Modeling of controlled biological treatment processes in the bioreactor of University of Cape Town

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Abstract. The paper is devoted to the study of processes in the bioreactor with the structural scheme of the University of Cape Town. The ASM1 mathematical model was used to study purification processes. Operating values of recycle flow rates are determined depending on input flow rate required for effective purification of ammonium nitrogen, and a method is proposed to expand the range of control of these values in combination with regulation of oxygen supply to the aerobic zone of the reactor. The specific role of the aerobic zone in the UCT reactor having a key role and affecting both nitrification and denitrification due to nitrate recycling is shown.

Introduction
The technological processes of the bioreactor with the structural scheme of the University of Cape Town (UCT-process) are studied in the work. The scheme under study is mainly used abroad; in Russian Federation you can also find examples of the use of this scheme at treatment plants, for example in Sestroretsk town.

The complexity of biochemical processes, the actions of disturbances associated with the instability of the concentrations of incoming contaminants, changes in the temperature of water and the environment, etc., lead to the need to develop a system for controlling bio-purification processes. The efficiency of such a system requires the creation of a mathematical model and the analysis of its dynamic properties.

1. Problem statement
Effective controlling of complex biochemical processes involves studying the dynamics of the UCT bioreactor using mathematical models. The task is to develop such a model and conduct behavior analysis for the subsequent synthesis of the control system.

A mathematical description of the chemical-biological processes in the reactor is possible using the ASM1 model (Activated Sludge Model 1) \cite{1}. Nitrification and denitrification processes are believed to occur independently of each other, and heterotroph bacteria are not used to feed oxygen, which is completely consumed in the nitrification zone.

The equations are made for concentrations of two groups of substances: soluble (S) and insoluble (suspended) - $X$. The concentrations of the first group include 6 components: alkalinity; concentration of ammonium and nitrate nitrogen, dissolved oxygen, dissolved organic nitrogen and dissolved biodegradable organic substance. The second group includes the following three concentrations:
nitrifying bacteria and denitrifying bacteria (autotrophs and heterotrophs) and suspended organic slowly decomposable nitrogen.

36 differential equations of balance are based on Petersen matrices for 4 zones and each of 9 components, the outputs of the previous zone corresponding to the inputs of the following. Below are the equations for each of the zones.

\[
\begin{align*}
dX_1 &= \frac{dX_1}{dt} = \frac{q_{in}X_{in} + q_{r_1}^T}{V_1} X_2 - \frac{q_{in} + q_{r_1}^T}{V_1} X_1 + r_{x1}; \\
dS_1 &= \frac{dS_1}{dt} = \frac{q_{in}S_{in} + q_{r_1}^T}{V_1} S_2 - \frac{q_{in} + q_{r_1}^T}{V_1} S_1 + r_{s1}; \\
dX_2 &= \frac{dX_2}{dt} = \frac{q_{in} + q_{r_2}^T}{V_2} X_1 + \frac{q_{r_2}^T}{V_2} X_4 - \frac{q_{in} + q_{r_2}^T + q_{r_4}^T}{V_2} X_2 + r_{x2}; \\
dS_2 &= \frac{dS_2}{dt} = \frac{q_{in} + q_{r_2}^T}{V_2} S_1 + \frac{q_{r_2}^T}{V_2} S_4 - \frac{q_{in} + q_{r_2}^T + q_{r_4}^T}{V_2} S_2 + r_{s2}; \\
dX_3 &= \frac{dX_3}{dt} = \frac{q_{in} + q_{r_3}^T + q_{r_4}^T}{V_3} X_2 - \frac{q_{in} + q_{r_3}^T + q_{r_4}^T}{V_3} X_3 + r_{x3}; \\
dS_3 &= \frac{dS_3}{dt} = \frac{q_{in} + q_{r_3}^T}{V_3} S_2 - \frac{q_{in} + q_{r_3}^T + q_{r_4}^T}{V_3} S_3 + r_{s3}; \\
dX_4 &= \frac{dX_4}{dt} = \frac{q_{in} + q_{r_3}^T + q_{r_4}^T}{V_4} X_3 - \frac{q_{in} + q_{r_3}^T + q_{r_4}^T}{V_4} X_4 + r_{x4}; \\
dS_4 &= \frac{dS_4}{dt} = \frac{q_{in} + q_{r_3}^T + q_{r_4}^T}{V_4} S_3 - \frac{q_{in} + q_{r_3}^T + q_{r_4}^T}{V_4} S_4 + r_{s4}.
\end{align*}
\]

