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Forward-Backward Propagation to Identify the Maximum Specific Growth Rates of a Bioreactor

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Abstract. In this article, we are interested in identifying the parameters of an aerobic bioprocess model used for wastewater treatment. In the field of biotechnology, various computer bugs caused by round- ing errors can induce an error interval that is too wide during data acquisition. For this reason, we are testing a new identification method using a set method based on interval arithmetic. The process studied is the chemical transformation of ammoniacal nitrogen which takes place in two stages: Re- action of nitrification-denitrification. The parameters chosen for the identification are the yields and the maximum growth rates. Initially, the study of observability by a differential algebraic method will simplify the study of the mathematical model. This nonlinear model is described by six differential equations. Subsequently, we apply a set method, in particular the propagation of constraints also called forwardbackward propagation, this technique allowed us to determine intervals containing the variable returns as well as the maximum specific growth rates defined from the Monod model which describes the operation of the bioreactor. This method also guarantees the result by rejecting all inconsistent values.

Introduction

In order to estimate the parameters of a bioreactor, we are interested in this study at a new identifi- cation method. This choice is motivated for several reasons. The first is due to an important problem faced by the scientific community and which concerns the various computer bugs caused by rounding errors [1]. The other reasons for our motivation is to find solutions to the problems of convergence and of estimates caused by the errors of modeling and noises of measurements [2], therefore, one cannot rely only on conventional methods of identification. The set approach based on interval arithmetic is well suited in the biotechnology field because in these cases the error interval introduced during data acquisition is too wide as is also the case in biology, chemistry or medical sciences. In this context, a variable is represented by a set called the likelihood set or domain, supposed to contain the real value x. The objective is to identify the parameters of a bioreactor as part of an ammoniacal nitrogen nitrification process, chemical reaction observed during depollution of wastewater. The first models to describe such processes are those reported by the international Association on Water Pollution Re- search and Control(IAWPRC) [3]. One of them is the activated sludge model [4] using Monod kinetics. It is a complete model describe by many parameters making it very complex and therefore identifi- cation by statistical methods is difficult or even impossible. These models are also not suitable for online control. Other models can be considered for the online control of an activated sludge process, using models like ARMAX [5], fuzzy logic [6] and neural networks [7]. The last two methods allow easier handling of nonlinearities. The identification of the parameters of a bioreactor using genetic al- gorithm are cited in [8]. The set techniques used in this study are an approach known for many years. The bases of these methods were established by R. Moore [9], then Neumaier [10] and Hansen [11]. There are applications in many fields for estimating uncertain parameters. This is the case in robotics for the identification of dynamic parameters [12, 13]. Due to the difficulties of acquiring measure- ments,the use of interval arithmetic is not new in the field of biotechnology [14, 15]. First, we apply a differential algebraic method [16, 17],[18], in order to study the observability and identifiability of the model. Indeed, models of biotechnological processes are often described in terms of differential

algebraic equations which therefore lend themselves well to this approach. The article is organized as follows, section 2 describes the essentials of the algebraic approach, and it will be followed in section 3 by the basic definitions of interval arithmetic as well as the principle of constraint propagation. In section 4, we present the bioreactor model whose dynamic parameters we want to identify. The results of the simulation and the discussion are given in section 5 followed by a conclusion.

The Algebraic Method

The study of observability and identifiability problems using differential algebraic methods dates back to the early 1990s [19, 20],[21]. The principle of the method used in this article consists in verifying the observability of a latent variable *x* compared, for example, to two variables *v* and *w*, if each com- ponent of *x* is solution of an algebraic equation not differential with coefficients dependent on *v* and *w* and a finite number of their time derivatives . In fact, to verify the observability of a variable *x* with respect to *v* and *w* of a system:

$$P_i\left(v, \frac{\partial v}{\partial t}, \frac{\partial^2 v}{\partial t^2}, \ldots, w, \frac{\partial w}{\partial t}, \frac{\partial^2 w}{\partial t^2}, \ldots, x, \frac{\partial x}{\partial t}, \frac{\partial^2 x}{\partial t^2}, \ldots, \xi, \frac{\partial \xi}{\partial t}, \frac{\partial^2 \xi}{\partial t^2}, \ldots\right) = 0 \quad (1)$$

