Paper presented at 1st IWA Conf. On Instrumentation, Control and Automation, Malmo, June 2001.

DYNAMIC COMPENSATION OF DISSOLVED OXYGEN PROBES FOR RESPIROMETRY

S. Marsili Libelli *, C. Barresi †

* *Department of Systems and Computers, University of Florence, via S. Marta, 3 - 50139 Florence, Italy. Email: marsili@ingfi1.ing.unifi.it*

† *Student, Faculty of Engineering, University of Florence, via S. Marta, 3 - 50139 Florence, Italy. Email: c.barresi@tin.it*

ABSTRACT

The accuracy of dissolved oxygen measurements in a dynamic environment is affected by the probe lag. This paper analyses the dynamic behaviour of the measuring device and proposes a new method to compensate the lag it introduces. This solution should be viewed in the context of a "software instrument" approach, including the sensor, its electronic circuitry and the process computer. The design of the software compensator is based on classical control design concepts and is aimed at improving the probe dynamic response thus reducing the error it introduces. The incorporation of this compensator into a software instrument, with self-tuning capabilities, is described and the accuracy improvement in measuring the oxygen transfer coefficient K_La is assessed. Though the numerical example refers to a case study, the procedure is general enough to be applied to any probe, provided the calibration experiment described in the paper is performed prior to normal operation.

KEYWORDS

Dissolved oxygen, Respirometry, Software instruments, Process control, Sampled systems, Wastewater treatment.

INTRODUCTION

The measurement of dissolved oxygen (DO) is at the basis of respirometry, a widely used technique in wastewater treatment to assess the state of microbial activity and for the calibration of microbial kinetic models. The principles of respirometry are thoroughly illustrated in Spanjers *et al.,* (1998).

The DO measuring principle with polarographic devices, described in Linek *et al.* (1988), is based upon the electrochemical reduction of oxygen in an amperometric cell. The electrodes are immersed in an electrolytic solution separated from the bulk liquid by a semi-permeable membrane, through which the oxygen molecules can penetrate, and are reduced at the cathode surface. The current flowing between the electrodes depends on two processes: the rate of the oxygen transport from the bulk liquid to the cathode surface and its reduction at the cathode with peroxide production. The number of electrons exchanged at the cathode is proportional to the concentration of peroxide and its rate of decomposition. This effect, combined to other rate limiting processes such as diffusion and disposal of produced peroxide, produce an overall low-pass dynamic behaviour, with the result that the measured current follows the rate change of dissolved oxygen concentration with a time lag depending on the probe design and chemistry.

Since all respirometric techniques rely on the rate of change of dissolved oxygen, ideally the measuring probe should be able to follow DO variations without introducing any additional lag. In practice this is not possible for the reasons explained above and the aim of this paper is to model the dynamic response of the DO probe and design a compensator to reduce this lag. This problem has rarely come to the fore in respirometric studies, it has nonetheless been considered by Philichi and Stenstrom (1989), Spanjers and Olsson (1992), Vanrolleghem *et al.,* (1998) in connection with the error introduced in dynamic DO response in a respirometer on for the measurement of the oxygen transfer coefficient K_La. In all these studies the DO probe has been modelled as a first order system. In this paper it is shown that the probe model should be modelled by a more complex system and its dynamic response can be tailored to compensate this undesirable behaviour.

Let $G(z^{-1})$ be a sampled-time rational transfer function representing the DO probe dynamics, with z^{-1} representing the backshift operator. The basic idea of this paper is the design of a compensator, to be implemented as an additional piece of software in the measuring device, for example a respirometer, in order to improve the DO dynamic characteristics. Basic design technique, normally applied to the design of discrete-time control systems will be used, for which a thorough survey can be found in Ogata (1987). Ideally, if $H(z^{-1})$ is the transfer function of the compensator, then the combination of the two systems should be a perfect all-pass filter

$$G(z^{-1})\times H(z^{-1})=1 \quad \Rightarrow \quad H(z^{-1})=G(\bar{z}^{1})^{-1} \quad \forall z=e^{jwT} \tag{1}$$

