U.P.B. Sci. Bull., Series C, Vol. 79, Iss. 2, 2017 ISSN 2286-3540

MATHEMATICAL MODELLING AND SIMULATION OF AQUATIC BIOMASS TRANSFORMATION PROCESSES

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This paper presents the mathematical model and the simulation of the aquatic biomass conversion processes for an urban effluent in a reactor. It is based on the kinetic equations which describe these processes, and which have been developed with Scilab-Xcos program. Therefore, we can see how the concentrations of carbonaceous substrate (S), heterotrophic bacteria (X_A), nitrosomonas (X_B), biomass nitrobacteria (X_C), ammonia nitrogen (NH_3-N), nitrite nitrogen (NO_2-N), nitrate nitrogen (NO_3-N) and the oxygen consumption (O_2) have evolved over time.

Keywords: biomass, oxygen consumption, mathematical modelling, simulation, Xcos

1. Introduction

In the aquatic ecosystems, the biomass goes through complex transformation processes which are usually called, kinetics of growth.

A Monod-type reaction equation has proved to be satisfactory for the mathematical representation of the microbial growth. With a few appropriate adjustments, this type of reaction has subsequently been used to describe other processes such as biodegradation of a substrate (organic matter, nitrogen, etc.), phytoplankton growth, etc.

In relation to the natural cycle of production and decomposition of organic matter schematized in Fig. 1, these reactions are found both in the decomposition phase, as well as in the aquatic biomass production.

In addition to solar energy, the following elements, oxygen and carbon dioxide in the atmosphere, oxygen generated/consumed by the produced/decomposing organic matter, carbon dioxide generated/consumed by the decomposing/emerging organic matter and the existing inorganic nutrients in the ecosystem or resulted from the decomposition of organic matter, participate to this process [1].

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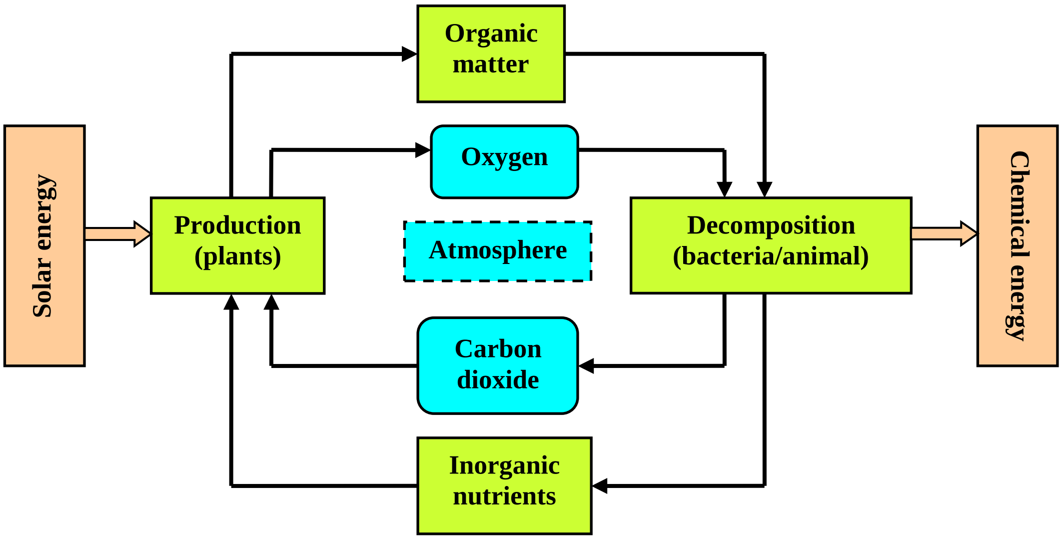


Fig. 1. Aquatic matter cycle in water system.

