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CALCULATION OF THE NITRIFICATION AND DENITRIFICATION PROCESSES IN TERMS OF A MATHEMATICAL MODEL

The essence of nitrogen and organic matter removal processes in one-sludge systems is discussed. Making use of the equations of biomass, BOD, and nitrogen compounds balance, a mathematical model is established. The model incorporates the following parameters: growth of biomass of heterotrophic and autotrophic microorganisms, degradation of organics, nitrification of ammonia, denitrification of nitrates, and assimilation of ammonia by growing microorganisms. It has been assumed that raw wastewater may contain organic nitrogen, ammonia nitrogen, and nitrate nitrogen.

Mathematical models are constructed for two configurations: 1) aeration tank placed before the denitrification tank, 2) denitrification tank arranged before the aeration tank. Configuration 1) may or may not use external carbon source (e.g., methanol) for denitrification.

The solutions to the mathematical models for steady state conditions are obtained as follows: a set of more than ten nonlinear equations is reduced to a single equation. Having solved this equation, all of the technological parameters in question can be calculated in terms of available formulae. This is illustrated by calculations carried out for both the configurations, and the obtained results are discussed.

NOTATION

- D_m – methanol dose, g/m^3 ,
- DO – dissolved oxygen, g/m^3 ,
- f – nitrifier fraction,
- K – saturation constant, g/m^3 ,
- M – nitrogen content in biomass, $g\ N/g\ vss$,
- m – maintenance coefficient, $g\ substrate/g\ vss \cdot d$,
- N_I – ammonia nitrogen concentration, $g\ N/m^3$,
- N_{II} – nitrate nitrogen concentration, $g\ N/m^3$,
- N_{III} – organic nitrogen concentration $g\ N/m^3$,
- N_{IV} – TKN, $g\ N/m^3$, $N_{IV} = N_I + N_{III}$,

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- Q – flow rate, m^3/d ,
 s – BOD_5 , g/m^3 ,
 x – biomass concentration, $g\ vss/m^3$,
 V – reactor volume, m^3 ,
 Y – growth yield, $g\ vss/g$ substrate,
 Y^{EG} – maximum growth yield, $g\ vss/g$ substrate,
 α – sludge recirculation ratio,
 β – denitrification tank feed ratio (for configuration I) or mixed liquor suspended solids recirculation ratio,
 μ – specific growth rate, d^{-1} ,
 μ^{max} – maximum specific growth rate, d^{-1} ,
 Θ – retention time, d ($\Theta = V/Q_o$),
 ΔA – excess autotrophic sludge, $g\ vss/d$,
 ΔH – excess heterotrophic sludge, $g\ vss/d$,
 Δx – excess sludge, $g\ vss/d$, $\Delta x = \Delta A + \Delta H$.

SUBSCRIPTS

- A – refers to autotrophs,
 H – refers to heterotrophs,
 a – refers to ammonia nitrogen,
 c – refers to BOD_5 ,
 n – refers to nitrate nitrogen,
 o – refers to dissolved oxygen,
 (1), (5) – refers to reactions itemized as (1) and (5), respectively,
 0, 1, 2, 3, 4, 5, 6, e – refers to items included in figs. 1 and 2.

EXAMPLES

- $Y_{A,a}^{EG}$ – maximum growth yield of autotrophs in relation to ammonia nitrogen, $g\ vss/g\ N-NH_4^+$,
 $m_{H(s)n}$ – maintenance coefficient of heterotrophs in the denitrification reaction – in relation to nitrate nitrogen, $g\ N-NO_3^-/g\ vss \cdot d$.

1. INTRODUCTION

Nitrogen removal has become a prerequisite to ensure a safe effluent for the potential user (e.g. for industrial reuses of water), on one hand, and to meet the demands made by pollution control authorities, on the other hand.

Biological nitrification and denitrification is among the methods of considerable popularity [7]. Both the processes have the inherent advantage of being modest in cost demand. Biological nitrification and denitrification may be carried out in attached growth reactors and suspended growth reactors, the latter being by far the most common case, and they may be arranged so as to form different technological systems.

Three major types of technological systems are as follows: three-sludge system, two-sludge system and one-sludge system. Thus, three-sludge systems involve separation of heterotrophic sludge contributing to the oxidation of organics in the aeration tank (oxic heterotrophs), of autotrophic sludge (nitrifiers), and of heterotrophic sludge contributing to the denitrification of nitrates (denitrifiers, unoxic heterotrophs). In the course of the treatment the three sludges of interest are settled in three separate tanks. In two-sludge systems, a mixture of oxic heterotrophs and nitrifiers is separated from denitrifiers. One-sludge systems involve no separation. Both oxidation of organics and nitrification occur in the aeration tank, whereas denitrification is conducted in a separate unoxic tank. Nitrification and denitrification tanks in many instances constitute one structural unit, wherein the nonaerated section acts as a denitrification tank. Denitrification is carried out by heterotrophic bacteria, which degrade organics in the aeration tank utilizing oxygen. Under unoxic conditions, the same bacteria soon begin to utilize nitrates as an acceptor of electrons. A major advantage of one-sludge system is the absence of intermediate settling tanks.

The effective design of one-sludge systems, however, raises serious trouble. It is necessary to take into account all the relations that might occur at the concurrence of a number of different reactions.

The efficiency of organic matter removal depends on the processes conducted by heterotrophs alternately under oxic and unoxic conditions. Moreover, the amounts of organics oxidized in the denitrification tank account for the amounts of nitrates reduced. The quantity of ammonia nitrogen removed is influenced by the efficiency of nitrification and by the building-in into the growing biomass. The nitrification rate depends on the quantity of nitrifiers contained in the activated sludge, whereas the quantity of nitrifiers shows a dependence on the composition of the wastewater under treatment, specifically on the ratio of total Kjeldahl nitrogen (TKN) to BOD.