where \(S\) – concentration of soluble substances, \(X\) – concentration of suspended substances, \(Q_{in}\) – wastewater flow rate at treatment plant inlet, \(Q_{r_1}\) – recycle flow rate from zone 4 in zone 2 (nitrate recycle), \(Q_{r_2}\) – recycle flow rate from zone 2 in zone 1 (anoxic recycle), \(V\) – zone volume; subscripts 1 – 4 mean the zone number, \(r\) – rate of kinetics of biochemical reactions.

The names of kinetics of biochemical reactions are nonlinear relationships and are summarized in Table 1. Enter variables \(F_1\) and \(F_2\) for ease of writing kinetics velocity expressions.

### Table 1. Dependences of the rates of kinetics of biochemical reactions

| Nitrification zone (zone 3) | Denitrification zone (zones 1, 2, 4) |
|-----------------------------|------------------------------------|
| \(F_1 = \mu a_{nh} \frac{S_{nh}}{S_{no}} + K_{nh} S_{no} X_{nh} \) | \(F_2 = \mu a_{nh} \frac{S_{nh}}{S_{no}} + K_{nh} S_{no} X_{nh} \) |
| \(r_{nh} = \frac{F_1}{Y_a} - k_X X_{nh} \) | \(r_{nh} = \frac{F_2}{Y_a} - k_X X_{nh} \) |
| \(r_{no} = \frac{F_1}{Y_a} \) | \(r_{no} = \frac{F_2}{Y_a} \) |
| \(r_{nh} = -\left(1 - Y_a \right) F_1 - k_X X_{nh} \) | \(r_{nh} = -\left(1 - Y_a \right) F_2 - k_X X_{nh} \) |
| \(r_{no} = \frac{F_1}{Y_a} \) | \(r_{no} = \frac{F_2}{Y_a} \) |
| \(r_{nh} = -\left(1 - Y_a \right) F_1 - k_X X_{nh} \) | \(r_{nh} = -\left(1 - Y_a \right) F_2 - k_X X_{nh} \) |
| \(r_{no} = \frac{F_1}{Y_a} \) | \(r_{no} = \frac{F_2}{Y_a} \) |
| \(r_{nh} = -\left(1 - Y_a \right) F_1 - k_X X_{nh} \) | \(r_{nh} = -\left(1 - Y_a \right) F_2 - k_X X_{nh} \) |
| \(r_{nh} = \frac{F_1}{Y_a} \) | \(r_{nh} = \frac{F_2}{Y_a} \) |
| \(r_{nh} = -\left(1 - Y_a \right) F_1 - k_X X_{nh} \) | \(r_{nh} = -\left(1 - Y_a \right) F_2 - k_X X_{nh} \) |
| \(r_{nh} = \frac{F_1}{Y_a} \) | \(r_{nh} = \frac{F_2}{Y_a} \) |
| \(r_{nh} = -\left(1 - Y_a \right) F_1 - k_X X_{nh} \) | \(r_{nh} = -\left(1 - Y_a \right) F_2 - k_X X_{nh} \) |

The names of the quantities are summarized in the Table 2.