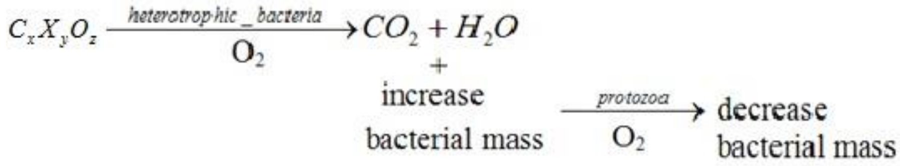
Biodegradation reactions of the organic matter (nutrient substrate) are inextricably linked to the existence of bacteria. Their contribution to the content of dissolved oxygen is reflected through a global quality parameter called BOD (biochemical oxygen demand), whose rate of change (corresponding to the oxygen consumption rate function of the bacterial metabolism) is called *dissolved oxygen in relation to the shaft balance*.

Generally, biochemical oxygen demand should include two types of microorganism activity:

- heterotrophic organisms which get their food and energy for their cell structure by metabolizing organic matter;
- autotrophic microorganisms able to synthesize organic compounds starting from simple inorganic compounds and using as an energy source, the energy resulting from the degradation of the organic matter (mostly represented by nitrosomonas and nitrobacteria, which are responsible for the nitrification processes) and oxygen consumption of the protozoa which destroy the bacteria. The latter is negligible in comparison with others.

Although bacterial growth phenomena are not independent, but rather consecutive and undergo multiple interactions, it is common for the two phases, the metabolism of organic matter and the nitrification, to be modelled separately.

In the initial phase, through the catalytic action of the enzymes produced by heterotrophic bacteria, the organic matter composed of long chains of carbon is decomposed into a simpler organic matter until it can be identified. This process takes place using dissolved oxygen in water, releases CO_2 and generates an increased bacterial mass (which is partially absorbed by protozoa) according to the following schema [1]:



Biological purification is carried out by means of micro-organisms, which remove the organic substances from water using them as a source of food or carbon. Part of the organic materials are used by microorganisms gives them the necessary energy to move and conduct other energy consuming reactions related to the synthesis of living matter, such as the reproduction [2].

The main objective of the biological treatment is to remove the unsettleable organic solids (dissolved and colloidal) and to stabilize the organic matter in sludge. It also reduces the nitrogen and phosphorus nutrients. This is a flexible process which can be easily adapted to a variety of wastewater concentrations and compositions. Biological processes are preceded by a physical treatment which is designed to retain sediment substances. This is followed by a secondary settlement - physical processes - intended to retain the products resulted from the biological treatment.

The factors influencing the biological process are: the contact time or the time during which the biological process takes place, the temperature, pH, oxygen, wastewater loading of the technological object (dilution), mud, nutrients, presence of the process inhibitors, and the hydrodynamic conditions of the process (mixing and blending) [3].

Biological processes, whether they are aerobic or anaerobic, are probably the most complex of the modern science. This is because they have different parameters: chemical, physical, biological. The modelling implies physical, chemical and biological considerations revealed by the equations which describe this process. Studies have failed to look at the problem of the biological reactors in all its complexity. Therefore, all kinetic reactions of the organic materials processing, take into account only the biologically pure cultures and not the totality of all microorganisms which conduct the biological degradation.

Moreover, the biological process does not take into account the aqueous medium where the biochemical reactions take place. The flow regime, the development of the turbulence of the water mass, the velocities and accelerations of the liquid environment do not occur under any circumstances in the equations and the biochemical process kinetics, although the latter is its basic environment.

Biological process modelling can be analysed in all its complexity. The kinetic parameters of the technological process vary each particular case as water is subjected to the treatment process. The biotechnological processes which occur in the biological reactors are very complicated and therefore, it is extremely difficult to predict their evolution. The number of parameters, the reactions involved, and the variety of bacterial species are very large and complicate a lot the problem. For this reason, a precise description of these complex systems is almost impossible. Consequently, we rely on the modelling of some simple processes [4].

