# A SOFTWARE SENSOR FOR A WASTEWATER TREATMENT PLANT

Teresa Lopez<sup>(1)</sup>, Anna Pulis<sup>(2)</sup>, Michela Mulas<sup>(2)</sup> and Roberto Baratti<sup>(2)</sup>

 <sup>(1)</sup> Instituto Mexicano del Petróleo, Programa de Matemáticas Aplicadas y Computación, A.P. 14-805, 07730 Mexico D.F., Mexico (e-mail: mtlopeza@imp.mx)
 <sup>(2)</sup> Dipartimento di Ingegneria Chimica e Materiali, Universita' di Cagliari, Piazza D'Armi, 09123 Cagliari, Italy

Abstract: In this work, a software sensor is presented in order to monitor the pollutant concentrations in an activated sludge process for industrial and municipal wastewater treatment. The software sensor consists of a model-based state estimator to infer the (unmeasured) biodegradable substrate and ammonia concentrations, based on a reduced process model with approximated model parameters and considering only on-line measurements of dissolved oxygen and nitrate concentrations. The software sensor performance is showed with experimental data from a real process and it is compared versus a complex process model, obtaining good estimated concentrations. *Copyright*  $\bigcirc$  2003 IFAC

Keywords: Biotechnology, Waste treatment, Detectors, Monitoring, Observability, State estimation.

## 1. INTRODUCTION

Biological wastewater treatment is an essential operation for the processing of liquid waste, where the main objectives are the degradation of the organic pollutant compounds and the removal of nutrients such as nitrogen that can damage the ecosystem. However during the wastewater treatment, variables such as concentrations are determined by off-line laboratory analysis, making a limitation for on-line monitoring and control purposes. Moreover, a control system design is not straightforward due to (Shimizu, 1996): the lack of reliable sensors, the significant model uncertainty, and the nonlinear time-varying nature of the system.

In a successful manner, concentrations can be on-line estimated using a software sensor (Aubrun et al., 2001; De Asís and Filho, 2000), which consists in using a state estimation technique in combination with a sensor that allows on-line measurements of some process variables, to reconstruct the time evolution of the unmeasured states. Having an important advantage since software sensors can be constructed based on a simple model with uncertain inputs and parameters (Stephanopoulos and San, 1984). Recently, several studies have been reported concerning the software sensor design in wastewater treatment for real time monitoring applications (Aubrun et al., 2001; Bernand et al., 2001; Larose and Jorgensen, 2001; Gomez-Quintero and Queinnec, 2001).

In this work, a software sensor is designed for on-line estimation of the pollutant concentrations in a wastewater treatment. In particular, we are considering a real case: the Tecnocasic plant (located near Cagliari, Italy), which collects industrial and municipal wastewater, and its biological treatment is done by the activated sludge process. The software sensor consists of a model-based state estimator to infer the (unmeasured) biodegradable substrate and ammonia concentrations, based on a reduced process model with approximated parameters and considering on-line measurements of dissolved oxygen and nitrate concentrations. The implementation is done with experimental data from the real process and it is compared versus a complex complete process model.

# 2. PROCESS MODEL

#### 2.1 Process description

In general, wastewater treatment includes as a first step a mechanical treatment to remove floating and settleable solids, then a biological treatment with activated sludge for removal of nitrogen and other organic pollutants, and after that other operations such as sludge treatment and water chemical treatment.

Here the continuous activated sludge process is considered for the biological wastewater treatment with the main purpose of nitrogen removal. This process (see Fig. 1) includes a reactor divided in two zones: a pre-denitrification step (in an anoxic zone) followed by a nitrification one (in an aerobic zone), and afterward by a settler from which the sludge is partly recirculated to the reactor (return activated sludge, RAS) and partly wasted as excess sludge (waste activated sludge, WAS). The global process is considered isothermal (around 20°C), and both anoxic (with low aeration for mixing purposes) and aerobic (with high aeration for reaction and mixing purposes) zones are controlled by the aeration supply in order to maintain a specific dissolved oxygen set point.

In particular, we are considering a real case: the Tecnocasic plant (located near Cagliari, Italy), which collects industrial and municipal wastewater, and its treatment is done by the activated sludge process as described previously.