### Table 2. Names of quantities, designations and units of measurement of the denitrification model

| № | Name of quantities and parameters | Symbol | Units |
|---|---------------------------------|--------|-------|
| 1 | Concentration of ammonium nitrogen | \(S_{nd}\) | g NH\(_4\)/m\(^3\) |
| 2 | Nitrate nitrogen concentration | \(S_{no}\) | g NO\(_3\)/m\(^3\) |
| 3 | Dissolved oxygen concentration | \(S_o\) | g O\(_2\)/m\(^3\) |
| 4 | Concentration of dissolved biodegradable organic matter | \(S\) | g COD/m\(^3\) |
The computer model of the bioreactor is compiled in the MATLAB/Simulink software based on the ASM1 model. Studies of the behavior of a multi-zone system make it possible to assert the inheritance of the dynamic properties of a single-zone model of nitrification and denitrification [2].

2. Analysis of the impact of inlet flow and recycle flows

A series of computational experiments were carried out to analyze the influence of the flow rate of the inlet wastewater stream on the treatment processes. As a result of the research, graphs of the static characteristics (steady-state values) of the concentrations of bacteria in various zones of the reactor and pollutants at the outlet were obtained depending on the input flow rate in the absence of recycle flow rates. The steady state concentrations are indicated by the symbols SS on the graphs.

The results of the computational experiments showed there is a critical value of the input wastewater flow, at which the active sludge is washed out and, as a result, the treatment is stopped (Figure 1). An increase in the concentration of pollutants at the inlet leads to an increase in the critical flow rate of the inlet stream, at which the active sludge is washed out in zones 1 and 2. However, the maximum flow rate for zones 3 and 4 remains substantially unchanged since the aerobic growth of sludge is determined by the concentration of dissolved oxygen.

![Fig. 1. Dependence of steady state concentrations of bacteria and pollutants at the outlet on nitrate recycle](image-url)
An increase in the flow rate of the anoxic recycle results in a decrease in the concentration of the denitrifying bacteria in zone 1 and an increase in the denitrifying bacteria in zone 2. The reason for this behavior is the shortage of nutrition for the bacteria of the first zone, which receives the flow from the second, with a higher concentration of bacteria and a small concentration of nitrates. The growth of the anoxic recycle increases the total flow through subsequent zones 3 and 4, which, with a relatively small number of bacteria, leads to their washing out. Therefore, effective purification can occur at anoxic recycle flow rates within certain limited limits.

Under conditions of mutual effect of recycles, gradual increase of nitrate recycle leads to narrowing of the range of permissible operating values of anoxic recycle, at that narrowing occurs faster than growth of nitrate recycle, at that zone 4 practically loses bacterial component.

Efficient purification is also possible in disengaged anoxic recycle if the nitrate recycle flow is comparable to the feed wastewater flow. Specificity of the aerobic zone of the UCT reactor is in its key role related to the effect on both nitrification and denitrification due to nitrate recycling. The preservation of denitrifying bacteria in the first two zones when the nitrifiers are washed out of zone 3 leads to deterioration in nitrate purification. An increase in the flow rate of the anoxic recycle results in a similar process.

The control of ammonium nitrogen concentrations is characterized by a narrow range of recycling flow rates – anoxic and nitrate, the excess of which no longer leads to effective purification due to washing out of the culture of nitrifying bacteria. Expansion of this range is possible due to increased oxygen supply to aerobic zone.

The optimum value of nitrate recycle flow rate for removal of ammonium nitrogen is set, Fig. 2. The increase in flow rate is accompanied by undesirable overregulation. We can talk about optimal control of nitrate recycle at the minimum steady state concentration of ammonium nitrogen in the absence of overregulation.

3. Analysis of the impact of input concentrations of pollutants
Computational experiments with different concentrations of ammonium and nitrate nitrogen at the inlet showed that in the absence of recycles, the concentrations of sludge in the first two zones are determined by the nutritional content in the source water. Therefore, when the dependence of bacterial growth on ammonium nitrogen in the source water is found, the steady-state concentrations of denitrifiers in these zones do not change. In the aerobic zone, the growth of bacteria directly depends on the ammonium content in the source water. Bacterial growth is absent when the substrate content is below the minimum critical point and the culture is washed out. This critical minimum concentration also affects zone 4.