In the modelling of biological processes is very important to describe the composition of the wastewater. It is impossible to consider all detectable compounds; therefore, they are grouped according to their characteristics. In general, in the modelling of biological purification there are three groups: bacteria, organic matter and nitrogen compounds [5].

This article presents a mathematical model of the biodegradation processes of organic matter which occur for an urban effluent in a reactor.

2. Mathematical Model of the Biodegradation Processes of Organic Matter

The mathematical equations which describe the biodegradation processes of organic matter for an urban effluent in a reactor are [1, 6]:

$$\frac{dX_A}{dt} = \left(\mu_{\max A} * \frac{S}{S + K_S} - m_A\right) * X_A \tag{1}$$

$$\frac{dS}{dt} = \left(-\frac{\mu_{\max A}}{Y} * \frac{S}{S + K_S} + \frac{m_A}{n_S} - q\right) * X_A \tag{2}$$

$$\frac{d(NH_3 - N)}{dt} = \frac{m_A}{n_B} * X_A - \frac{\mu_{\max B}}{Y_B} * \left(e^{\frac{-(NH_3-N)}{p_{1i}}} - e^{\frac{-(NH_3-N)}{p_{1s}}}\right) * X_B \tag{3}$$

$$\frac{dX_B}{dt} = \mu_{\max B} * \left(e^{\frac{-(NH_3-N)}{p_{1i}}} - e^{\frac{-(NH_3-N)}{p_{1s}}}\right) * X_B - m_B * X_B \tag{4}$$

$$\frac{d(NO_2 - N)}{dt} = \frac{f_B * \mu_{\max B}}{Y_B} * \left(e^{\frac{-(NH_3-N)}{p_{1i}}} - e^{\frac{-(NH_3-N)}{p_{1s}}}\right) * X_B - \frac{\mu_{\max C}}{Y_C} * \frac{(NO_2 - N)}{\left((NO_2 - N) + p_{2s}\right) * \left(1 + \frac{(NO_2 - N)}{p_{2i}}\right)} * X_C \tag{5}$$

$$\frac{dX_C}{dt} = \left(\mu_{\max C} * \frac{(NO_2 - N)}{\left((NO_2 - N) + p_{2s}\right) * \left(1 + \frac{(NO_2 - N)}{p_{2i}}\right)} - m_C \right) * X_C \quad (6)$$

$$\frac{d(NO_3 - N)}{dt} = \frac{f_C * \mu_{\max C}}{Y_C} * \frac{(NO_2 - N)}{\left(NO_2 - N + p_{2s}\right) * \left(1 + \frac{NO_2 - N}{p_{2i}}\right)} * X_C \quad (7)$$

where:

X_A – heterotrophic bacteria concentration [mg/l];

S – carbonaceous substrate concentration [mg/l];

μ_{maxA} – maximum velocity of growth [h^{-1}];

K_S – half-saturation constant or Michaelis constant (substrate concentration for which the growth rate is half the μ_{maxA});

m_A – rate of disappearance/death of bacteria [h^{-1}];

Y – conversion coefficient of substrate into biomass [g biomass generated by g metabolism substrate];

q – substrate consumption rate to cover metabolic needs of living cells [g substrate consumed by g cell biomass per unit of time];

n_S – rate of replenishment by autolyse [g biomass autolysis to release 1 g metabolisable products];

K_A – metabolic consumption rate of O_2 [h^{-1}];

NH_3-N – ammonium concentration in solution [mg N-NH_3/l];

X_B – concentration of nitrosomonas [mg-B/l];

Y_B – substrate-biomass conversion factor for XB species (of the order of 0.05÷0.1);

n_B – coefficient of nitrogen supply by autolyse (of the order of 50);

μ_{maxB} – maximum rate for nitrosomonas (of the order of 0.05÷0.1 h^{-1});

p_{1i} – constant (of the order of 800 mg/l NH_3);

p_{1s} – a constant (of the order of 20 mg/l NH_3);

m_B – extinction rate of B species (of the order of 0.005÷0.01 h^{-1});