One-sludge systems involve three configurations (figs. 1 and 2). Of these, one may appear to be the most advantageous under given conditions in engineering

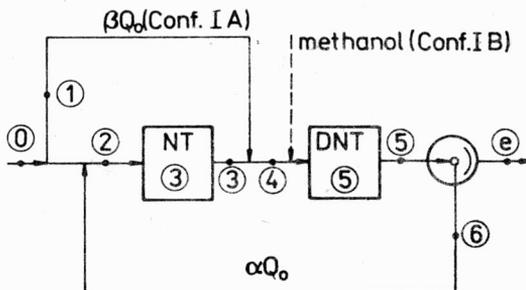


Fig. 1. Configuration I

NT - nitrification tank, DNT - denitrification tank

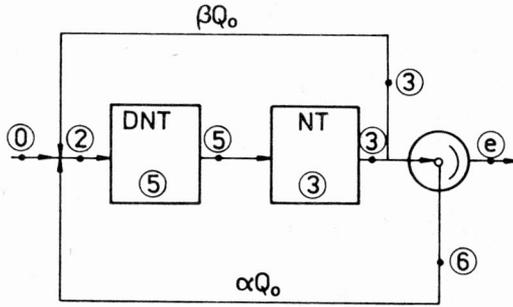


Fig. 2. Configuration II

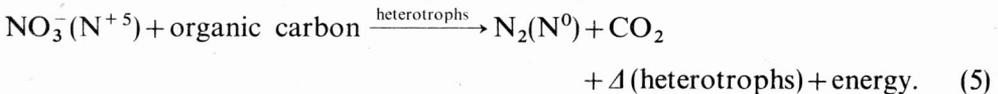
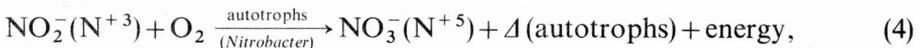
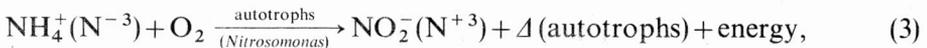
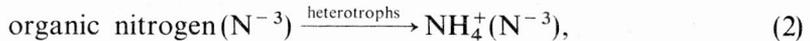
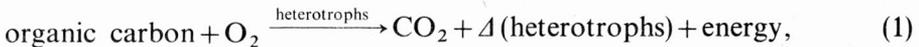
DNT - denitrification tank, NT - nitrification tank

practice. It is, therefore, useful to have a tool which could be helpful in determination of how each of the three configurations works. The recommended procedure of choosing the best configuration involves analysis of mathematical models, thus allowing a favourable change of the scope of technological investigations on laboratory and pilot scales. Laboratory investigations should aim at establishing the unknown kinetics coefficients for the process. Using the coefficient values and mathematical models, it is possible to select the most advantageous configuration and to determine approximate technological parameters. The parameters may be established more precisely by pilot tests.

In this paper, the mathematical models for three configurations of the one-sludge system are discussed. A comparison of treatment effects is given as well.

2. MATHEMATICAL MODELS OF THE PROCESS

The treatment of municipal sewage, wherein nitrogen compounds are removed during nitrification and denitrification, involves transformations which may be described by the following reactions:



Ammonification of organic nitrogen (2) is concurrent with reaction (1) in the aeration tank or with reaction (5) in the denitrification tank when the influent stream contains organic nitrogen.

In one-sludge system the heterotrophs, that under aerobic conditions carry out reaction (1), are ready to change their abilities and to utilize nitrates as hydrogen acceptor in reaction (5) in the absence of oxygen [4]. Nitrifiers are active under aerobic conditions only. The rate of reaction (4) is markedly higher than the rate of reaction (3), [7], and this means that under typical conditions of operation no significant accumulation of nitrites occurs. Thus, the nitrification rate depends on the rate of ammonia-to-nitrites oxidation (3). Reaction (2) precedes biodegradation of organic nitrogen compounds. If a high degree of organic matter degradation (which is a major goal of biological treatment) is expected, it may be assumed that, practically, reaction (2) runs to completion [7]. For the purpose of calculations, we can assume that organic nitrogen is equivalent to an appropriate amount of ammonia nitrogen. Thus, we shall consider here only the TKN value.

In reactions (1)–(5), biomass growth is associated with the assimilation of a certain portion of TKN. At high growth yield, nitrogen removal may be considerable.

2.1. KINETICS

The following has been anticipated:
biomass growth is expressed as

$$dx = \mu x dt; \quad (6)$$

substrate consumption takes the form

$$ds = -\frac{dx}{Y}; \quad (7)$$

growth yield is a function of specific growth rate [5]

$$\frac{1}{Y} = \frac{1}{Y^{EG}} + \frac{m}{\mu}; \quad (8)$$

specific growth rate for heterotrophs in reaction (1), i.e. under oxic conditions, becomes [2]

$$\mu_{H(1)} = \mu_{H(1)}^{\max} \frac{s}{K_c + s}. \quad (9)$$

Parameters of kinetics for autotrophic

Process	m	K
Oxidation of organics in the aeration tank	$\mu_{H(1)}^{\max} = 6 \times 1.03^{T-20} \text{ d}^{-1}$, ref [1] $\mu_{H(1)}^{\max} = 1.05 \times 10^{10} \exp\left(-\frac{6290}{273+T}\right)$, ref [3]	$K_c = 150 \text{ g BOD}_5/\text{m}^3$, ref [3] $K_c = 350 \text{ g BOD}_5/\text{m}^3$, ref [1]
Denitrification with methanol as organic carbon source	$\mu_{H(5)}^{\max} = 0.27 \text{ d}^{-1}$ for $T = 25^\circ\text{C}$ $\mu_{H(5)}^{\max} = 0.18 \text{ d}^{-1}$ for $T = 20^\circ\text{C}$ $\mu_{H(5)}^{\max} = 0.11 \text{ d}^{-1}$ for $T = 15^\circ\text{C}$ $\mu_{H(5)}^{\max} = 0.07 \text{ d}^{-1}$ for $T = 10^\circ\text{C}$	ref [7] $K_n = 0.15 \text{ g N-NO}_3^-/\text{m}^3$, ref [7]
Denitrification with municipal sewage as organic carbon source	$\mu_{H(5)}^{\max} = 0.675 \text{ d}^{-1}$ for $T = 25^\circ\text{C}$ $\mu_{H(5)}^{\max} = 0.0540 \text{ d}^{-1}$ for $T = 20^\circ\text{C}$ $\mu_{H(5)}^{\max} = 0.0450 \text{ d}^{-1}$ for $T = 15^\circ\text{C}$ $\mu_{H(5)}^{\max} = 0.0360 \text{ d}^{-1}$ for $T = 10^\circ\text{C}$ $\mu_{H(5)}^{\max} = 0.135 \cdot 1.2^{T-20} \text{ d}^{-1}$ ref [1]	ref [7] $K_n = 0.15 \text{ g N-NO}_3^-/\text{m}^3$
Nitrification	$\mu_A^{\max} = 0.47 P \exp[0.098(T-15)] \text{ d}^{-1}$, ref [7] $P = 1 - 0.833(7.2 - \text{pH})$, ref [7] $\mu_A^{\max} = 0.18 \times 1.12^{(T-15)}$, ref [1]	$K_a = 10^{(0.051T-1.158)} \text{ g N-NH}_4^+/\text{m}^3$, ref [7] $K_o = 1.3 \text{ g DO}/\text{m}^3$, ref [7]

^a - values calculated from other constants reported in the literature.