with T_s representing the sampling period. This result cannot be achieved in practice, since if $G(z^{-1})$ is strictly proper, the compensator $H(z^{-1})$ resulting from eq. (1) would not be physically realizable. However, an approximation $\tilde{H}(z^{-1})$ can be found such that the series $G(z^{-1})\times\tilde{H}(z^{-1})$ approaches unity in a suitably defined low-pass band. In the paper, then the criteria for designing the approximate sampled-time compensator $\tilde{H}(z^{-1})$ are discussed and the improvement which it introduces are assessed. It is then shown how this compensator can be incorporated into a software instrument to complement the basic hardware to perform dynamic DO measurements.

EXPERIMENTAL SET-UP

The dynamic DO response is identified from experimental data collected with the equipment illustrated in figure 1. The dynamic probe response is obtained by alternatively dipping the probe in a stirred beaker containing distilled water, either oxygen-saturated or fully deoxygenated by addition of sodium sulphide (Na_2SO_3). Twenty runs for each step (upward and downward) were performed and the average response and standard deviations computed. The experimental set-up includes a DO probe (OXI - 91, WTW, Weilheim, Germany) with a 45 μm teflon membrane and related measuring unit, a multifunction analogue/digital data acquisition board (PCI 6024E, National Instruments, Austin TX, USA) and a PC equipped with an AMD K6/350 Mhz processor. The *software instrument*, including the compensator, the automation of the measurement and calibration procedure was developed in Labview 5.1 (National Instruments, Austin TX, USA) for the real-time part, whereas the modelling and calibration software was developed in Matlab 5.3. Software modules developed in the two environments could be intertwined using Labview 5.1 "Matlab Node" capability through which a segment of Matlab code can be incorporated into a Labview diagram and executed in real-time. The A/D converter has been software programmed for an input range of 1 V, corresponding to a resolution of $2^{-12}=2.4414\times10^{-4}\ V$. Since the probe constant is 14.922 mgO_2/l to 1 V output, the final resolution in the DO scale is $3.643\times10^{-3}\ mgO_2/l$, which is at least one order of magnitude better than the intrinsic probe accuracy. A sampling time T_s = 50 msec was used throughout.

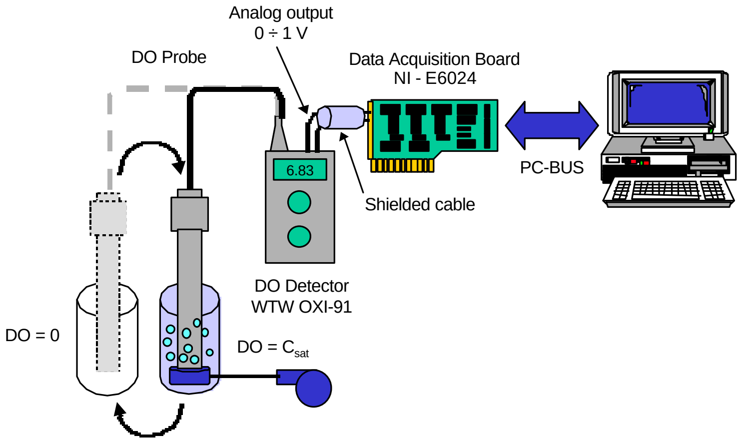

Fig. 1 - Experimental set-up with the two stirred beakers in which the probe is alternatively dipped.

DO PROBE MODELLING AND PARAMETER CALIBRATION

From the collected data two probe models were determined, one for the downward and one for the upward step, using a second-order transfer function. This was considered an acceptable compromise between accuracy and complexity, in view of compensator design. The parameters of the two transfer functions were determined through least-squares optimisation using a modified flexible polyhedron algorithm (Marsili-Libelli, 1992). They are shown in Table 1 and their response is compared to the data in figures 2 and 3. Two separate transfer functions were used, since a single transfer function proved inadequate to model both behaviours.

