ANALYTICAL MODEL AND SIMULATION OF OXYGEN SOLUBILITY IN WASTEWATER

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Abstract
The research paper discusses oxygen transfer process in the water of the sewage biological treatment system, and provides mathematical model and simulation of oxygen solubility process in wastewater. Oxygen supply to wastewater is one of the most important components of the biological treatment process from energy point of view because of substantial energy consumption and need for continuous operation. Thus, understanding process of oxygen transfer and development of analytic expressions describing oxygen solubility under different environmental conditions is cruical. Impact of temperature, air pressure, oxygen concentration in supplied air, composition of dissolved chemicals, and air supply unit submerging depth was taken into account, and the mathematical model of oxygen solubility in water was compiled. Oxygen solubility process was simulated using Matlab `Simulink` software. Analytical model of oxygen solubility in water can be used in wastewater treatment plants in order to develop an improved control system for the aeartion system, which would result in a decrease in energy consumption.
Key words: oxygen solubility, mathematical modeling, simulation, wastewater aeration, control.

Introduction

Modern wastewater treatment systems (WWTS) utilize bological sewage treatment approach, in which activated sludge is being used. Activated sludge is a process in sewage treatment in which air or oxygen is forced into sewage liquor to develop a biological environment consisting of different microorganisms which are processing the pollutents of the sewage. In the process, large quantities of air are bubbled through wastewaters that contain dissolved organic substances in open aeration tanks. Air is being supplied to the WWTS using air blowers driven by asynchronous electric motors, and this system is the largest energy consumer in WWTS (accounting 40–80% of all WWTS energy consumption, value varies depending on aeration technology used and WWTS geographical location) (Šnīders, 2004; Wang, 2007), and precise air supply to WWTS and dissolved oxygen control are becoming very important tasks taking into account the global trend of energy prices increase.

Oxygen is required by bacteria and other types of microorganisms present in the system to live, grow, and multiply in order to consume the dissolved organic `food`, or pollutants in the waste. As the wastewater composition, physical, chemical properties and waste concentration, as well as external environment (temperature, moisture content, air presure and composition, etc.) vary along time, it is very important to create the system which could supply appropriate amount of oxygen, at the same time using an economically affordable energy amount.

Optimal control of the operation of WWTS electric motors is very important in order to obtain the optimum technical and economical solution, while at the same time, optimal control requires the creation of appropriate mathematical model which high quality and realistic process adequately addresses the oxygen delivery. Lack of a common mathematical model that describes the non-stationary oxygen transfer process in the aeration tank sets limitations for the sewage treatment plant designers and operators to use the optimal (energy-efficient and high quality) aeration engineering system control algorithm, which takes into account the dynamics of the aeration tank. Studies on oxygen solubility in wastewater had been looking at influence of different individual factors, but no complex analytic model taking into account the set of factors affecting solubility of oxygen was developed and used in wastewater aeration control systems.

Oxygen dissolving in water is a complicated physical process influenced by different factors. In order to evaluate the aerotank dynamic response, it was necessary to introduce in the mathematic model of aerotank the analytic equation of oxygen solubility, which takes into consideration the main influencing factors – oxygen concentration in the air supplied, wastewater temperature and salinity, as well as air pressure, and to validate the simulation model.

Materials and Methods

Observations of oxygen concentration in air prove substantial seasonality. Oxygen concentration change diapason is between 20.84% and 20.97 %, showing lowest scores during winter (BIO2 International, s.a.). Oxygen concentration fluctuations are considerable, and this factor will be included in oxygen solubility formula, which then will be used for the development of highly efficient wastewater aeration control system. The main reasons for such seasonality in oxygen concentration in air are the following: plants are producing oxygen mostly in warm season, oxygen solubility in water increases due to water temperature decrease, as well as seasonal changes in human activities – increased oxygen consumption due to increased fuel burning for heating in cold weather. Observations also confirm assumption that oxygen concentration in urban area is lower than in countryside and in forests (Moiseeva, 1995; Keeling, 1998).