#### 2.2 Mathematical modeling

The mathematical modeling was done first by the plant simulation in the GPS-X (a commercial software of Hydromantis), using the two-step-mantis model (Technical reference manual, 2001) which corresponds to the so-called IAWQ Activated Sludge Model No. 1 (Henze et al., 1987) with two modifications: (a) the nitrification is modeled by a two-step process (the conversion of ammonia to nitrite by the nitrosomona bacteria and the conversion of nitrite to nitrate by the nitrobacters), and (b) the hydrolysis of rapidly biodegradable substrate is included. This complex model, that will be referred as GPS-X model, consists of 18 state variables (particle and soluble concentrations) for each anoxic and aerobic reactor, so that the process is modeled with 36 ordinary differential equations, including 15 reaction rates and 30 model parameters. The GPS-X model is included in this work in order to show the advantages of using simple models together with the available measurements, since a great problem for having an exact model is the parameter identification which strongly changes for each waste and biomass type (Maria et al., 2000).



Fig. 1. Diagram of the activated sludge process.

Since we are interested on having estimates of soluble concentrations before the settler, a reduced model proposed by Gomez-Quintero et al. (2000) is considered. Differently from the complete GPS-X model, this model consists of eight state variables:

$$\boldsymbol{x} = \begin{bmatrix} x_{1}, \dots, x_{8} \end{bmatrix}^{T} = \begin{bmatrix} S_{NO_{3}}^{p}, S_{O_{2}}^{p}, S_{NH_{4}}^{p}, S_{S}^{p}, S_{NO_{3}}^{n}, S_{O_{2}}^{n}, S_{NH_{4}}^{n}, S_{S}^{n} \end{bmatrix}^{T}$$

where  $S_{O2}$ ,  $S_{NO3}$ ,  $S_{NH4}$ , and  $S_S$  are the dissolved oxygen, nitrate, ammonia and biodegradable substrate concentrations for each reactor zone (*p* and *n* denote pre-denitrification and nitrification, respectively). The exogenous inputs

$$d = [d_1, \dots, d_6]^T = [S_{NO_3}^{in}, S_{NH_4}^{in}, S_S^{in}, Q_{in}/V, Q_r/V, Q_w/V]^T$$

are the influent concentrations and flow rates. The model needs of only five reaction rates given by

$$\begin{aligned} r_1^{p/n} &= \frac{S_{No3}^{p/n}}{K_{NO3} + S_{No3}^{p/n}}, \quad r_2^{p/n} &= \frac{K_{O2,H}}{K_{O2,H} + S_{O2}^{p/n}}, \\ r_3^{p/n} &= \frac{S_{NH4}^{p/n}}{K_{NH4} + S_{NH4}^{p/n}}, \quad r_4^{p/n} &= \frac{S_{O2}^{p/n}}{K_{O2,A} + S_{O2}^{p/n}}, \\ r_5^{p/n} &= \frac{S_{O2}^{p/n}}{K_{O2,H} + S_{O2}^{p/n}} \end{aligned}$$

and it has twelve model parameters  $p = [p_1, \dots, p_{12}]^T = [Y_H, i_{XB}, K_{O2,H}, K_{O2,A}, K_{NO3}, K_{NH4}, \eta_g, \eta_H, \alpha_1, \alpha_2, \alpha_3, \alpha_4]^T$ 

The reactor model is given as follows:

$$x_{2} = d_{5}x_{6} - (d_{4} + d_{5})x_{2} + k_{La}^{p} (S_{OST} - x_{2}) - Ex_{4}r_{5}^{p} - Fr_{3}^{p}r_{4}^{p} := f_{2} (x_{2}, x_{3}, x_{4}, x_{6}, d, p)$$
(1b)

$$x_{3} = d_{2}d_{4} + d_{5}x_{7} - (d_{4} + d_{5})x_{3} - Bx_{4}(r_{5}^{p} + r_{1}^{p}r_{2}^{p}) - \alpha_{2}r_{3}^{p}r_{4}^{p} + \alpha_{3} := f_{3}(x_{1}, x_{2}, x_{3}, x_{4}, x_{7}, d, p)$$
(1c)

$$\dot{x}_{4} = d_{3}d_{4} + d_{5}x_{8} - (d_{4} + d_{5})x_{4} + (\alpha_{4} - Dx_{4})r_{5}^{p} + (C - Dx_{4})r_{1}^{p}r_{2}^{p} := f_{4}(x_{1}, x_{2}, x_{4}, x_{8}, d, p)$$
(1d)