T - temp °C.

Specific growth rate for heterotrophs in reaction (5), i.e. under unoxic conditions, is [1]

$$\mu_{H(5)} = \mu_{H(5)}^{\max} \frac{N_{II}}{K_n + N_{II}}, \quad (10)$$

and specific growth rate for *Nitrosomonas* is given by [7]

$$\mu_A = \mu_A^{\max} \frac{N_I DO}{(K_a + N_I)(K_o + DO)}. \quad (11)$$

The values of the parameters included in formulae (8)–(11) are listed in tab. 1.

2.2. PROCESS CONFIGURATIONS

Two major configurations will be discussed here, namely configuration I (fig. 1) and configuration II (fig. 2). For configuration I, two variants will be considered:

Table 1

and heterotrophic biomass growth

Y^{EG}	m
$Y_{H(1)c}^{EG} = 0.6 \text{ g vss/g BOD}_5$, ref [1]	$m_{H(1)} = 0.083 \text{ g BOD}_5/\text{g vss d}$, (a) ref [1]
$Y_{H(5)c}^{EG} = 0.32 \text{ g vss/g meth}$, ref [7, 5]	$m_{H(5)c} = 0.125 \text{ g meth/g vss d}$, (a) ref [7, 5]
$Y_{H(5)n}^{EG} = 0.9 \text{ g vss/g N-NO}_3^-$, (a) ref [7]	$m_{H(5)n} = 0.044 \text{ g N-NO}_3^-/\text{g vss d}$, (a) ref [7]
$Y_{H(5)c}^{EG} = 0.39 \text{ g vss/g BOD}_5$, (a) ref [1]	$m_{H(5)c} = 0.128 \text{ g BOD}_5/\text{g vss d}$, (a) ref [1, 5]
$Y_{H(5)n}^{EG} = 0.9 \text{ g vss/g N-NO}_3^-$, ref [1]	$m_{H(5)n} = 0.056 \text{ g N-NO}_3^-/\text{g vss d}$, (a) ref [1]
$Y_{A,a}^{EG} = 0.05 \text{ g vss/g N-NH}_4^+$, ref [1]	$m_{A,a} = 0.47 \text{ g N-NH}_4^+/\text{g vss d}$, (a) ref [2]
$Y_{A,a}^{EG} = 0.15 \text{ g vss/g N-NH}_4^+$, ref [7]	

denitrification without methanol (IA) and denitrification using methanol (IB) ($\beta = 0$).

The following assumptions have been made:

a) there is a complete mixing both in the aeration tank and in the denitrification tank,

b) the system works under steady-state conditions; the values of the parameters of kinetics and the values of the wastewater components are all constant and equivalent to their averages.

c) $s_5 = s_e$, $N_{1,5} = N_{1,e}$, $N_{11,5} = N_{11,e}$ (for configuration I),

d) $s_3 = s_e$, $N_{1,3} = N_{1,e}$, $N_{11,3} = N_{11,e}$ (for configuration II).

2.2.1. CONFIGURATION IA

Age of sludge

Denoting excess sludge by Δx and assuming that the nitrifiers fraction is f , we can write

Sludge balance for NT

$$\alpha x_6 - (1 + \alpha - \beta) x_3 = 0. \quad (\text{IA6})$$

Sludge balance for DNT

$$(1 + \alpha - \beta) x_3 - (1 + \alpha) x_5 = 0. \quad (\text{IA7})$$

TKN balance for NT

$$(1 - \beta) Q_0 N_{\text{IV},0} + \alpha Q_0 N_{\text{I},e} - V_3 \frac{\mu_A x_3 f}{Y_{A,a}} - Y_{H(1)c} Q_0 [(1 - \beta) s_0 + \alpha s_e - (1 + \alpha - \beta) s_3] M - (1 + \alpha - \beta) Q_0 N_{\text{I},3} = 0. \quad (\text{IA8})$$

(TKN built-in in heterotrophic sludge) (effluent)

$N\text{-NO}_3^-$ balance for NT

$$(1 - \beta) Q_0 N_{\text{II},0} + \alpha Q_0 N_{\text{II},e} + V_3 \frac{\mu_A x_3 f}{Y_{A,a}} - Y_{A,a} Q_0 [(1 - \beta) N_{\text{IV},0} + \alpha N_{\text{I},e} - (1 + \alpha - \beta) N_{\text{I},3}] M - (1 + \alpha - \beta) Q_0 N_{\text{II},3} = 0 \quad (\text{IA9})$$

(TKN built-in in heterotrophic sludge) (effluent)
(TKN built-in in autotrophic sludge) (effluent)

BOD_5 balance for NT

$$(1 - \beta) Q_0 s_0 + \alpha Q_0 s_e - V_3 \frac{\mu_{H(1)} x_3 (1 - f)}{Y_{H(1)c}} - (1 + \alpha - \beta) Q_0 s_3 = 0. \quad (\text{IA10})$$

(influent) (effluent)
(decay)

BOD_5 balance for DNT

$$(1 + \alpha - \beta) Q_0 s_3 + \beta Q_0 s_0 - V_5 \frac{\mu_{H(5)} x_5 (1 - f)}{Y_{H(5)c}} - (1 + \alpha) Q_0 s_e = 0. \quad (\text{IA11})$$

(influent) (effluent)
(decay)

$N\text{-NO}_3^-$ balance for DNT

$$(1 + \alpha - \beta) Q_0 N_{\text{I},3} + \beta Q_0 N_{\text{II},0} - V_5 \frac{\mu_{H(5)} x_5 (1 - f)}{Y_{H(5)n}} - (1 + \alpha) Q_0 N_{\text{II},e} = 0. \quad (\text{IA12})$$

(influent) (effluent)
(decay)