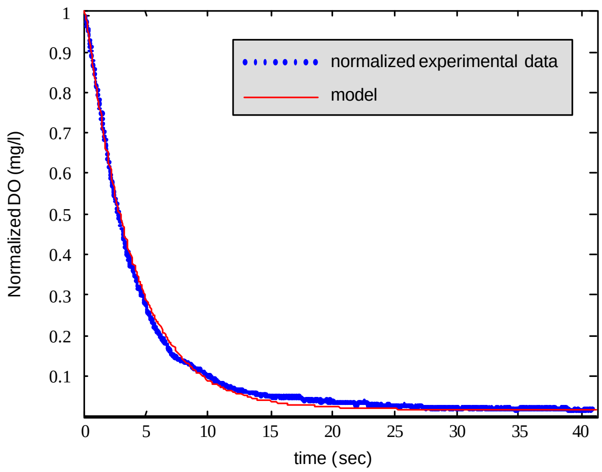

Fig. 2 - Model response compared to experimental data in the downward step (from O$_2$-saturated to deoxygenated water).

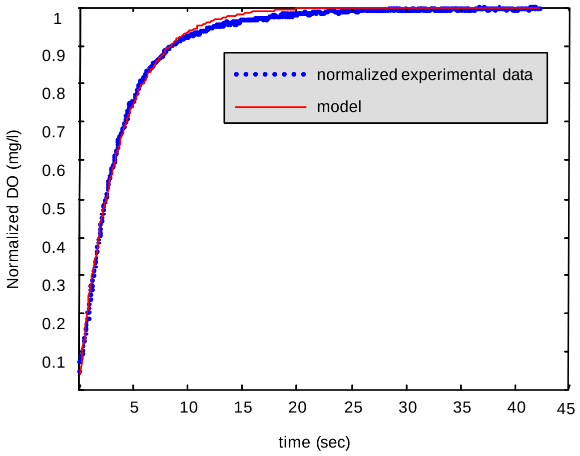

Fig. 3 - Model response compared to experimental data in the upward step (from deoxygenated to O$_2$-saturated water).

Table 1
Sampled-time modelling of the DO probe

Step	**Transfer function**	**poles (p)/zeros (z)**
up	$G_{up}(z^{-1}) = -3.855 \cdot 10^{-5} \dfrac{1 - 12.153 z^{-1} - 19.978 z^{-2}}{1 - 1.9014 z^{-1} + 0.9026 z^{-2}}$	$z_1^{up} = 10.866$ $\quad z_2^{up} = 1.2863$ $p_1^{up} = 0.98627$ $\quad p_2^{up} = 0.9151$
down	$G_{down}(z^{-1}) = -1.33 \cdot 10^{-6} \dfrac{1 + 577.409 z^{-1} - 2758.22 z^{-2}}{1 - 1.7675 z^{-1} + 0.7704 z^{-2}}$	$z_1^{down} = -582.147$ $\quad z_2^{down} = 4.738$ $p_1^{down} = 0.9868$ $\quad p_2^{down} = 0.7807$

COMPENSATOR DESIGN

The problem of dynamic compensation consists of reducing the probe lag as much as possible, so that the transfer function has unity gain over the required frequency band $\left(0,w_b\right)$. Ideally, the perfect compensator could be obtained by inverting the given transfer function and therefore cancelling out the probe dynamics altogether, i.e. $G(z^{-1})\times G^{-1}(z^{-1})=1 \quad w\in\left(0,w_b\right)$. However, exact compensation is not possible since the inverse system $G^{-1}(z^{-1})$ would not be a proper transfer function, hence only approximate compensation can be obtained. A compensating digital transfer function $\tilde{H}(z^{-1})$, to be placed in series with the probe dynamics, is now determined so that the response of the combined system $G(z^{-1})\times\tilde{H}(z^{-1})\approx 1 \quad w\in\left(0,w_b\right)$ introducing the least possible lag over the required bandwidth. The compensator $\tilde{H}(z^{-1})$ is designed so that its zeros cancel out the poles of $G(z^{-1})$. Its poles are selected in order to shape the system response according to rise-time reduction and monotonic response (i.e. no overshoot). To meet these design criteria, it was assumed that the input is not an exact step function, but a pseudo-step composed of a steep ramp as the leading edge reaching the maximum value in 2.5 s, which is considered a satisfactory compromise (see figures 4 and 5). The poles of $\tilde{H}(z^{-1})$ are designed to minimise the response error to the pseudo-step y_{pstep} input, namely,