NO_2-N – nitrite nitrogen concentration in water [mg/l];

f_B – ammonium-nitrogen transformation coefficient (of the order of 1);

Y_C – conversion factor of nitrites into nitrates (of the order of 0.1);

X_C –biomass concentration of nitrobacteria [mg-C/l];

μ_{maxC} – maximum rate for nitrobacteria (of the order of 0.05÷0.1 h^{-1});

p_{2i} – constant (of the order of 750 mg/l de NO_2);

p_{2s} – constant (of the order of 110 mg/l de NO_2);

m_C – extinction coefficient (of the order 0.001 h^{-1});
NO_3-N – nitrate nitrogen concentration in water [mg/l];
f_C – nitrite-nitrate nitrogen transformation coefficient (of the order of 1);
Total oxygen consumption is given by [1, 6]:

$$\frac{dO_2}{dt} = \left(K_A + \frac{Y_0 * \mu_{\max A}}{Y} * \frac{S}{S+K_S}\right) * X_A + \left[K_B + \frac{Y_{B0} * \mu_{\max B}}{Y_B} * \left(e^{\frac{-(NH_3-N)}{p_{1i}}} - e^{\frac{-(NH_3-N)}{p_{1s}}}\right)\right] * \\ * X_B + \left[K_C + \frac{Y_{C0} * \mu_{\max C}}{Y_C} * \frac{(NO_2-N)}{\left((NO_2-N)+p_{2s}\right) * \left(1 + \frac{(NO_2-N)}{p_{2i}}\right)}\right] * X_C \tag{8}$$

where:
Y_0 – velocity ratio of O_2 consumption - growth substrate [-];
K_B – metabolic rate of O_2 consumption in nitrosomonas (of the order 10^{-2} h^{-1});
Y_{B0} – velocity ratio of O_2 consumption - ammonia increase (of the order of 3.2);
K_C – metabolic rate of O_2 consumption in nitrobacteria (of the order 10^{-2} h^{-1});
Y_{C0} – velocity ratio of O_2 consumption - growth nitrogen (of the order of 1.1);

Based on the above equations, we performed in Scilab-Xcos [7] the program in Figs. 2, 3 and 4 which can make simulations for various scenarios. Thus, for an urban effluent we can see the way in which the carbonaceous substrate concentration (S), the concentrations of heterotrophic bacteria (X_A), nitrosomonas (X_B), nitrobacteria biomass (X_C), ammonia nitrogen (NH_3-N), nitrite nitrogen (NO_2-N), nitrate nitrogen (NO_3-N) and the oxygen consumption (O_2) evolve over time in a reactor.

The program developed in Scilab-Xcos uses the Sundials / CVODE-BDF-NEWTON integration method and for the following example we used the time reference of 1 hour for a simulation period of 800 hours.

Scilab-Xcos environment has free license. The program created in this environment enables immediate implementation without costs in wastewater treatment plants. By doing simulations with this program, its biological processes can be improved. This program is useful also for professionals working in the design of wastewater treatment plants and those who carry out mathematical modeling and simulation programs.