Then, for $i = 1, 2, \ldots$ we compute a characteristic set of all differential polynomials v, w, x, ξ …

we compute a characteristic set of all differential polynomials with respect to a classification whose order {{v, w}, {x}, {ξ}} must be respected. This classification means that all the derivatives of v and w are less than x and all the derivatives of x are less than ξ. This characteristic set will be represented by a set E of differential polynomials, each directed by one and only one of the variables. We conclude that x is observable with respect to v and w if and only if, each component of it leads to a differential polynomial in E. To do this, a REDUCE package called astb (Diop S, 2002) is used.

Constraint Propagation

Interval arithmetic

An interval, denoted by [x], is a bounded and connected set of $\mathbb{R}$, which is defined by:

$$[x]=(\underline{x}, \overline{x})= \{ x \in R \mid \underline{x} \leq x \leq \overline{x} \} \quad (2)$$

The real numbers $\underline{x}$ and $\overline{x}$ are the lower and upper bounds of [x], respectively all intervals within R are denoted by $\mathbb{IR}$, basic mathematical operations are extended to intervals.

Let $[x] \in \mathbb{IR}$, then, we define.

Its lower bound**:** inf ([x]) = $\underline{x}$

Its upper bound**:** sup ([x]) = $\overline{x}$

$$\text{Its width: } w([x]) = \overline{x} - \underline{x} \geq 0 \quad (3)$$

Its Middle: mid ([x]) = $\frac{\overline{x}+\underline{x}}{2}$

Its radius**:** rad ([x] = $\frac{\overline{x}-\underline{x}}{2} \geq 0$

A box (or interval vector) [**x**] is a compact of R*n* , defined by the Cartesian product of n intervals.Therefore,

$$[\mathbf{x}] = [\underline{x}_1, \overline{x}_1] \times [\underline{x}_2, \overline{x}_2] \times, \ldots, [\underline{x}_n, \overline{x}_n]$$

$$= [x_1] \times [x_2] \times, \ldots, [x_n] \quad (4)$$

Elementary mathematical operations are extended to intervals. The result of an operation between two intervals of finite terminals is an interval obtained by working only on their bonds.

Let [x], [y] $\in \mathbb{IR}$ and $\circ \in \{+, -, *, /\}$, then

$$[\mathbf{x}] \circ [\mathbf{y}] = \{x \circ y \ / \ x \in [\mathbf{x}], \ y \in [\mathbf{y}] \ \} \quad (5)$$

In practice, we use less abstract equations:

$$\begin{aligned}
[\mathbf{x}] + [\mathbf{y}] &= [\,\underline{x} + \underline{y}\,,\, \overline{x} + \overline{y}\,] \\
[\mathbf{x}] - [\mathbf{y}] &= [\,\underline{x} - \overline{y}\,,\, \overline{x} - \underline{y}\,] \\
[\mathbf{x}] * [\mathbf{y}] &= [\min\{\underline{x}\,\underline{y}, \underline{x}\,\overline{y}, \overline{x}\,\underline{y}, \overline{x}\,\overline{y}\}, \max\{\underline{x}\,\underline{y}, \underline{x}\,\overline{y}, \overline{x}\,\underline{y}, \overline{x}\,\overline{y}\}] \\
[\mathbf{x}]^2 &= [\min(\underline{x}^2, \overline{x}^2)\,,\, \max(\underline{x}^2, \overline{x}^2)\,] \text{ if } 0 \notin [\underline{x}\,,\, \overline{x}\,] \\
&= [0, \max(\underline{x}^2, \overline{x}^2)\,] \quad \text{otherwise}
\end{aligned} \tag{6}$$

The division is defined by:

$$\begin{aligned}
1/[y] &= \emptyset && \text{if } [y] = [0, 0] \\
&= [\,1/y, 1/y\,] && \text{if } 0 \notin [y] \\
&= [\,1/y, \infty[&& \text{if } y = 0 \text{ et } y > 0 \\
[x]/[y] &= [x] * (1/[y]) && \text{if } 0 \notin [y]
\end{aligned}$$