$$x_{7} = (d_{4} + d_{5})(x_{3} - x_{7}) - Bx_{8}(r_{5}^{n} + r_{1}^{n}r_{2}^{n}) - \alpha_{2}r_{3}^{n}r_{4}^{n} + \alpha_{3} := f_{7}(x_{3}, x_{5}, x_{6}, x_{7}, x_{8}, d, p)$$
(1g)

$$x_{8} = (d_{4} + d_{5})(x_{4} - x_{8}) + (\alpha_{4} - Dx_{8})r_{5}^{n} + (C - Dx_{8})r_{1}^{n}r_{2}^{n} := f_{8}(x_{4}, x_{5}, x_{6}, x_{8}, d, p)$$
(1h)

where

$$A = \alpha_1 (1 - Y_H) / 2.86Y_H , B = \alpha_1 i_{XB}, C = \alpha_4 \eta_h$$
  
$$D = \alpha_1 / Y_H , E = \alpha_1 (1 - Y_H) / Y_H , F = 4.57\alpha_2$$

# 2.3 Test motion

As it was mentioned before, the experimental data correspond to the Tecnocasic plant (Cagliari, Italy) for industrial and municipal wastewater treatment. The experimental motion is shown in Fig. 2 (where the data were taken one per day), with an operation condition around the mean value  $\overline{d} \approx [0.0 \text{ gN/m}^3, 16.25 \text{ g N/m}^3, 118.3 \text{ g COD/m}^3, 3.10 \text{ d}^{-1}, 3.90 \text{ d}^{-1}, 0.28 \text{ d}^{-1}]^{\text{T}}$  with some disturbances. For the dissolved oxygen control, a PI-controller was used to calculate the airflow supply to each reactor (equivalent to calculate the necessary oxygen mass transfer coefficient, k<sub>La</sub>). And the identified model parameters (according Gomez-Quintero et al., 2000) are given in Table 1.

In Fig. 2 the test motion for the two considered models are shown in comparison with the experimental one. As we can see, the GPS-X model gives a very good approximation, while the reduced model gives the motion tendency but with significant offsets due to the errors in the model assumptions and parameter identification. With these results, it can be stated one of the tasks that the software sensor should do: using the reduced model, the software sensor should give a good inference of the modeling errors in order to reach the actual (experimental) concentration motions.

Table 1. Reduced model parameters

Parameter (p)	Value
$Y_{\rm H}$	0.7
i <sub>XB</sub>	$0.086 \text{ g N} (\text{g COD})^{-1}$
K <sub>O2,H</sub>	$0.2 \text{ g O}_2 \text{ m}^{-3}$
K <sub>O2,A</sub>	$0.23 \text{ g } \text{O}_2 \text{ m}^{-3}$
K <sub>NO3</sub>	0.1 g N m <sup>-3</sup>
K <sub>NH4</sub>	0.8 g NH <sub>3</sub> -N m <sup>-3</sup>
$\eta_{ m g}$	0.5
$\eta_{ m H}$	0.4
$\alpha_1$	163.9 d <sup>-1</sup>
$\alpha_2$	224.63 g m <sup>-3</sup> d <sup>-1</sup>
$\alpha_3$	92.12 g m <sup>-3</sup> d <sup>-1</sup>
$\alpha_4$	739.74 g m <sup>-3</sup> d <sup>-1</sup>



Fig. 2. Performance of the GPS-X (\_\_\_\_\_) and reduced (- - -) models, in comparison with the experimental data (•).

#### 2.4 On-line monitoring problem

In our experimental study, the on-line monitoring problem consists on designing a software sensor for estimating mainly the ammonia and biodegradable substrate concentrations in the reactor exit (before the settler), from available measurements of dissolved oxygen in both reactor zones and the ammonia concentration in the (aerobic) nitrification zone. Meaning that the measured output is given by

$$y = [y_1, y_2, y_3]^T = [S_{O2}^p, S_{NO3}^n, S_{O2}^n]^T$$
(2)

The software sensor will be based on the reduced model [Eqs. (1)] and these three measurements [Eq. (2)], and it should be robust to have tolerance to the modeling error and to the uncertain inputs and measured outputs.