TKN balance for DNT

$$(1 + \alpha - \beta) Q_0 N_{1,3} + \beta Q_0 N_{IV,0} - Y_{H(5)c} [(1 + \alpha - \beta) s_3 + \beta s_0 - (1 + \alpha) s_e] M$$

(influent) (TKN built-in in heterotrophic sludge)

$$-(1 + \alpha) Q_0 N_{1,e} = 0. \quad (\text{IA13})$$

(effluent)

The values of the x_5 , x_6 , s_e , $N_{II,e}$, $N_{I,3}$, as well as DO and pH in NT are assumed. Adoption of concentration values of $N_{II,e}$ and $N_{I,3}$ according to formulae (10) and (11) is equivalent to the adoption of the calculated values $\mu_{H(5)}$ and μ_A , respectively. Considering the safety factor (*SF*) concept developed by LAWRENCE and McCARTY [3], it is advisable that biological processes be designed so as to keep the value of μ below the maximum value which may be achieved under given conditions ($\dot{\mu}$)

$$SF = \frac{\dot{\mu}}{\mu}. \quad (12)$$

A conservative *SF* is recommended to minimize process variations caused by extreme values of pH, low DO concentrations in NT, and toxicants [7]. The *SF* can be also used to ensure that substrate breakthrough does not occur during diurnal peaks in load [6]. To achieve this, we have to keep the *SF* somewhat above the value of the ratio of hourly peak to average influent load [6].

Taking these into account and considering formulae (10)–(11), we obtain the conditions for adoption of $N_{II,e}$ and $N_{I,3}$. Thus

$$N_{II,e} \leq \frac{K_n}{SF - 1}, \quad N_{I,3} \leq \frac{K_a}{SF - 1}.$$

From (IA6) and (IA7) it follows that

$$\alpha = \frac{x_5}{x_6 - x_5}. \quad (\text{IA14})$$

By virtue of (IA3), (IA4), and (IA8)–(IA13), we may derive equation (IA15), which should be solved numerically with respect to s_3

$$\frac{[B + N_{II,0} - N_{II,e} - (s_0 - s_3) M Y_{H(1)c} - (s_3 - s_e) C] (1 - \alpha)}{B - (s_0 - s_3) [C - (1 + 2\alpha) M Y_{H(1)c}]} + \frac{\frac{s_3 - s_e}{s_0 - s_3} [1 + \alpha(D + 1)] - D}{1 + D} = 0 \quad (\text{IA15})$$

where:

$$B = (N_{IV,0} - N_{I,3})(1 - M Y_{A,a}),$$

$$C = (1 + \alpha) \frac{Y_{H(5)c}}{Y_{H(5)n}} + \alpha M [Y_{H(1)c} + Y_{H(5)c} (1 - MY_{A,a})],$$

$$D = \left(\frac{\mu_A}{\mu_{H(1)}} - 1 \right) \frac{Y_{H(1)c}}{Y_{H(5)c}}.$$

Making use of (IA1a), (IA1b), (IA3), and (IA4), we can derive the condition that should be fulfilled by the constants μ of autotrophs and heterotrophs in both tanks

$$\frac{\mu_A}{\mu_{H(1)}} = 1 + \frac{\mu_{H(5)} \Theta_5 x_5}{\mu_{H(1)} \Theta_3 x_3}. \quad (\text{IA16})$$

It follows that $\mu_A > \mu_{H(1)}$. Thus, considering eqs. (9) and (11), it is possible to determine the range of concentrations s_3 , in which the solution of eq. (IA15) is to be sought

$$0 < s_3 < \frac{K_c}{[(\mu_{H(1)}^{\max})/(\mu_A)] - 1}. \quad (\text{IA17})$$

Having calculated s_3 , we may determine β in terms of the following equation

$$\beta = \frac{\frac{s_3 - s_e}{s_0 - s_3} [1 + \alpha(D + 1)] - D}{1 + D}. \quad (\text{IA18})$$

By virtue of (IA7)

$$x_3 = \frac{1 + \alpha}{1 + \alpha - \beta} x_5. \quad (\text{IA19})$$

By virtue of (IA13)

$$N_{1,e} = N_{1,3} + \frac{\beta}{1 + \alpha} [N_{IV,0} - N_{1,3} - (s_0 - s_3) MY_{H(5)c}] - (s_3 - s_e) MY_{H(5)c}. \quad (\text{IA20})$$

Considering (IA1a), (IA2b), (IA3), and (IA4), we have

$$f = \frac{1}{1 + \frac{1}{E}} \quad (\text{IA21})$$

where

$$E = \frac{(N_{IV,0} - N_{1,e}) Y_{A,a}}{Y_{H(1)c} [(1 - \beta) s_0 + \alpha s_e - (1 + \alpha - \beta) s_3] + Y_{H(5)c} [(1 + \alpha - \beta) s_3 + \beta s_0 - (1 + \alpha) s_e] - MY_{A,a}}.$$

Taking into account (IA8), we get

$$\Theta_3 = \frac{V_3}{Q_0} = \frac{Y_{A,a}}{\mu_A x_3 f} \{ (1-\beta) N_{IV,0} + \alpha N_{I,e} - (1+\alpha-\beta) N_{I,3} - MY_{H(1)c} [(1-\beta) s_0 + \alpha s_e - (1+\alpha-\beta) s_3] \}. \quad (\text{IA22})$$

Using (IA9), we obtain

$$N_{II,3} = \frac{(1-\beta) N_{II,0} + \alpha N_{II,e} + \frac{\Theta_3 \mu_A x_3 f}{Y_{A,a}} - [(1-\beta)(N_{IV,0} - N_{I,3}) + \alpha(N_{I,e} - N_{I,3})] MY_{A,a}}{1+\alpha-\beta}. \quad (\text{IA23})$$

By virtue of (IA12), we have

$$\Theta_5 = \frac{V_5}{Q_0} = \frac{Y_{H(5)n}}{\mu_{H(5)} x_5 (1-f)} [(1+\alpha)(N_{II,3} - N_{II,e}) - \beta(N_{II,3} - N_{II,0})]. \quad (\text{IA24})$$

By virtue of (IA2b), (IA3), and (IA5), we get

$$\Delta x = \frac{Y_{H(1)c} [(1-\beta) s_0 + \alpha s_e - (1+\alpha-\beta) s_3] + Y_{H(5)c} [(1+\alpha-\beta) s_3 + \beta s_0 - (1+\alpha) s_e]}{1-f} \cdot Q_0. \quad (\text{IA25})$$