In order to reduce an interval or block, bisection techniques are used. However, the result of operations between intervals is not minimal because of pessimism **(**Tarek Raissi, 2004) .Contraction techniques have been developed (Luc Jaulin, Michel Kieffer, Olivier Didrit, and Eric Walter, 2001), (Tarek Raissi, Nacim Ramdani, and Yves Candau ,2003) in order to reduce pavement without sometimes having to use bisections. So, a contractor $\mathcal{C}$ is an operator who makes it possible to contract or reduce an initial search pavement [x] without bisection and keeping all the solutions, i.e. eliminating inconsistent values. Constraint propagation on intervals allows on a predefined domain of variables, a considerable reduction in the size of a box [x] without resorting to bisections. The contractor that we use in our study is based on the principle of projection constraints **(**Isabelle Braems, 2002).

Consider a set $\mathbb{S}$, let us note $\mathcal{C}s$ ([x]) containing the smallest pavement $\mathbb{S} \cap$ [x]. $\mathcal{C}s$ is called the contraction operator. This operator is able to replace a box [x] by a box $\mathcal{C}s$ ([x]) with lower size while preserving the entire of solution set.

A contractor must therefore verify the following two properties (*Fig*1):

$$\forall\, [x] \in \mathbb{IR}^n \begin{cases} \forall\, [x] \subseteq \mathbb{X}, \mathcal{C}_s([x]) \subset [x] & \text{(contractance)} \\ \forall\, [x] \subseteq \mathbb{X},\ [x] \cap \mathbb{S} \subset \mathcal{C}_s([x]) & \text{(correctness)} \end{cases} \tag{7}$$

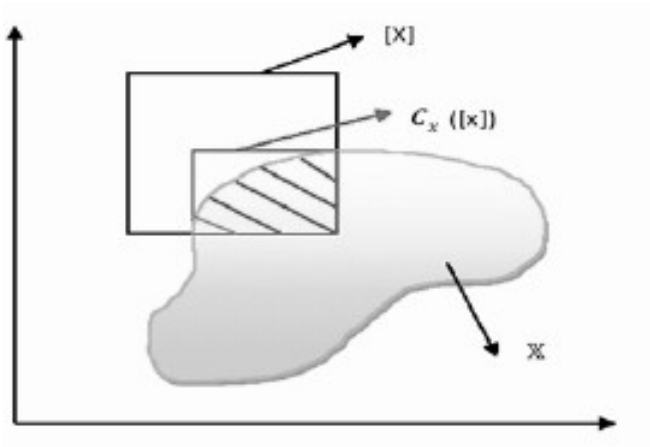

Fig. 1: Contraction of a set

Application to the bioreactor

In practice, modeling bacteria is difficult due to its living nature. Consequently,they are described by complex functions involving poorly known parameters. We focus on the interval approach, in order to represent the uncertainties that affect these parameters. For this application, a mathematical model is used to describe a biological wastewater treatment with activated-sludge process. Ammonia nitrogen is treated by nitrification-denitrification reaction, involving two populations of

autotrophic bacteria. Nitrification is the biological oxidation of ammoniacal nitrogen, it occurs through two steps: First, nitratation by ammonium-oxidizing bacteria, Nitrosomonas (AOB) and second, nitritation by nitride- oxidizing bacteria,Nitrobacter (NOB).

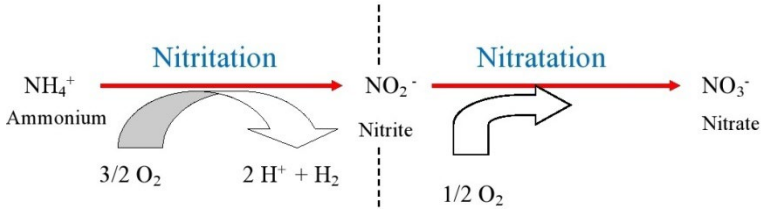

Fig. 2: The two stages of nitrification

The state of this bioreactor is described by six variables: the bacterial concentrations, called biomass and denoted X_1 and X_2, as well as the concentrations of substrate S_1, S_2 and S_3, S_{in} is the concen- tration of the incoming substrate. The above model represents the dynamic evolution of these state variables. The model represents the dynamic evolution of these state variables.