#### 3. SOFTWARE SENSOR DESIGN

For this purpose, the design is based on the geometric nonlinear estimation methodology developed in Alvarez and Lopez (1999) and Lopez (2000), which has a systematic construction, with a robust convergence criterion connected to the convergence rate, and with a simple tuning procedure.

Next the observability analysis, the estimator construction and tuning are presented for our specific case study.

## 3.1 Observability analysis

According to Alvarez and Lopez (1999), the motion x(t) of the reactor [Eqs. (1) and (2)] is *RE (robustly exponentially)* - *detectable* (i.e. partial observable) with the observability indices

$$(\kappa_1, \kappa_2, \kappa_3)^{\mathrm{T}} = (2, 2, 2)^{\mathrm{T}}$$
 (4)

and with the state partition  $(x_I \text{ and } x_{II} \text{ are the observable and unobservable states, respectively})$ 

$$x_{I} = [x_{2}, x_{3}, x_{5}, x_{6}, x_{7}, x_{8}]^{I}$$
(5a)

$$\boldsymbol{x}_{II} = \begin{bmatrix} \boldsymbol{x}_1, \boldsymbol{x}_4 \end{bmatrix}^T \tag{5b}$$

if the two following conditions are met along the reactor motion x(t):

- (i) The map  $\phi(x, d, p)$  is invertible for x<sub>I</sub>, and
- (ii) The motions of the unobservable dynamics  $x_{II}(t)$  are stable.

Where the map  $\phi$  is given by the measured outputs and some of their time-derivatives:

$$\phi(x,d,p) = [y_1, y_1, y_2, y_2, y_3, y_3]^{t}$$
  
=  $[x_2, f_2(x,d,p), x_5, f_5(x,d,p), x_6, f_6(x,d,p)]^{T}$  (6)

To verify that the plant is detectable for all time, next the two conditions are verified.

Assessment of the invertibility condition. Here it is important to mention that the observability matrix Q corresponds to

$$Q = \frac{\partial \Phi}{\partial x_i} \tag{7}$$

Such that the invertibility condition [condition (i)] is equivalent to verify that  $Rank[Q] = \kappa_1 + \kappa_2 + \kappa_3 = 6$ , or else,  $det[Q] \neq 0$  for all time. In fact this condition was evaluated numerically as can be seen in Fig. 3, showing that det[Q] < 0 for all time.

Assessment of the stability condition. The stability condition [condition (ii)] is equivalent to verify that the dynamics of

$$x_1 = f_1\left(x_1, \overline{x}_2, \overline{x}_3, x_4, \overline{x}_5, \overline{d}\right)$$
(8a)

$$\mathbf{x}_4 = f_4\left(\mathbf{x}_1, \overline{\mathbf{x}}_2, \mathbf{x}_4, \overline{\mathbf{x}}_8, \overline{d}\right) \tag{8b}$$

are stable, considering  $\overline{x}_2$ ,  $\overline{x}_3$ ,  $\overline{x}_5$ ,  $\overline{x}_8$  and d as nominal known motions. These equations are stable if the eigenvalues of its linear system have strictly negative real part. This is verified also numerically along the reactor motion and is shown in Fig. 4, concluding that the unobservable dynamics are stable.



Fig. 3. Determinant of the observability matrix.

![](_page_3_Figure_28.jpeg)

Fig. 4. Eigenvalues of the unobservable dynamics.

As the two conditions are met, therefore the reactor motion is RE-detectable, and a state estimator can be implemented.

#### 3.2 Construction

Considering the previous state partition [Eqs. (5)], the plant [Eqs. (1) and (2)] can be rewritten as

$$\mathbf{x}_{I} = f_{I}\left(\mathbf{x}_{I}, \mathbf{x}_{II}, d, p\right)$$
(9a)

$$x_{II} = f_{II}(x_I, x_{II}, d, p)$$
 (9b)

$$y = h(x_I) \tag{9c}$$

The construction of the geometric estimator (Luenberguer-like high-gain) follows from a straightforward consequence of the detectability property, according to the following expression (see Theorem 1 in Alvarez and Lopez, 1999). So that the estimator for our case is given by

$$\dot{\hat{x}}_{I} = f_{I}\left(\hat{x}_{I}, \hat{x}_{II}, d, p\right) + Q^{-1}K_{o}\left[y - h\left(\hat{x}_{I}\right)\right]$$
(10a)