Considering (IA3), we obtain

$$SA = \frac{(\Theta_3 x_3 + \Theta_5 x_5) Q_0}{\Delta x}. \quad (\text{IA26})$$

Assuming that the oxygen required for nitrification and biodegradation of organics amounts to 4.6 g O₂/g N-NH₄⁺ [7] and 1 g O₂/g BOD₅, respectively, it is possible to determine the oxygen demand for biochemical processes. Thus,

$$OD = [(1-\beta) s_0 + \alpha s_e - (1+\alpha-\beta) s_3 + 4.6(N_{IV,0} - N_{I,e})] Q_0 - 4.6 \Delta x M (1-f). \quad (\text{IA27})$$

2.2.2. CONFIGURATION IB

Almost all of the balance equations derived for configuration IA are valid for configuration IB provided that $\beta = 0$ and $s_3 = s_e$ (which means that during denitrification methanol is the only carbon source). Now, the value of s_e is no longer adopted by assumption; it is obtained by calculation. It is only necessary to

introduce some changes to eqs. (IA2b), (IA11), and (IA13). Hence, we can write

$$\Delta H = [(s_0 - s_e) Y_{H(1)c} + D_m Y_{H(5)c}] Q_0. \quad (\text{IB2b})$$

It has been assumed that BOD₅ for methanol amounts to approximately 1 g O₂/g methanol

$$(1 + \alpha) Q_0 s_e + Q_0 D_m - V_5 \frac{\mu_{H(5)} x_5 (1-f)}{Y_{H(5)c}} - (1 + \alpha) Q_0 s_e = 0, \quad (\text{IB11})$$

$$(1 + \alpha) Q_0 N_{1,3} - Y_{H(5)c} Q_0 D_m M - (1 + \alpha) Q_0 N_{1,e} = 0. \quad (\text{IB13})$$

By virtue of (IA19) we have $x_3 = x_5$.

Using (IA1a), (IA1b), (IA8)–(IA13), we may derive eq. (IB15) which is to be solved numerically with respect to s_e :

$$\frac{Y_{H(5)n}}{Y_{H(5)c}} [B + N_{11,0} - N_{11,e} - (s_0 - s_e) M Y_{H(1)c}] - (s_0 - s_e) D = 0. \quad (\text{IB15})$$

$$1 + \frac{\alpha}{1 + \alpha} M Y_{H(5)n} (1 - M Y_{A,a})$$

The interval of the s_e values is defined in terms of (IA17) after having inserted $s_3 = s_e$.

Having calculated s_e , we can determine D_m , using (IB18). Hence,

$$D_m = (s_0 - s_e) D. \quad (\text{IB18})$$

Considering (IB13), we have

$$N_{1,e} = N_{1,3} - \frac{M Y_{H(5)c} D_m}{1 + \alpha}. \quad (\text{IB20})$$

Making use of (IA1b), (IB2b), (IA3), and (IA4) and assuming

$$E = \frac{(N_{11,0} - N_{11,e}) Y_{A,a}}{(s_0 - s_e) Y_{H(1)c} + Y_{H(5)c} D_m} - M Y_{A,a},$$

it is possible to prove that f should be calculated in terms of (IA21).

Θ_3 is calculated by virtue of (IA22), $N_{11,3}$ by virtue of (IA23), and Θ_5 by virtue of (IA24). Making use of (IA3), (IA5), and (IB2b), we obtain

$$\Delta x = \frac{[(s_0 - s_e) Y_{H(1)c} + Y_{H(5)c} D_m]}{1-f} Q_0. \quad (\text{IB25})$$

SA may be calculated in terms of (IA26), whereas OD can be determined by virtue of (IA27).

2.2.3. CONFIGURATION II

What has been said about the age of the sludge for configuration I is also valid for configuration II. This means that eqs. (IA1)–(IA5), as well as (IA1a), (IA1b) and (IA2a), along with the conclusions drawn by using the formulae mentioned, still hold. Here, the expression for increment of heterotrophic biomass by virtue of the balance of utilized organic matter for configuration I (IA2b) becomes

$$\Delta H = Y_{H(1)c}(1 + \alpha + \beta)(s_5 - s_e)Q_0 + Y_{H(5)c}[s_0 + (\alpha + \beta)s_e - (1 + \alpha + \beta)s_5]Q_0. \quad (\text{II2b})$$

Sludge balance

For DNT

$$\alpha x_6 + \beta x_3 - (1 + \alpha + \beta)x_5 = 0. \quad (\text{II6})$$

For NT

$$(1 + \alpha + \beta)x_5 - (1 + \alpha + \beta)x_3 = 0. \quad (\text{II7})$$

TKN balance for NT

$$(1 + \alpha + \beta)Q_0 N_{1,5} - V_3 \frac{\mu_A x_3 f}{Y_{A,a}} - Y_{H(1)c}(1 + \alpha + \beta)Q_0(s_5 - s_e)M - (1 + \alpha + \beta)Q_0 N_{1,e} = 0. \quad (\text{II8})$$

N-NO₃⁻ balance for NT

$$(1 + \alpha + \beta)Q_0 N_{11,5} + V_3 \frac{\mu_A x_3 f}{Y_{A,a}} - (1 + \alpha + \beta)Q_0 N_{11,e} - Y_{A,a}(1 + \alpha + \beta)Q_0(N_{1,5} - N_{1,e})M = 0. \quad (\text{II9})$$

BOD₅ balance for NT

$$(1 + \alpha + \beta)Q_0 s_5 - V_3 \frac{\mu_{H(1)} x_3 (1-f)}{Y_{H(1)c}} - (1 + \alpha + \beta)Q_0 s_e = 0. \quad (\text{II10})$$

BOD₅ balance for DNT

$$Q_0 s_0 + (\alpha + \beta)s_e - V_5 \frac{\mu_{H(5)} x_5 (1-f)}{Y_{H(5)c}} - (1 + \alpha + \beta)Q_0 s_5 = 0. \quad (\text{II11})$$

N-NO₃⁻ balance for DNT

$$Q_0 N_{11,0} + (\alpha + \beta)Q_0 N_{11,e} - V_5 \frac{\mu_{H(5)} x_5 (1-f)}{Y_{H(5)n}} - (1 + \alpha + \beta)Q_0 N_{11,5} = 0. \quad (\text{II12})$$

TKN balance for DNT

$$Q_0 N_{IV,0} + (\alpha + \beta) Q_0 N_{I,e} - Y_{H(5)c} Q_0 [s_0 + (\alpha + \beta) s_e - (1 + \alpha + \beta) s_5] M - (1 + \alpha + \beta) Q_0 N_{I,5} = 0. \quad (\text{II13})$$

The values of the x_3 , x_6 , $N_{II,e}$, $N_{II,5} \leq K_n/(SF - 1)$, $N_{I,e} \leq K_d/(SF - 1)$ as well as DO and pH in NT are assumed.