$$\begin{aligned}
\dot{S}_1 &= D\,(S_{in} - S_1) - k_1\,\mu_1(s_1)\,X_1 \\
\dot{X}_1 &= (\mu_1\,(s_1) - D)\,X_1 \\
\dot{S}_2 &= k_1\,\mu_1\,(s_1)\,X_1 - k_2\,\mu_2\,(s_2)\,X_2 - S_2\,D \\
\dot{X}_2 &= (\mu_2\,(s_2) - D)\,X_2 \\
\dot{S}_3 &= k_2\,\mu_2\,(s_2)\,X_2 - S_3\,D
\end{aligned} \tag{8}$$

with:

$$\mu_1\,(s_1) = \mu_{max1}\,\frac{S_1}{S_{1+}\,ks_1} \quad \text{and,} \quad \mu_2\,(s_2) = \mu_{max2}\,\frac{S_2}{S_{2+}ks_2} \tag{9}$$

$\mu_1(S_1)$ and $\mu_2(S_2)$ are the biomass growth rates. They are modeled by Monod kinetics[26]. $\mu_{max1}(S_1)$ and $\mu_{max2}(S_2)$ are the maximum specific growth rates, k_1 and k_2 are the stoichiometric coefficients which represent the respective yields of biomasses X_1 and X_2, k_{s1} and k_{s2} are the half-saturation con- stants for the growth corresponding to the cell affinity for the substrate of each bacterial population. D is the dilution rate, such that $D = \frac{Q_{in}}{V}$, where Q_{in} is the input flow of the bioreactor and V its volume.

Results and Discussions

The observability of the yields k_1 and k_2 of the system described by Equations (8) cited above is tested by calculating the characteristic set of the following set of differential polynomials. First, we simu- lated the model with parameters and measurements taken from the literature [27] over a period of 220 days. The yields k_1 and k_2 are obtained by the algebraic method [28]:

$$\begin{aligned}
k_1 &= \frac{D(Sin - y3) - \dot{y3}}{Dy1 + \dot{y1}} \\
k_2 &= \frac{D(Sin - y4 - y3) - (y4 + \dot{y3})}{Dy2 + \dot{y2}}
\end{aligned} \tag{10}$$

In order to illustrate the propagation of constraints, we construct the directed acyclic graph(DAG) for k_1 and k_2 which are represented by Figure 3