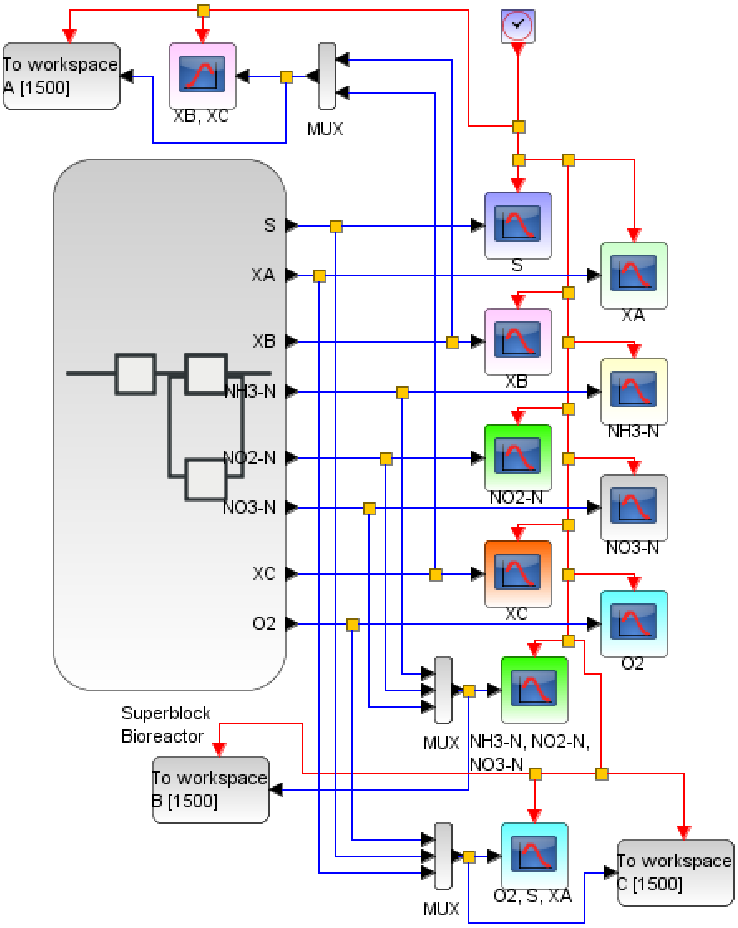


Fig. 2. Xcos simulation diagram of biodegradation processes and evolution of dissolved oxygen concentration in water.

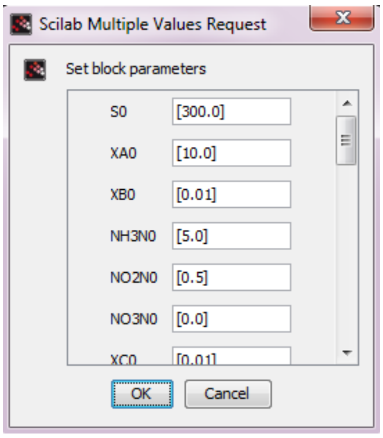
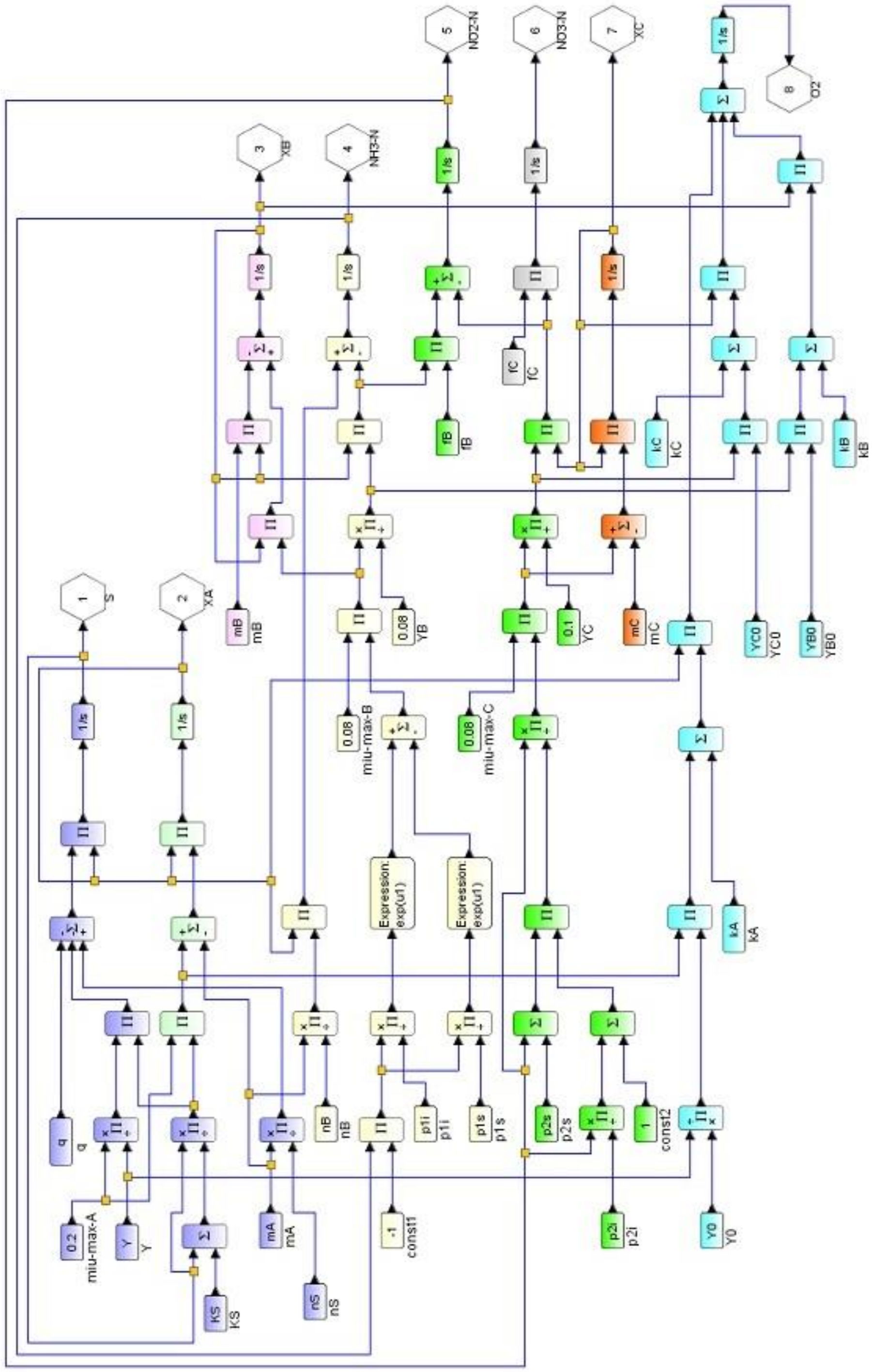