By virtue of (II6)

$$\alpha = \frac{x_5}{x_6 - x_5}. \quad (\text{II14})$$

Using eqs. (IA1a), (IA2a), (IA4), (IA5), and (II8)–(II13), it is possible to derive eq. (II15), which should be solved with respect to s_e included in it. Hence,

$$\frac{(N_{IV,0} - N_{I,e})(1 - MY_{A,a}) + N_{II,0} - N_{II,e} - (s_0 - s_e) MY_{H(1)c}}{1 + G} - \frac{(s_0 - s_e) \frac{Y_{H(5)c}}{Y_{H(5)n}}}{1 + \frac{1}{D}} = 0 \quad (\text{II15})$$

where

$$G = MY_{H(5)n} \left(1 - MY_{A,a} - \frac{Y_{H(1)c}}{Y_{H(5)c}} \right).$$

The interval of the s_e values is defined by condition (IA17) after inserting $s_3 = s_e$. Then, we calculate by virtue of (II18)

$$\beta = \frac{\frac{(s_0 - s_e) \frac{Y_{H(5)c}}{Y_{H(5)n}}}{1 + \frac{1}{D}} + N_{II,e} - N_{II,0}}{N_{II,e} - N_{II,5}} - 1 - \alpha. \quad (\text{II18})$$

Considering (II7), we have

$$x_5 = x_3. \quad (\text{II19})$$

Using (II11)–(II13) gives

$$N_{I,5} = \frac{N_{IV,0} + (\alpha + \beta) N_{I,e} - [N_{II,0} + (\alpha + \beta) N_{II,e} - (1 + \alpha + \beta) N_{II,5}] Y_{H(5)n}}{1 + \alpha + \beta}. \quad (\text{II20})$$

From (II11) and (II12) we obtain

$$s_5 = \frac{s_0 + (\alpha + \beta) s_e - \frac{Y_{H(5)n}}{Y_{H(5)c}} [N_{II,0} + (\alpha + \beta) N_{II,e} - (1 + \alpha + \beta) N_{II,5}]}{1 + \alpha + \beta}. \quad (\text{II23})$$

If (IA3), (IA4), (IA1b), and (II2b) is taken into account and

$$E = \frac{(N_{IV,0} - N_{I,e}) Y_{A,a}}{Y_{H(5)c} [s_0 + (\alpha + \beta) s_e - (1 + \alpha + \beta) s_5] + Y_{H(1)c} (1 + \alpha + \beta) (s_5 - s_e)} - M Y_{A,a}$$

adopted, f should be calculated in terms of (IA21).

From (II9)

$$\Theta_3 = \frac{Y_{A,a}}{\mu_A x_3 f} (1 + \alpha + \beta) [N_{II,e} - N_{II,5} + (N_{I,5} - N_{I,e}) M Y_{A,a}]. \quad (\text{II22})$$

By virtue of (II11)

$$\Theta_5 = \frac{Y_{H(5)c}}{\mu_{H(5)} x_3 (1-f)} [s_0 + (\alpha + \beta) s_e - (1 + \alpha + \beta) s_5]. \quad (\text{II24})$$

Considering (IA3), (IA5), (II2b) yields

$$\Delta x = \frac{Y_{H(1)c} (1 + \alpha + \beta) (s_5 - s_e) + Y_{H(5)c} [s_0 + (\alpha + \beta) s_e - (1 + \alpha + \beta) s_5]}{1-f} Q_0. \quad (\text{II25})$$

Using (IA3) and (II19), we have

$$SA = \frac{(\Theta_3 + \Theta_5) Q_0 x_3}{\Delta x}. \quad (\text{II26})$$

Oxygen demand is calculated as follows:

$$OD = [(1 + \alpha + \beta) (s_5 - s_e) + 4.6 (N_{IV,0} - N_{I,e})] - 4.6 \Delta x M (1-f). \quad (\text{II27})$$

3. DISCUSSION

The models presented without transformation in the form of (IA), (IB) and (II) (1-13) for configuration IA, configuration IB and configuration II, respectively, are sets of nonlinear algebraic equations. Their nonlinearity is associated with the nonlinear dependence of μ and Y on the substrate concentration ($N_{I,3}$, $N_{II,5}$, s_3). That is why these sets can be solved numerically only.

The transformation of the models to equations (IA), (IB) and (II) (14-27), respectively, involves a partial elimination of nonlinearity. In consequence, instead

of numerical solving of a set of more than ten equations, it is necessary to solve numerically one equation only (IA15), (IB15), (II15)). Needless to say that it is much easier and more convenient to solve one equation, the more so as this can be done even without a computer.

The design of the process by using the model in question is quite simple. After s_3 has been calculated in terms of (IA15), or s_e from (IB15), or s_e from (II15) for configuration IA, configuration IB or configuration II, respectively, the remaining process parameters may be determined direct from successive formulae.

For calculation, special computer programmes in BASIC have been developed. Two versions, NIDE and NIDES, are available for microcomputer ZX81 and microcomputer ZX SPECTRUM, respectively, and the design procedure is quick and easy. Although the model is rather complex it does not take into account all details. Thus nitrogen and organic matter concentrations, measured in the effluent from the sewage treatment plant, will be higher than those calculated in terms of the model. It is, therefore, advisable to add the following to the calculated values: a certain amount of organic substances either nondegradable or resistant to biodegradation, as well as a certain quantity of organics contained in the sludge escaping from the secondary settling tank. Also organic nitrogen included in the escaping biomass should be added to the nitrogen in the effluent.

To prove that the model-based predictions are logical, a series of calculations was carried out, using the two computer programmes.