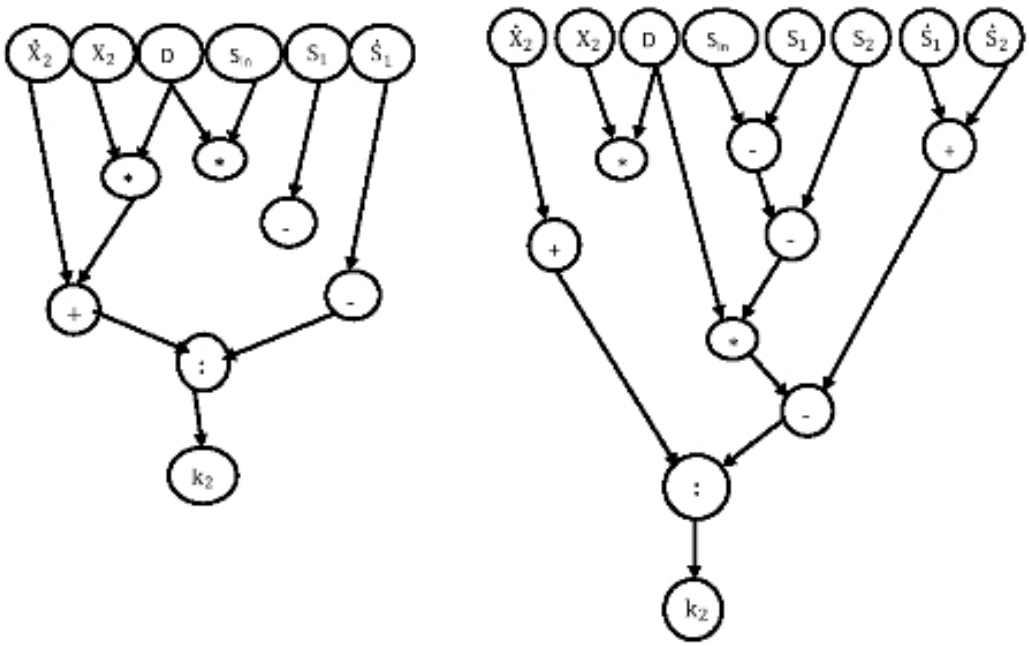

Fig. 3: The directed acyclic graph (DAG) for k_1 and k_2

We apply the forward-backward propagation after having developed the expressions (10) in primitive functions (see Appendix). For the simulations, we have chosen X_1=0.975X;
X_2= 0.035X and for the additive error due to disturbances and the modeling error, we chose e=0.01. The principle of forward-backward propagation is to select the primitive constraints to be used for the contractions according to an optimal order, in the sense of the size of the domains obtained at the end.
All the intervals of a_i are chosen]-∞, + ∞[, k_1 and k_2 are initialized with [0, + ∞[
The intervals are obtained by simulation on Matlab, using the Intlab toolbox.

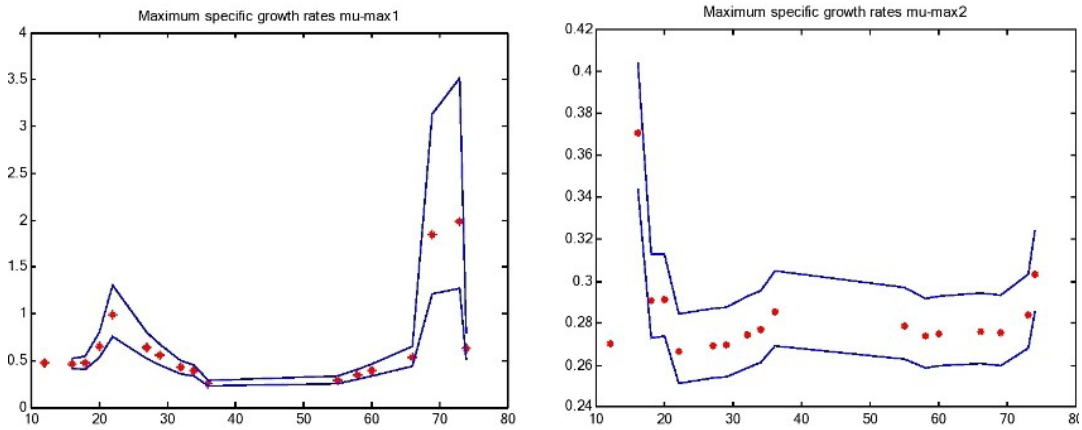

Fig. 4: Yield k_1 (right) , k_2 (left)

In Figure (4) are represented on the right the yield k_1 and on the left the yield k_2, in blue framing obtained by propagation of constraints, in red star model a priori We obtain the intervals for the yields:

k_1 = [0.6266, 1.3216]

k_2 = [0.0572, 10.75]

Such as: $\mu_{max1}=\frac{\mu_1 (S_1+ ks1)}{S_1}$ and $\mu_{max2}=\frac{\mu_2 (S_2+ ks2)}{S_2}$

We apply the same principle to determine interval for the maximum specific growth rates μ_{max1} and μ_{max2}. The directed acyclic graph (DAG) are represented by figure 4 In the same way, all the intervals of the primitives constraints b_i are chosen $]-\infty, +\infty[$, μ_{max1} and μ_{max2} are initialized with $[0, +\infty[$