$$\hat{x}_{II} = f_{II} \left( \hat{x}_{I}, \hat{x}_{II}, d, p \right)$$
 (10b)

$$\hat{y} = h(\hat{x}_l) \tag{10c}$$

Here  $Q^{-1}$  is the inverse of the observability matrix [Eq. (7)], and K<sub>o</sub> is the gain matrix which should be chosen such that the estimation error dynamics are stable (this will be discussed in next subsection). It can be seen that the observable part [Eq. (10a)] of the estimator has two terms: (i) a predictor term given by the model, and (ii) a corrector term driven by the error in the measurements. While the unobservable part [Eq. (10b)] only has a predictor term given by the model.

#### 3.3 Tuning

Some strategies for the estimator tuning are also given in Alvarez and Lopez (1999) and Lopez (2000). According to this, the gains can be calculated as follows

$$K_{o} = \begin{bmatrix} k_{11} & 0 & 0 \\ k_{12} & 0 & 0 \\ 0 & k_{21} & 0 \\ 0 & k_{22} & 0 \\ 0 & 0 & k_{31} \\ 0 & 0 & k_{32} \end{bmatrix}, \qquad k_{i1} = 2\zeta\omega_{i} \qquad (11)$$

Where  $\zeta$  is the damping factor, which can be set according the literature (Stephanopoulos, 1984) as  $\zeta$ = 0.71 in order to have a response with moderate oscillations. While  $\omega_i$  is the characteristic frequency, which can be selected such that the estimator response is faster than the reactor response. For this purpose, first we calculated the residence time as  $\theta = 0.1428$  d, then to obtain an estimator response faster, we selected the estimator characteristic time as  $\omega_i > 10 / \theta$ . Meaning that a good initial test can be  $\omega_i = 70 \text{ d}^{-1}$ . In fact after some trials, the final tuning values were set as  $\omega_1 = \omega_2 = \omega_3 = 150 \text{ d}^{-1}$  ( $\approx 20$  times faster than the natural dynamics).

### 5. IMPLEMENTATION RESULTS

Here it is worth of mention that the experimental data (shown in Fig. 2) are off-line laboratory analysis taken one per day, however with purpose of implementation of the software sensor [Eqs. (10)], the outputs [Eq. (2)] are incorporated as on-line measurements. So that when the software sensor is implemented there is exact converge for the measured states  $(S_{O2}^{p}, S_{NO3}^{n}, S_{O2}^{n})$  as was expected, while for the other states good estimates are obtained. In Fig. 5, the inference of the two main (ammonia  $S_{NH4}^{n}$  and biodegradable substrate  $S_{S}^{n}$ ) concentrations of interest in the reactor exit is shown. In this figure, we can see that the estimated ammonia concentration reaches closely the experimental data, in fact better than the GPS-X model estimation (shown in Fig. 2). With this result, we can say that the biodegradable substrate estimation should be reliable, in spite of no having experimental data for comparison.

![](_page_4_Figure_18.jpeg)

Fig. 5. Software sensor (\_\_\_\_\_) in comparison with the off-line experimental data (•).

### 6. CONCLUSIONS

In this study, the on-line estimation of unmeasurable concentrations of ammonia and biodegrable substrate in a wastewater treatment has been investigated, using a software sensor based upon a reduced model and considering only on-line measurements of dissolved oxygen and nitrate concentrations. The positive results, validated with experimental data, displays that the estimated concentrations are reliable in spite of the presence of input disturbances and of using a simple reduced model with uncertain parameters. Showing that not always the use of complex models is the best way to obtain a good process representation for monitoring and control purposes.

The solution of using a software sensor gives promising guidelines to tackle in the future the problem of real time control of wastewater treatment plants.

Acknowledgments. The work was supported by a contribution from MIUR (2002095147). The authors are very grateful to the Instituto Mexicano del Petroléo (MEXICO) and to the Regione Sardegna.