3.1. TREATMENT EFFECTS OBTAINED FOR THE SAME SEWAGE BY MAKING USE OF THE THREE CONFIGURATIONS

3.1.1. EXAMPLE 1 (TYPICAL TKN AND BOD)

$Q_0 = 20\,000 \text{ m}^3/\text{d}$, $s_0 = 300 \text{ g O}_2/\text{m}^3$, $N_{1,0} = 35 \text{ g N-NH}_4^+/\text{m}^3$, $N_{11,0} = 10 \text{ g N-NO}_3^-/\text{m}^3$, $N_{111,0} = 50 \text{ g N}/\text{m}^3$, $T = 10 \text{ }^\circ\text{C}$, $\text{pH} = 6.9$ (nitrification tank), $\text{DO} = 3 \text{ g O}_2/\text{m}^3$, $SF = 1.5$, $x_5 = 3000 \text{ g smo}/\text{m}^3$ (for IA and IB) or $x_3 = 3000 \text{ g smo}/\text{m}^3$ (for II), $x_6 = 8000 \text{ g smo}/\text{m}^3$.

Major computational results are listed in tab. 2a. As shown by these data, effluent nitrogen concentration for configuration IA is high, with N-NH_4^+ as the main contributor. This is to be attributed to the intensive wastewater stream ($\beta = 0.48$) which has been sent direct to the denitrification tank, wherein only a slight part of TKN is assimilated by the heterotrophs. Thus, most of the TKN enters the effluent.

The application of methanol as the sole carbon source for denitrification (configuration IB) enables an almost complete removal of nitrogen, as only small amounts of TKN are passed to the denitrification tank. However, this configuration needs the expenditures for methanol and for the dosing installation.

Comparison of configuration

Configuration	Parameter												
	Θ_3, h / V_3, m^3	Θ_5, h / V_5, m^3	$\Theta_3 + \Theta_5, h$ / $(V_3 + V_5), m^3$	$N_{I,e}$ g N/m ³	$N_{II,e}$ g N/m ³	$\sum Ne$ g N/m ³	Se g O ₂ /m ³	OD kg O ₂ /d	Δx kg smo/d	f	α	β	D_m g meth/m ³
a) Example 1, $M = 0.123$													
IA	$\frac{4.4}{3667}$	$\frac{6.2}{5166}$	$\frac{10.2}{8833}$	24.46	0.3	24.76	5	7850	1579	0.057	0.6	0.48	0
IB	$\frac{12.7}{10583}$	$\frac{7.5}{6250}$	$\frac{20.2}{16833}$	< 0.45	0.3	< 0.75	2.6	12105	2985	0.04	0.6	0	221.8
II	$\frac{5.7}{4750}$	$\frac{8.1}{6750}$	$\frac{13.8}{11500}$	0.45	10	10.45	2.3	9531	1426	0.095	0.6	6.21	0
b) Example 2, $M = 0.123$													
IA	$\frac{12}{9971}$	$\frac{3.9}{3227}$	$\frac{15.9}{13198}$	3.7	0.3	4.0	5	9032	3410	0.005	0.6	0.19	0
IB	$\frac{21.3}{17712}$	$\frac{3.6}{2996}$	$\frac{24.9}{20708}$	0.45	0.3	0.75	3.15	10724	4242	0.004	0.6	0	111
II	$\frac{13.7}{11393}$	$\frac{3.9}{3221}$	$\frac{17.6}{14614}$	0.45	3.5	3.95	3.21	9364	3434	0.007	0.6	2.53	0
c) Example 2, $M = 0$													
IA	$\frac{10.5}{8726}$	$\frac{5.7}{4771}$	$\frac{16.2}{13497}$	6.4	0.3	6.7	5	9858	3176	0.015	0.6	0.28	0
IB	$\frac{17.7}{14738}$	$\frac{5.8}{4850}$	$\frac{23.5}{19588}$	< 0.45	0.3	< 0.75	2.98	13119	4442	0.014	0.6	0	181.6
II	$\frac{12.6}{10494}$	$\frac{6}{5013}$	$\frac{18.6}{15507}$	0.45	3.5	3.95	3.05	10318	3163	0.019	0.6	9.2	0

Configuration II yielded effluent nitrogen concentration which was less than half that achieved in configuration IA. It should be noted that configuration II has one more advantage because the main contributor to the effluent nitrogen concentration is nitrate nitrogen. And nitrate concentration may be further reduced by applying more intensive recirculation (by increasing the β value) from the nitrification tank. Thus, with $\beta = 43.4$, the following values were obtained: $N_{II,e} = 2$, $N_{I,e} = 0.45$, $s_e = 2$, $\Theta_3 + \Theta_5 = 14.3$, $OD = 9205$, $\Delta x = 1302$ (units as in tab. 2). When β increases, so does the dissolved oxygen load ($\beta Q_0 DO$) entering the denitrification tank. Hence, it may happen that once a certain high β value is achieved, it will no longer be possible to obtain unoxic conditions in the denitrification tank. But this trouble may be overcome. The problem of how to overcome it, will be discussed in a separate report.

The volume of the nitrification tank for configuration IA is quite small. This should be attributed to the fact that only 52% of raw wastewater enters the nitrification tank.

Volume V_3 for configuration IB is much larger. This should be attributed to two factors (direct and indirect) – 1) nitrification involves the total amount of wastewaters under treatment, and 2) the content of nitrifiers in the biomass is decreased ($f = 0.04$). What accounts for the decrease in nitrifier content, is the unfavourable change in the ratio of nitrified nitrogen load to the load of BOD removed (because of the application of additional methanol BOD).

The nitrified nitrogen load for configuration II is practically the same as that for configuration IB, but there is a difference in the nitrification tank volume between the two configurations. That for configuration II is markedly smaller, which should be attributed to the substantially greater content of nitrifiers in the biomass.

Compared to configuration IB, configuration II has the inherent advantage of using less oxygen and producing less amounts of excess sludge. This is because in configuration IB, the whole BOD load of the wastewater should be removed under oxic conditions, whereas in configuration II a considerable part of it is removed in the denitrification tank. The application of methanol brings about large amounts of excess sludge in configuration IB.

Comparison of results shows that configuration II and configuration IB yield effluents of higher quality than does configuration IA. On the other hand, configuration II involves lower expenditures and running costs, as compared to configuration IB.

3.1.2. EXAMPLE 2 (LOWER TKN, HIGHER BOD)

$N_{I,0} = 17$, $N_{II,0} = 30$, $N_{III,0} = 5$, $s_0 = 500$ (the remaining data are the same as in example 1). Major results are given in tab. 2b. As shown by these data, each of the three configurations yields sufficiently good effluents, but configuration IB is the most expensive.