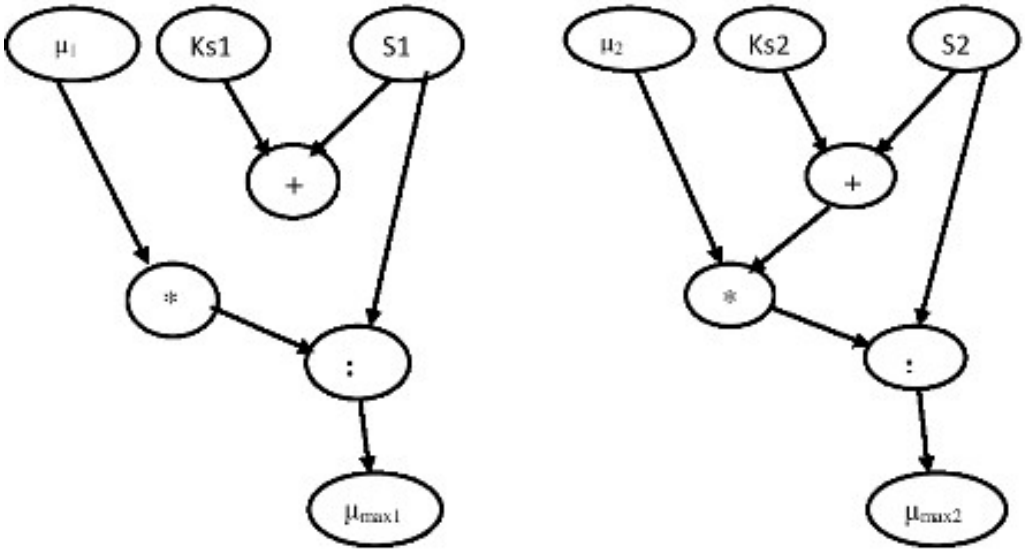

Fig. 5: DAG for μ_{max1} and μ_{max2}

In Figure (5) are represented on the right the the maximum specific growth rates μ_{max1} and on the left the maximum specific growth rates μ_{max2}, in blue framing obtained by propagation of constraints,in red star model a priori We obtain the intervals for the maximum specific growth rates

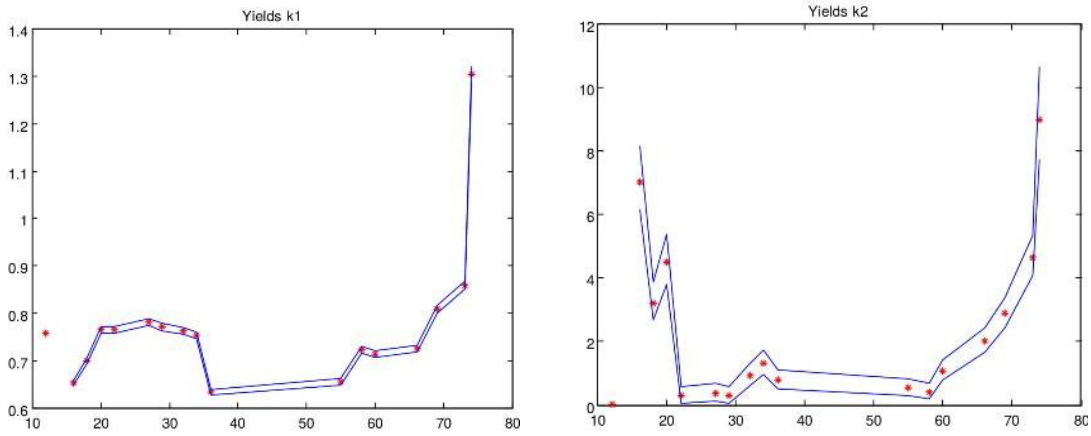

Fig. 6: The maximum specific growth rates μ_{max1} and μ_{max2}

$\mu_{max1} = [0.2486, 0.4045]$

$\mu_{max2} = [0.4009, 3.51]$

As a result, we have been able to associate with the yield parameters k_1 and k_2, as well as with maximum specific growth rates μ_{max1} and μ_{max2} the smallest intervals contain the a priori values obtained by the propagation of constraints

Conclusion

One of the difficulties in the study of biological or biotechnological systems is due to the experimental samples which can be counted in days. Therefore, the error interval may be too wide. The set methods based on interval arithmetic that we have already used are well suited in these areas. However, it has a drawback which concerns the problem of pessimism due to two phenomena

which can lead to an overestimation of the desired interval. There is a phenomenon of wrapping (wrapping effect) and of dependence or multi-occurrence because each variable is considered to be different. In this study, we tested this technique to identify the parameters of an aerobic bioprocess model for wastewater treatment. In order to avoid pessimism by studying a model with five equations, an algebraic method allowed us to determine simpler expressions for the yield k_1 and k_2 then to apply the principle of propagation constraints. The Forward-backward propagation technique allowed us to find a minimum interval for the return k_1 and k_2 as well as for the maximum unobservable specific growth rates μ_{max1} and μ_{max2} The advantage of this method is that it allows to obtain an interval containing the real value by rejecting the inconsistent values. We can extend our method to the identification of half-saturation constants for the growth k_{s1} and k_{s2} unobservable parameters