$$\hat{\mathbf{p}}_H = \underset{\mathbf{p}_H}{arg\,min}\left(\int_0^{t_{step}}\left(y_{DO}-y_{pstep}\right)dt\right) \tag{2}$$

where t_{step} is the duration of the step experiment, typically 40 s, as shown in figures 2 and 3. A numerical optimization procedure based on a modified version of the Nelder and Mead flexible polyhedron (Marsili-Libelli, 1992) was used to obtain the optimal compensator poles $\hat{\mathbf{p}}_H$, obtaining the design values reported in Table 2. The transfer function $\tilde{H}(z^{-1})$ was then software-implemented as a LabView *Virtual Instrument* (VI) supervising DO measurements, using a Matlab Node in the data acquisition *while* structure.

Table 2
Transfer function of the optimal compensator for the DO probe dynamics of Table 1

Step	Transfer function	poles (p)
up	$\tilde{H}_{up}\left(z^{-1}\right)=-0.1579\dfrac{1-1.914z^{-1}+0.9026z^{-2}}{1-1.9697z^{-1}+1.0237z^{-2}-0.0522z^{-3}}$	$p_1^{down}=0.9749$ $p_2^{down}=0.9372$ $p_3^{down}=0.0575$
down	$\tilde{H}_{down}\left(z^{-1}\right)=-296.55\dfrac{1-1.7675z^{-1}+0.7704z^{-2}}{1-1.389z^{-1}-0.039z^{-2}-0.432z^{-3}}$	$p_1^{down}=0.9391$ $p_2^{down}=0.9387$ $p_3^{down}=-0.4902$

The performance of the combined system (DO probe and software compensator) was tested with the same experimental set-up of figure 1 and the results of figures 4 and 5 were obtained. It can be seen that the system response is still monotonic and much faster than in the original case. The frequency analysis of figure 6 shows the increased 3 dB bandwidth as a result of compensator design.

To take into account the possibility of changing probe characteristics and to make the design as portable as possible, the complete VI has auto-tuning capabilities. If a new set-up is used, then the two-beaker experiment should be repeated and the optimization routine run again, to determine the best compensator $\tilde{H}(z^{-1})$ for the given probe. If a new set-up is used, then the two-beaker experiment should be repeated and the optimization routine run again, to determine the best compensator $\tilde{H}(z^{-1})$ for the given probe.

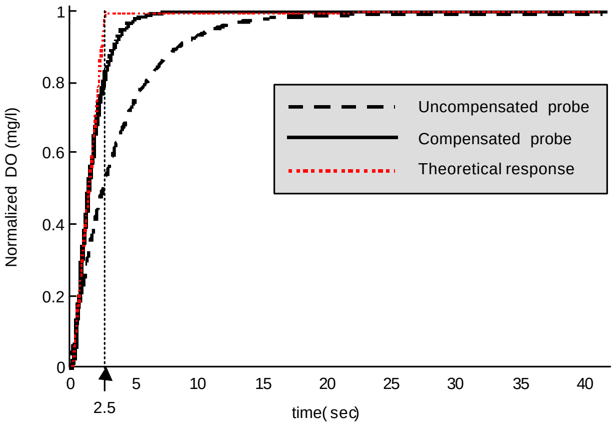

Fig. 4 - Experimental response of the compensated probe in the upward step.

