=0}^{T}\dot{V}dt = \left(V_T - V_0 \right)/T \le \rho_Q - \frac{\alpha_Q}{T}\int_{t=0}^{T}\|\Delta_t\|_P^2\,dt$$

Taking the upper limit on T completes the proof.