Appendix

S_{in}	Concentration of the incoming substrate
S_1	Concentrations of substrate 1
S_2	Concentrations of substrate 2
S_3	Concentrations of substrate 3
X_1	Biomass 1
X_2	Biomass 2
μ_1	Biomass growth rates 1
μ_2	Biomass growth rates 2
μ_{max1}	Maximum specific growth rates 1
μ_{max2}	Maximum specific growth rates 2
k_1	Yields of biomasse 1
k_2	Yields of biomasse 2
K_{s1}	Half-saturation constants for the growth 1
K_{s2}	Half-saturation constants for the growth 2
D	Dilution rate

Fig. 7: Notations

Forward propagation

$a_1=S_{in}- S_1$
$a_2=D.a_1$
$a_3=a_2- \dot{S}_1$
$a_4=D.X_1$
$a_5=a_4+\dot{X}_1$
$k_1= (a_3 / a_5) \cap k_1$
$a_7=S_{in}- S_2;$
$a_8=a_7- S_1;$
$a_9=D.a_8;$
$a_{10}= \dot{S}_2+\dot{S}_1$
$a_{11}=a_9-a_{10}$
$a_{12}=D. X_2;$
$a_{13}=a_{12}+\dot{X}_2$
$k_2=(a_{11} / a_{13}) \cap k_2$

$b_1= S_1+Ks_1$
$b_2= \mu_{max1}. S_1$
$\mu_1 =(b_2 / b_1) \cap \mu_1$
$b_3=S_2+Ks_2$
$b_4= \mu_{max2}.S_2$
$\mu_2= (b_4 / b_3) \cap \mu 2$

Backward propagation

$\dot{X}_2 = (a_{13}-a_{12}) \cap \dot{X}_2$
$a_{12} = (a_{13} - \dot{X}_2) \cap a_{12}$
$a_{11}= (a_{13}.k_2) \cap a_{11}$

$b_4= (\mu_2.b_3) \cap b_4$
$b_3= (b_4/ \mu_2) \cap b_3$
$\mu_{max2}= (b_4 /S_2) \cap \mu_{max2}$

$a_{13}= (a_{11} / k_2) \cap a_{13}$
$\dot{X}_2= (a_{13}-a_{12}) \cap \dot{X}_2$
$X_2= (a_{12} / D) \cap X_2$
$a_9= (a_{11}+a_{10}) \cap a_9$
$a_{10}= (a_9 - a_{11}) \cap a_{10}$
$\dot{S}_2= (a_{10} - \dot{S}_1) \cap \dot{S}_2$
$\dot{S}_1= (a_{10} - \dot{S}_2) \cap \dot{S}_1$
$a_8= (a_9/D) \cap a_8$
a7= (a8+SS1) ∩ a7
$S_1= (a_7 - a_8) \cap S_1$
$S_{in}= (a_7+ S_2) \cap S_{in}$
$S_2= (S_{in}-a_7) \cap S_2$
$a_3= (a_5.k_1) \cap a_3$
$a_5= (a_3 / k_1) \cap a_5$
$a_4= (a_5 -\dot{X}_1) \cap a4$
$\dot{X}_1=(a_5-a_4) \cap \dot{X}_1$
$X_1=(a_4 / D) \cap X_1$
$a_2=(a_3+\dot{S}_1) \cap a2$
$\dot{S}_1=(a_2-a_3) \cap \dot{S}_1$
$a_1=(a_2 / D) \cap a_1$
$S_{in}=(a+S_1) \cap S_{in}$
$S_1=(S_{in}-a_1) \cap S_1$