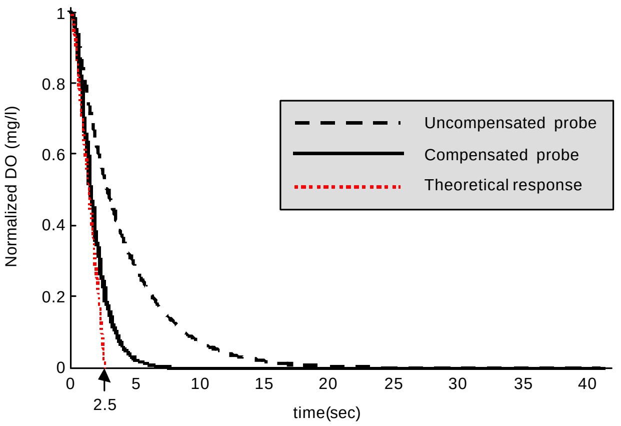

Fig. 5 - Experimental response of the compensated probe in the downward step.

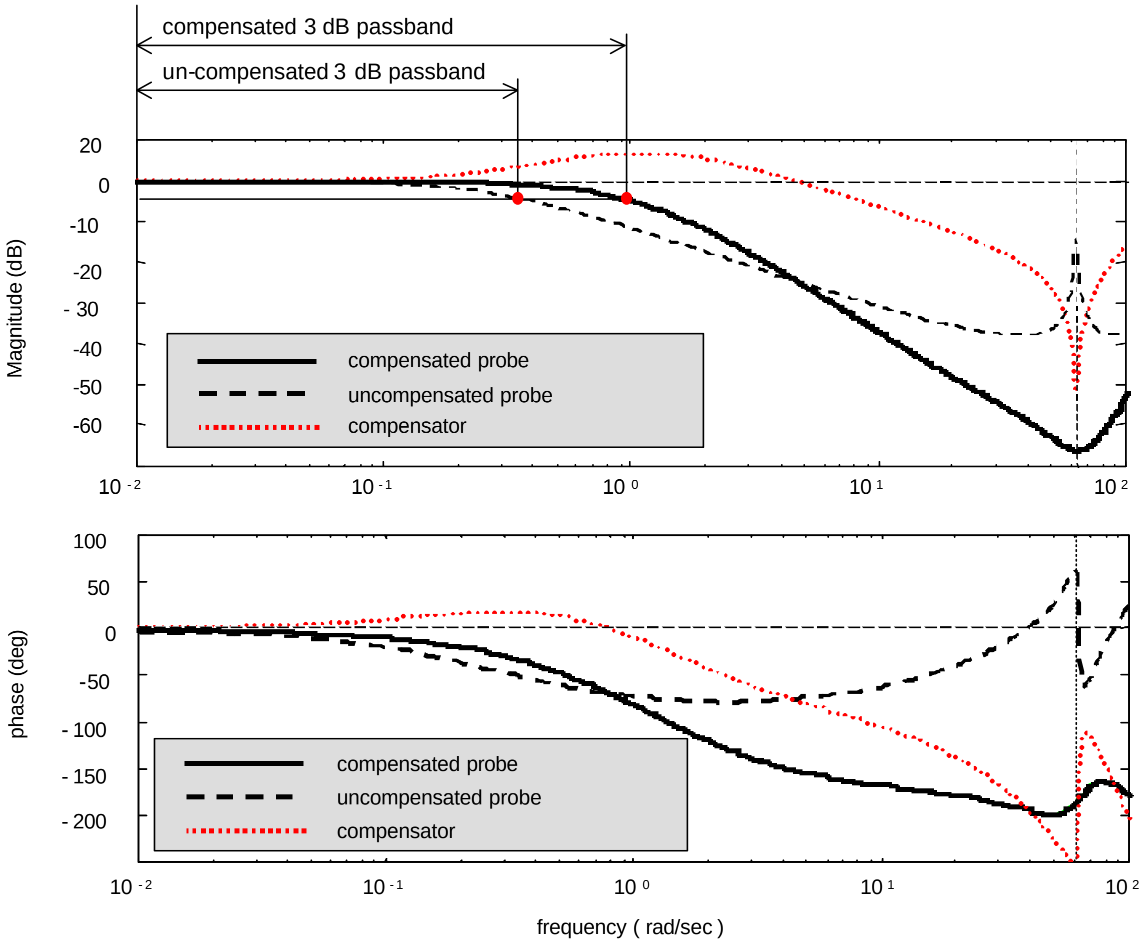

Fig. 6 - Bandwidth extension as a result of probe compensation.