Fig. 3. Bioreactor Superblock Parameters in figure



2.

Fig. 4. Bioreactor Superblock Xcos diagram in Fig. 2.

3. Example of Simulation

Initial data:

- rate of disappearance/death of bacteria $m_A=0.02\ h^{-1}$;
- maximum velocity rate $\mu_{maxA}=0.2h^{-1}$;
- semi-saturation constant $K_S=100$;
- conversion ratio of biomass substrate $Y=0.5$;
- substrate consumption rate covering the metabolic needs of living cells $q=10^{-3}$;
- refuelling rate autolysis $n_S=2$;
- metabolic consumption rate O_2, $K_A=10^{-2}h^{-1}$;
- velocity ratio of O_2 consumption - growth substrate $Y_0=0.5$;
- substrate-biomass conversion factor for X_B species, $Y_B=0.08$;
- supply rate of nitrogen by autolysis $n_B=50$;
- constant $p_{1i}=800$ mg/l de NH_3;
- constant $p_{1s}=20$ mg/l de NH_3;
- extinction rate of B m_B species $=0.008\ h^{-1}$;
- ammonium-nitrogen transformation coefficient $f_B=1$;
- conversion factor of nitrites into nitrates $Y_C=0.1$;
- max growth rate of nitrobacteria $\mu_{maxC}=0.08\ h^{-1}$;
- constant $p_{2i}=750$ mg/l de NO_2;
- constant $p_{2s}=110$ mg/l de NO_2;
- extinction coefficient $m_C=0.001\ h^{-1}$;
- nitrogen-nitrate nitrogen transformation coefficient $f_C=1$;
- metabolic rate of O_2 consumption in nitrosomonas $K_B=10^{-2}\ h^{-1}$;
- velocity ratio of O_2 consumption - ammonia for growth $Y_{B0}=3.2$;
- metabolic rate of O_2 consumption in nitrobacteria $K_C=10^{-2}\ h^{-1}$;
- velocities ratio of O_2 consumption - for nitrogen growth $Y_{C0}=1.1$;
- simulation time $t=800$ *hours*;
- initial conditions: $S_0=300$ *mg/l*; $X_{A0}=10$ *mg/l*; $(NH_3\text{-}N)_0=5$ *mg/l*; $X_{B0}=0.01$ *mg/l*; $(NO_2\text{-}N)_0=0.5$ *mg/l*; $X_{C0}=0.01$ *mg/l*; $(NO_3\text{-}N)_0=0$ *mg/l*; $(O_2)_0=0$ *mg/l* [1].