$S_2= (b_4 / \mu_{max2}) \cap S_2$
$S_2= (b_3-Ks_2) \cap S_2$
$Ks_2= (b_3-S_2) \cap Ks_2$
$b_2= (\mu_1.b_1) \cap b_2$
$b_1= (b_2 / \mu_1) \cap b_1$
$\mu_{max1}= (b_2 /S_1) \cap \mu max1$
$S_1= (b_2 / \mu_{max1}) \cap S_1$
$Ks_1= (b_1-S_1) \cap Ks_1$
$S_1= (b_1-Ks_1) \cap S_1$

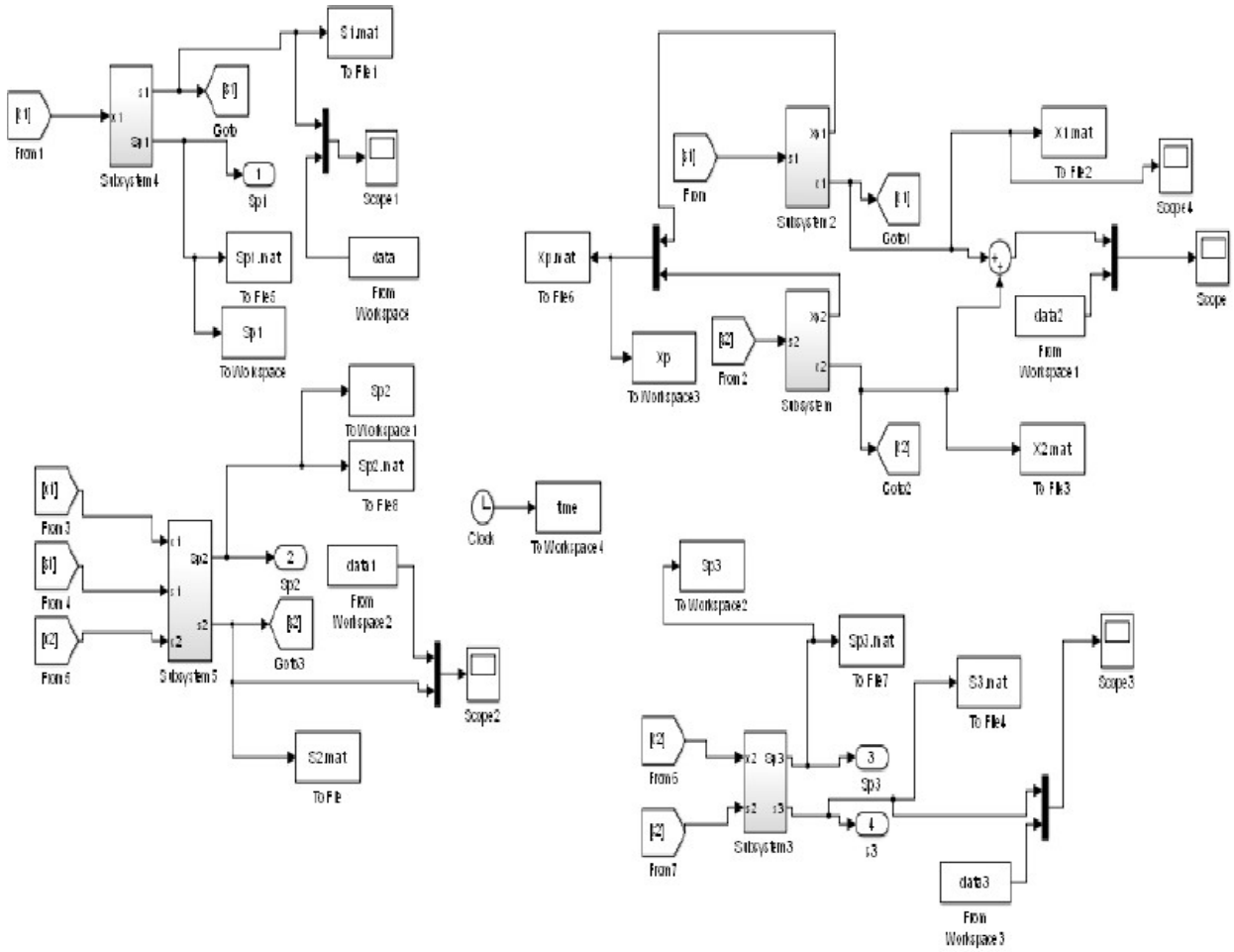

Fig. 8: Simulink

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