APPLICATION TO AN OPEN RESPIROMETER

This compensation technique may have several applications, whenever it is important to correct the dynamic response of the DO probe. For example, consider the calibration of the oxygen transfer coefficient K_La from oxygenation experiments. If the reaction tank is small and the oxygenation capacity of the aerator is large, the DO kinetics may be of the same order of magnitude as the probe rise time, hence the need to compensate its response.

The compensated probe was applied to the measurement of Dissolved Oxygen in an open respirometer operated in a RODTOX mode (Vanrolleghem *et al.,* 1990). The following simulation experiment shows the accuracy improvement, which can be achieved with the compensated probe. Suppose that a given amount of biodegradable substance is injected into the system, then the deoxygenation curve follows the behaviour of figure 7. The hatched area below the endogenous DO level C_e represents the oxygen consumed to metabolise the injected substrate S_o, which is supposed to be completely biodegradable. A yield factor Y = 0.47 is assumed.

OUR estimation

The relationship between the area C_o and the injected substrate S_o, can be obtained from the dynamic oxygen balance, with OUR_{ex} representing exogenous oxygen uptake rate.

$$\frac{dC}{dt} = K_L a\left(C_e - C\right) - OUR_{ex} \tag{3}$$

Integration over the respiration interval (0, T_{resp}) yields the following relation between consumed oxygen C_o and injected biodegradable substrate S_o.

$$K_L a \int_0^{T_{resp}} \left(C_e - C\right) dt = \int_0^{T_{resp}} OUR_{ex} dt = -\left(1 - Y\right) \int_{S_o}^{0} dS \quad \Rightarrow \quad K_L a \cdot C_o = \left(1 - Y\right) S_o \tag{4}$$

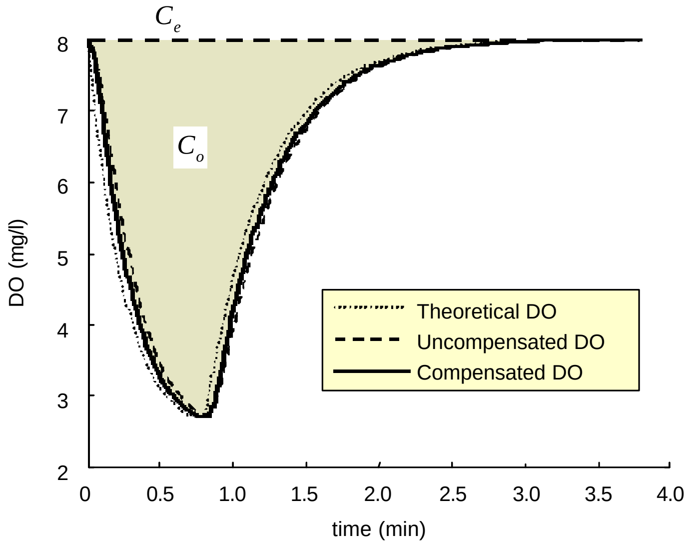

Fig. 7 – Simulation of dissolved oxygen deoxygenation curves: comparison of the theoretical curve (hatched area) with those taking into account the DO probe dynamics, both in the compensated and uncompensated case.

This experiment has been simulated using the ASM1 kinetics for carbonaceous substances and no start-up lag (Vanrolleghem *et al.,* 1998) was considered for simplicity. Three different simulations were performed: the theoretical one, without probe dynamics (labelled 'Theo-retical DO'), and with compensated and uncompensated probe models from Tables 1 and 2. Table 3 compares the areas under the curves in the three cases and the resulting estimation errors. It can be seen that the compensated probe yields a better approximation of the theoretical area.