This minimum concentration is visible as a plateau in all zones and most of all in the fourth zone (Figure 3) in the graphs of steady-state concentrations versus ammonium concentrations. This situation is explained by the fact that heterotrophic bacteria feed on nitrates, which are additionally produced by autotrophic bacteria. To the last zone 4, this power practically does not remain.
The inclusion of a single anoxic recycle results in an increase in the minimum concentration of ammonium nitrogen sufficient for bacterial growth in zone 4. The inclusion of nitrate recycle alone results in the effect of bacterial concentrations in zones 3 and 4 on their concentration in zone 2 depending on the nitrate content of the recycle. After the growth of bacteria in zone 3, the concentration of bacteria in zone 2 also begins to grow.

Simultaneous inclusion of anoxic and nitrate recycles leads to similar processes in the first zone. Nitrate recycle has a more beneficial effect on the removal of ammonium nitrogen than anoxic.

Since there is no point of minimum nitrate nitrogen input concentration in zones 1 and 2, only ammonium nitrogen is sufficient to ensure the operation of the UCT reactor. Experiments show that the reactor successfully copes with contaminants in the absence or low content of nitrate nitrogen in the source water and high values of ammonium nitrogen, the growth of which affects almost only the growth of denitrifiers in zone 1. The reason for this behavior is that the aerobic zone is capable of producing substrate (nitrates) for denitrifiers.

It was found that with an increase in the input concentration of nitrates, anaerobic growth of denitrifier bacteria in zones 1 and 2 increases. However, this is only relevant for small concentrations of ammonium nitrogen in the source water. The increase in the consumption of any of the recycles leads to the fact that the increase in ammonium nitrogen in the source water practically ceases to affect the nitrates in the purified water. In this case, it is necessary to further enhance the growth of aerobic bacteria by adding oxygen.

4. Analysis of the impact of dissolved oxygen concentration in the nitrification zone

Computational experiments in the absence of recycle streams made it possible to obtain the dependence of steady-state concentrations of bacteria and pollutants on the concentration of oxygen in the nitrification zone. It follows there is a point of minimum dissolved oxygen concentration necessary for the growth of nitrifying bacteria in zone 3 and denitrifying bacteria in zone 4.

Switching on recycles increases the minimum concentration of oxygen in zone 4 (Figure 4). Due to the presence of nitrate recycle in zone 2, an increase in the concentration of denitrifying bacteria is observed. This is due to the entry of nitrates together with recycle streams.
5. Results
The studies made it possible to establish the dependence of recycle costs on inlet flow and the mutual limiting effect of recycles on each other. The control of ammonium nitrogen concentration has a narrow range of recycling costs - anoxic and nitrate, the excess of which no longer leads to a decrease in the concentration of contaminants due to the washing out of the culture of nitrifying bacteria.

It has been found that there is an optimal nitrate recycle flow rate for the removal of ammonium nitrogen. Nitrate recycle has a more beneficial effect on the removal of ammonium nitrogen than anoxic at the same flow rates both in separate recycle operation and simultaneously.

The UCT reactor is capable of operating in the absence of nitrate nitrogen in the source wastewater or at a very small content. The concentration of ammonium nitrogen can and should reach sufficiently high values.

The research is based on the development of a system for controlling biological processes of wastewater treatment with a logic-dynamic regulator, which was previously successfully used to control processes in a 3-zone reactor.

References
[1] Henze M, Harremoes P, Jes la Cour Jansen, Arvan E 2009 Wastewater Treatment (Moskow: Mir) p 480
[2] Grudyaeva E K, Dushin S E 2017 Simulation of Controlled Biological Wastewater Treatment Processes (Saint Petersburg.: Publishing House SPbGETU «LETi») p 222