Following the simulation, we can see graphically how the carbonaceous substrate (S), heterotrophic bacteria (X_A), nitrosomonas (X_B) nitrobacteria biomass (X_C) ammonia nitrogen ($NH_3\text{-}N$), nitrite nitrogen ($NO_2\text{-}N$), nitrate nitrogen ($NO_3\text{-}N$) and the oxygen consumption (O_2) have evolved over time for the simulated conditions, in the water of an urban type of effluent (Figs. 5, 6 and 7).

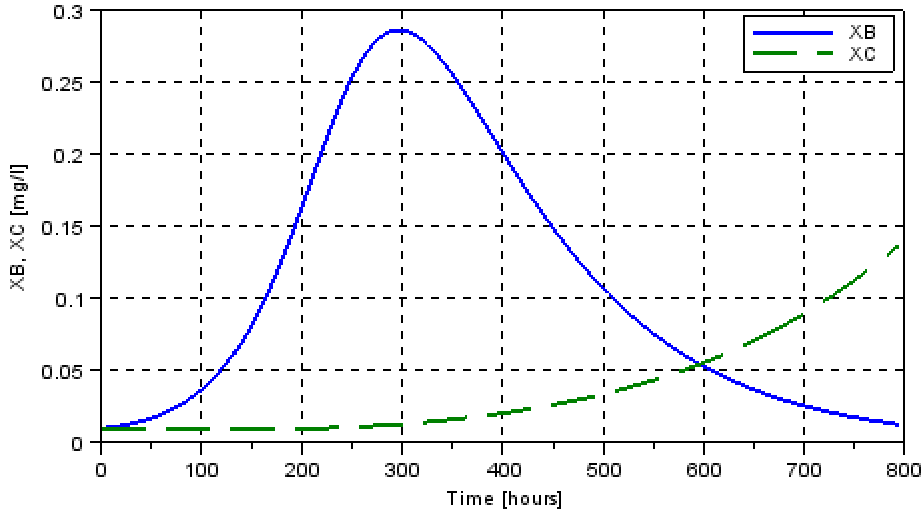


Fig. 5. Time evolution of the concentration of nitrosomonas (X_B) and nitrobacteria biomass (X_C) in a reactor effluent.