3.2. SIGNIFICANCE OF BUILT-IN TKN

It is a frequent practice that calculations for the needs of design do not include TKN built-in in the biomass [7]. Furthermore, it is believed that the resulting error is insignificant. To verify this, the models derived in this paper were made use of. Comparison of results was carried out for $M = 0.123$, and for $M = 0$ for the data of example 2 (tabs. 2b and 2c). As shown by this comparison, assuming $M = 0$ yields too short times of nitrification (Θ_3) and too long times of denitrification (Θ_5). For configuration IB the overestimation of Θ_5 in the example considered amounted to approximately 40%. Similar degree of overestimation pertains to the methanol dose. Summing up, it is obvious that neglecting the TKN building-in problem may lead to serious inaccuracy of design. The trouble may easily be overcome by applying the mathematical models presented here.

3.3. RELATION BETWEEN WASTEWATER COMPOSITION AND THE COMPOSITION OF THE BIOMASS

The formula describing the nitrifier content in the biomass (f) shows that the composition of the biomass depends on the ratio of nitrified TKN load to the load of BOD removed (more precisely on $\Delta A/\Delta H$ ratio which is dependent on TKN/BOD ratio).

Thus, it is interesting to note that the increase of TKN concentration in the wastewater at constant BOD does not lead to a proportional extension of the nitrification time. This is so because the increased TKN load is nitrified by an increased number of nitrifiers. From the expressions for Θ_3 it is obvious that the amount of nitrifiers has a strong influence on the nitrification time required. Thus, for example 1 and configuration II (provided that $s_0 = 500 \text{ g O}_2/\text{m}^3$), the rise in $N_{1,0}$ from 35 to $100 \text{ g N-N}_4/\text{m}^3$ brought about the following: the increase of f from 0.037 to 0.106, the decrease of Θ_3 from 12.6 to 9.0 h, the increase of Θ_5 from 6.5 to 14.7 h, and the decrease of Δx from 3162 to 2271. As shown by these data, the 76% increase of TKN accounted for an approximately 30% decrease of the nitrification time required. This curiosity is the result of an almost threefold increase of f . The substantial increase of f should be attributed to the overlapping of two effects – the effect of the increased TKN load in raw wastewater and the effect of the markedly increased contribution of BOD₅ load degraded in the denitrification tank. The previous one brings about increment of excess nitrifiers sludge (ΔA) from 116 to 241 kg vss/d. The increased contribution of BOD₅ load oxidized in the denitrification tank is due to the increment of nitrate load being reduced there. The growth yield of heterotrophs in the denitrification tank is nearly one third that occurring in the aeration tank ($Y_{H(5)c} = 0.127$, $Y_{H(1)c} = 0.331 \text{ g vss/g BOD}_5$), and this brings about decrement of excess heterotrophic sludge (ΔH) from 3046 to 2030 kg vss/d. Taking into account the more than

doubled increase of denitrification time, the total time of retention ($\Theta_3 + \Theta_5$) showed an approximately 25% increase only, although the TKN load increased by some 76%.

4. CONCLUSIONS

The mathematical models presented in this paper include some significant factors affecting the nitrification and denitrification efficiencies in different configurations of the one-sludge system. The predictions established in terms of these models for each of the three configurations are consistent and in good agreement with the results of qualitative analysis making use of the theory of the phenomena involved. The models are fit for the design of the process. When the wastewater under treatment is municipal sewage or a liquid of similar properties, it is advisable to use the parameters of kinetics listed in tab. 1. The models presented here may also be of utility in the treatment of any other wastewater provided that the values of the parameters of kinetics are determined or estimated.

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PROJEKTOWANIE PROCESU NITRYFIKACJI I DENITRYFIKACJI W OPARCIU O MODEL MATEMATYCZNY

Przedyskutowano podstawowe zasady usuwania azotu i związków organicznych w procesie jednego osadu. Na podstawie równania bilansu dla BZT, azotu i biomasy zbudowano model matematyczny procesu. W modelu uwzględniono następujące elementy: przyrost biomasy heterotroficznej i autotroficznej, rozkład związków organicznych, nitryfikację azotu amonowego, denitryfikację azotanów i asymilację azotu amonowego przez przyrastającą biomasę. Zakładano, że ścieki surowe mogą zawierać azot organiczny, amonowy i azotanowy.

Zbudowano modele matematyczne dla następujących konfiguracji: 1) komora napowietrzania przed komorą denitryfikacji, 2) komora denitryfikacji przed komorą napowietrzania. W konfiguracji 1) uwzględniono możliwość wykorzystania zewnętrznego źródła węgla (np. metanola) w denitryfikacji.

Rozwiązania modeli matematycznych dla warunków ustalonych zostały uzyskane przez przekształcenie układu ponad dziesięciu równań nieliniowych w jedno równanie. Po jego rozwiązaniu wszystkie parametry procesu mogą być obliczone wprost z podanych wzorów. Aby zilustrować sposób korzystania z modeli, przedyskutowano przykładowe wyniki obliczeń dla obu konfiguracji.

ПРОЕКТИРОВАНИЕ ПРОЦЕССА НИТРИФИКАЦИИ И ДЕНИТРИФИКАЦИИ НА БАЗЕ МАТЕМАТИЧЕСКОЙ МОДЕЛИ

Обсуждены основные принципы удаления азота и органических соединений в процессе одного осадка. Опираясь на уравнения баланса для ВЗТ, азота и биомассы, построили математическую модель процесса. В модели учли следующие элементы: приращение гетеро- и автотрофической массы, распределение органических соединений, нитрификацию аммиачного азота через прирастающую биомассу. Предполагалось, что сырые сточные воды могут содержать органический, аммиачный и нитратный азот.

Простроены математические модели для следующих конфигураций: 1) аэротанк перед камерой денитрификации, 2) камера денитрификации перед аэротанком. В первой конфигурации учтена возможность использования внешнего источника угля (напр. метанола) в денитрификации. Решения математических моделей для установленных условий были получены путём преобразования системы свыше десяти нелинейных в одно уравнение. После его решения все параметры процесса могут вычисляться непосредственно из данных в работе формул. С целью иллюстрации способа пользования моделями обсуждены примерные результаты вычислений для обеих конфигураций.