However, the estimated area C_o is the least affected by the probe dynamics, with percentage errors below 1% in both cases. This is not surprising, given the integral nature of this quantity.

Table 3
Computation of deoxygenation curve area taking into account the dynamics of compensated and uncompensated DO probe (Y = 0.47).

	$C_o\ (mg\,O_2)$	DC_o %	$K_La\ (min^{-1})$	DK_La %	$S_o\ (mg\,O_2)$	DS_o %
Theoretical	5,374886		2,194800		22,2581	
Uncompensated	5,381654	0.126	1,824878	-16.854	18,5299	16,749
Compensated	5,377796	0.054	1,967200	-10.370	19,9607	10,321

K_La estimation

From the oxygen integral balance (4) and the results of Table 3 it can be seen that K_La directly affects the relationship between consumed oxygen C_o and injected substrate S_o. In fact K_La and S_o are almost equally affected by the errors introduced by the probe dynamics. A further investigation into K_La errors is now considered. Figure 8 shows a typical reoxygenation experiment in an open respirometer with endogenous sludge (OUR_{end}=const). The DO model is fitted to the DO data through adjustment of the K_La parameters, since OUR_{end} was previously measured known. This experiment is repeated with different DO models including compensated and uncompensated probe dynamics.

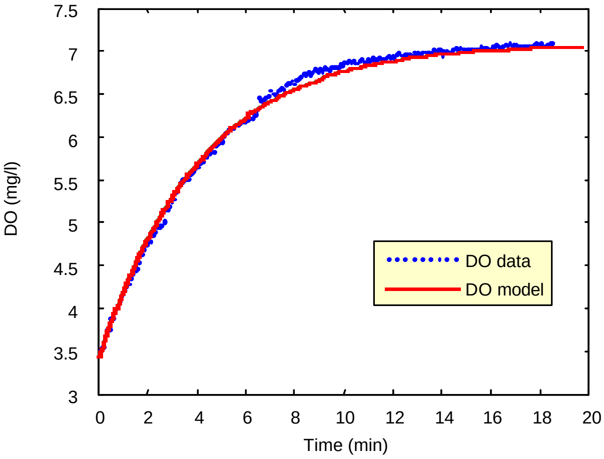

Fig. 8 - Measurement of the K_La during the respirometer calibration procedure.

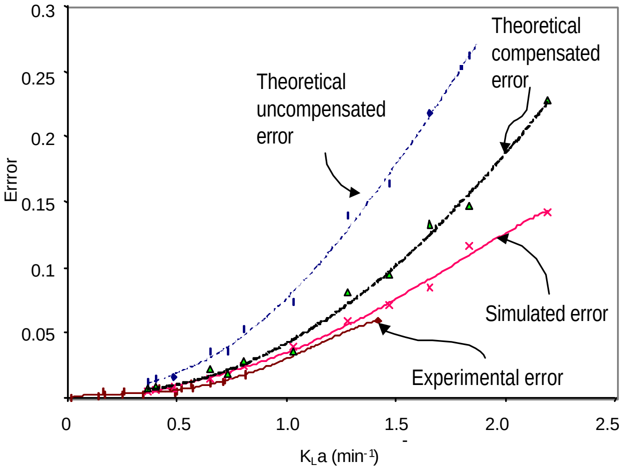

Fig. 9 - K_La estimation error with the compensated and uncompensated probe model.

The influence of probe compensation on K_La estimation error has been assessed with two different sets of experiments, one performed through simulation and the other with the experimental respirometer.

K_La experimental error evaluation. Several reoxygenation curves were obtained starting with a low-oxygen condition (around 2 mg/l) and increasing the air flow rate. The data couples for the compensated $\left(\hat{t}_i,\hat{C}_i^{(c)}\right)$ and uncompensated $\left(\hat{t}_i,\hat{C}_i^{(nc)}\right)$ case were recorded for a number of differing air-flow settings and the corresponding $K_La^{(nc)}$ and $K_La^{(c)}$ estimated. With the available equipment a maximum value of $K_La = 1.5\ min^{-1}$ could be obtained. Larger values were obtained through simulation.