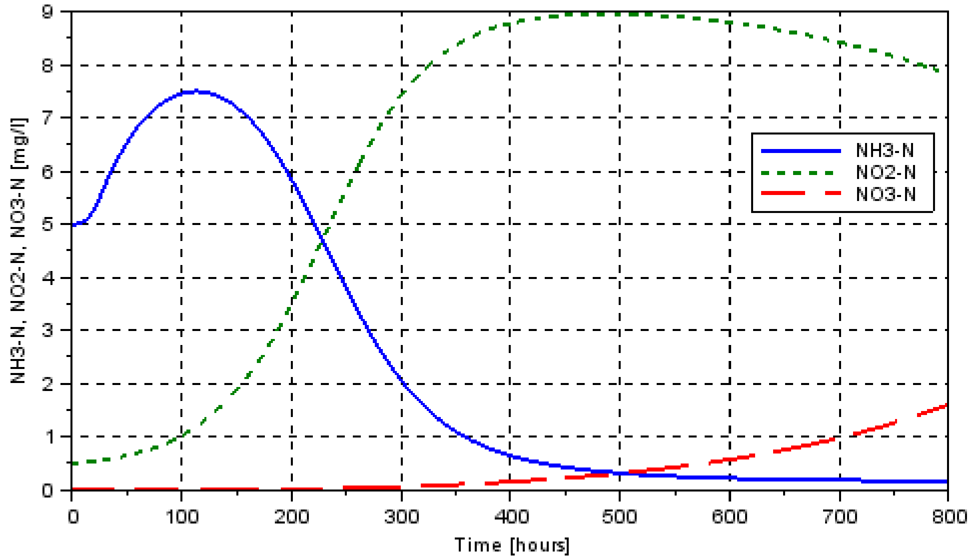


Fig. 6. Time evolution of the concentrations of nitrogen ammonia (NH_3-N), nitrite nitrogen (NO_2-N) and nitrate nitrogen (NO_3-N) in a reactor effluent.

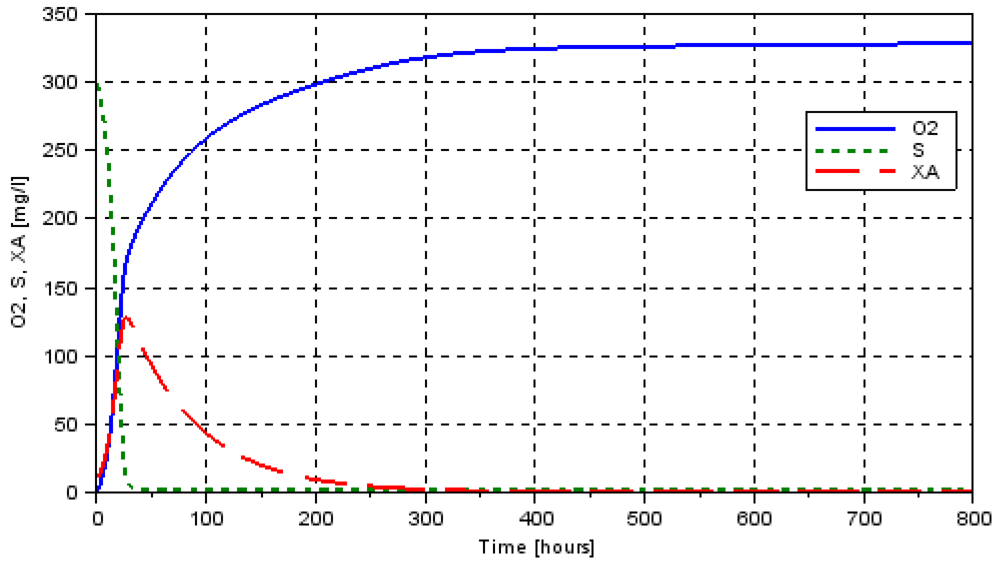


Fig. 7. Time evolution of the concentrations of carbonaceous substrate (*S*), heterotrophic bacteria (X_A) and the oxygen consumption (O_2) in a reactor effluent.

4. Conclusions

The calculation program (Figs. 2, 3 and 4) developed by the author of this article in Scilab-Xcos, solves mathematical equations (1 ÷ 8) which describe the over time evolution of the concentrations of carbonaceous substrate (*S*), heterotrophic bacteria (X_A), nitrosomonas (X_B), nitrobacteria biomass (X_C), ammonia nitrogen (NH_3-*N*), nitrite nitrogen (NO_2-*N*), nitrate nitrogen (NO_3-*N*) and the oxygen consumption (O_2) in the water of an urban type effluent. This program is able to make simulations, which show the overtime evolution of the above-mentioned parameters function of each specific case and therefore, it is useful to design and operate the biological reactors of wastewater treatment plants.

R E F E R E N C E S

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