## NOMENCLATURE

d	exogenous input
f	model map
i <sub>XB</sub>	Mass N/ mass COD in biomass
Ko	observability matrix gain
$k_{La}$	oxygen mass transfer coefficient $(d^{-1})$
$K_{O2,H}$	Aerobic oxygen half-saturation coefficient
$K_{O2A}$	Aerobic/anoxic oxygen half-sat. coefficient
$K_{NO3}$	Nitrate half-saturation coefficient
$K_{NH4}$	Ammonia half-saturation coefficient
p	model parameter
Q	observability matrix
$Q_n$	flow rate, $m^{3}/d$ ( $n = in, out, r, w$ )
$r_i$	i-th reaction rate $(1 \le i \le 5)$
$S_{NO3}$	nitrate concentration (g $N/m^3$ )
$S_{O2}$	dissolved oxygen concentration (g $O_2/m^3$ )
$S_{NH4}$	ammonia concentration (g N/m <sup>3</sup> )
$S_S$	biodegradable substrate conc. (g COD/m <sup>3</sup> )
$S_{OST}$	dissolved oxygen saturation conc. $(g O_2/m^3)$
V	reactor volume (m <sup>3</sup> )
x	process state
у	measured output
$Y_H$	Heterotrophic yield
Greek symbols	
$\alpha_i$	i-th reduced model parameter $(1 \le i \le 4)$
•	

- $\alpha_i$  1-th reduced model parameter (1  $\leq$  1  $\eta_g$  Correction factor for anoxic growth
- $\eta_{H}$  Correction factor for anoxic hydrolysis
- $\phi$  observable map
- $\kappa_i$  observability index  $(1 \le i \le 3)$
- $\zeta$  damping factor
- $\omega_i$  characteristic frequency  $(1 \le i \le 3)$

Subscripts

- *in* influent
- r RAS
- w WAS
- out reactor exit
- *eff* (clean) effluent
- *I* observable partition
- *II* unobservable partition

#### **Superscripts**

- *p* pre-denitrification
- *n* nitrification
- ^ estimated

### REFERENCES

- Alvarez, J., and Lopez, T. (1999). Robust dynamic state estimation of nonlinear plants. *AIChE J.*, 45(1), 107.
- Aubrun, C., Therilliol, D., Harmand, J., Steyer, S.P. (2001) Software sensor design for COD estimation in an anaerobic fluidized bed reactor. *Water Sci. Tech.*, 43 (7), 115.
- Bernard, O., Polit, M., Hadj-Sadok, A., Pengov, M., Docahin, D. Estaben, M., Labat, P. (2001) Advanced monitoring and control of anaerobic wastewater treatment plants: Software sensors and controllers for an anaerobic digester. *Water Sci. Tech.*, 43 (7), 175.
- De Asís, A.J., Filho, W.M. (2000) Soft sensors development for on-line bioreactor state estimation. *Comp. Chem. Eng.*, 24, 1099.
- estimation. Comp. Chem. Eng., 24, 1099. Gomez-Quintero, C., Queinnec, I. (2001) Robust filtering for a reduced nonlinear model of an activated sludge process. Proc. Conf. On Decision and Control 2001.
- Gomez-Quintero, C., Queinnec, I., Babary, J.P. (2000) A reduced nonlinear model for an activated sludge process. *Proc. ADCHEM 2000*, 1037.
- GPS-X Technical reference manual (2001), Hydromantis Inc.
- Henze, M., Leslie Grady, C.P., Gujer, W., Maris, G.V.R., Matsuo, T. (1987) Activated sludge model No. 1, I.A.W.Q. Sci. and Tech. Report No. 1, London, U.K.
- Larose, A., Jorgensen, S.B. (2001). State estimation for a biological phosphorus removal process using an asymptotic observer. *Water Sci. Tech.*, 43 (11), 205.
- Lopez, T. (2000). Estimacion y control no lineal de reactores de copolimerizacion. Ph. D. Thesis, Universidad Autonoma Metropolitana, Mexico.
- Maria, G., Maria, C., Salcedo, R., Feyo de Azevedo, S. (2000) Databank transfer-of-information, shortcut and exact estimators used in the wastewater biological treatment process identification. *Comp. Chem. Engng.*, 24, 1713.
- Shimizu, K. (1996). A tutorial review on bioprocess systems engineering. *Comp. Chem. Eng.*, 20 (6/7), 915.
- Stephanopoulos, G. (1984) *Chemical Process Control*, Prentice Hall, Englewood Cliffs, New Jersey.
- Stephanopoulus, G., San K. (1984) Studies on on-line bioreactor identification. I. Theory. *Biotech. Bioeng.*, 26, 1179.