K_La simulated error evaluation. This test is similar to the experiment leading to figure 7. After selecting a K_La value a reoxygenation curve was simulated and the three data couples recorded: $\left(t_i,\tilde{C}_i^{(T)}\right)$ for the theoretical case (no probe dynamics), $\left(t_i,\tilde{C}_i^{(nc)}\right)$ for the uncompensated and $\left(t_i,\tilde{C}_i^{(c)}\right)$ for the compensated probe dynamics. The corresponding estimated values of K_La were labelled $K_La_{(S)}$, $K_La^{(nc)}_{(S)}$ and $K_La^{(c)}_{(S)}$ respectively. The errors labels of figure 9 correspond to the following error computations

Table 4
K_La estimation errors shown in figure 9

Experimental error	Simulated error	Theoretical compensated error	Theoretical uncompensated error
$K_L a^{(c)} - K_L a^{(nc)}$	$K_L a^{(c)}_{(S)} - K_L a^{(nc)}_{(S)}$	$K_L a_{(S)} - K_L a^{(c)}_{(S)}$	$K_L a_{(S)} - K_L a^{(nc)}_{(S)}$

CONCLUSION

The dynamic accuracy of dissolved oxygen measurements can be improved by reducing the low-pass response of polarographic DO probes. This time lag is a consequence of the chemical reactions at the basis of the measuring principle. A software compensator has been proposed to obtain a partial cancellation of this effect and it was shown that the resulting virtual instrument can be used in an open respirometer to improve the accuracy of DO measurements and K_La estimation. The compensator is based on the identification of the probe dynamic response as a discrete-time transfer function. From this basis a digital compensator was designed to cancel the probe dynamics and substitute the original poles with others providing a tailored response to a quasi-step input. The compensated dynamics was determined by optimal pole allocation, based on a least-squares objective function with several constraints, such as monotonic response and minimum rise time. An application of this procedure was the accuracy assessment of respirometric quantities. For this, the virtual instrument was incorporated into the software driving a bench-scale open respirometer and the K_La estimation error with and without compensation was obtained. Though this application was demonstrated with the help of a practical example, the procedure is general enough to be applied to any probe, which can be quickly compensated prior to normal operation using the illustrated procedure.

REFERENCES

Linek V., Vacek V. Sinkule J. and Beneš P. (1988). *Measurement of oxygen by membrane-covered probes*. Ellis Horwood Ltd. Chichester.

Marsili-Libelli S. (1992). Parameter estimation of ecological models. *Ecological Modelling,* **62**: 233 – 258.

Ogata K. (1987) *Discrete-time control systems,* Prentice-Hall, New York.

Philichi T.L. and Stenstrom M.K. (1989). Effects of dissolved oxygen probe lag on oxygen transfer parameter estimation, *J. WPCF,* **51** (1): 83 – 86.

Spanjers H. and Olsson G. (1992). Modelling of the dissolved oxygen probe response in the improvement of the performance of a continuous respiration meter. *Water Res.,* **26** (7): 945 – 954.

Spanjers H., Vanrolleghem P.A., Olsson G. and Dold P.L. (1998). Respirometry in control of the activated sludge process: principles. *IAWQ Scientific and Technical Report n. 7.*

Vanrolleghem P. A., Dries D. and Verstraete W. (1990). RODTOX: biosensor for rapid determination of the biochemical oxygen demand and the on-line monitoring of the toxicity of wastewaters. In *Proc. 5th European Congress on Biotechnology,* Copenhagen, Denmark, July 8 - 13, 1990, Vol. 1, pp. 161 - 164.

Vanrolleghem P.A., Gernaey K., Petersen B., De Clercq B., Coen F. and Ottoy J-P. (1998). Limitations of short-term experiments designed for identification of activated sludge biodegradation models by fast dynamic phenomena, Proc. *7th IFAC Conference on Computer Applications in Biotechnology* CAB7. Osaka, Japan, pp. 567-572.