Experimental research revealed that the water of open basins in summer (temperature 21°C) contains on average 13 g·m^{-3} of nitrogen (N_2), 9 g·m^{-3} of oxygen (O_2), and 35 g·m^{-3} of carbon dioxide (CO_2) (Meck, s.a.; Mack, s.a.). Saturation level of gases dissolved in water differs, and depends on water temperature (Colby, s.a.; Colt, 1984). With water temperature increase the solubility of gases in water decreases (Colt, 1984; FAO, 1998). Saturation level of oxygen solubility usually is being acquired from ready-made tables, which were developed from experimental data (Colt; 1984; YSI, s.a.). There are only few analytic expressions available currently (Weiss, 1970; Garcia, Gordon, 1992; Tromans, 2000; Sniders, 2003), which have very limited use in automatic conrol systems.

Wastewater contains a mixture of different dissolved salts, suspended solids, and live creatures – microorganisms, bacteria, etc. Experimental research shows that concentration and composition of salts dissolved have direct impact on oxygen concentration in water – the higher is salinity, the lower is oxygen saturation level in water (Colt, 1984). For simplified oxygen saturation calculations, usually non-dimensional coefficient is being introduced, which should take into account wastewater salinity (YSI, s.a.), but the quality of the simulation is questionable. Obviously, such approach does not allow adjusting oxygen saturation level neither to specifics of particular WWTP with its own composition and concentration of dissolved salts, nor to changes in dissolved salts composition and concentration.

Observations (Colt, 1984) show that atmospheric pressure has an impact on oxygen solubility in water – with diminishing atmospheric pressure the oxygen solubility in water decreases. No analytical expressions were find which describe this solubility impacting factor.

Air supply to aerotank must be provided with overpressure, if aeration is provided from a bottom of aerotank, because wastewater layer above the diffuser creates overpressure, and air blower must provide air pressure which is larger than that created by the wastewater layer – air pressure must be higher than the pressure in the diffuser submerging depth *h* in wastewater.

Water density changes have an impact on the necessary air blower output pressure. At the same time water in its liquid stage substantially differs from other liquids – its density changes nonlinearly with the changes in water temperature. None of the known oxygen solubility models takes into account this nonlinear impact.

Oxygen solubility process was simulated using Matlab `Simulink` software in order to evaluate how the variables influence this process.

Results and Discussion

Regression analysis application on the experimental data gathered about the relation between the water temperature and oxygen saturation in water (Colt, 1984) revealed the formula describing this relation:

$$C_S(\Theta) = 14.208 \cdot \exp\left(-0.0219 \cdot \Theta\right). \qquad (1)$$

The obtained exponential expression which joins together oxygen saturation in water $C_S(\Theta)$ and temperature Θ (in Celsius degrees) with high accuracy describes the interdependence of the two factors (R^2= 0.997). At the same time it can be used as a basic analytic expression for the development of an oxygen solubility multifactorial model.

Modified analytic expression which takes into account the composition and concentration of dissolved salts in wastewater (using Mack, s.a.; Han, 2002) was created:

$$C_S = C_0 \cdot \exp\left(\sum_{i=1}^{n} K_i c_i\right)^{-1}, \qquad (2)$$

where

- C_0 – oxygen solubility in clean water, g·m^{-3};
- i – index of the ione dissolved in water;
- K_i – semiempyrical constant for the indexed ione;
- c_i – molarity of the indexed ione in water solution;
- C – oxygen solubility in water with dissolved indexed iones, g·m^{-3}.

An analytic expression which describes interrelation between air pressure and oxygen solubility was developed using a modified Henry's formula:

$$C_x = p_x \cdot k_H^x = p_x \cdot A \cdot N_A \cdot \alpha^x, \qquad (3)$$

where

- C_x – solubility of gas x, g·m^{-3};
- k_H^x – Henry's constant for gas x (particularly – for oxygen), (g/m^3)·Pa^{-1};
- p_x – partial pressure of gas x (in this formula – oxygen), Pa;
- N_A – Avogadro's constant, mol^{-1};
- A – coefficient taking into account oxygen density;

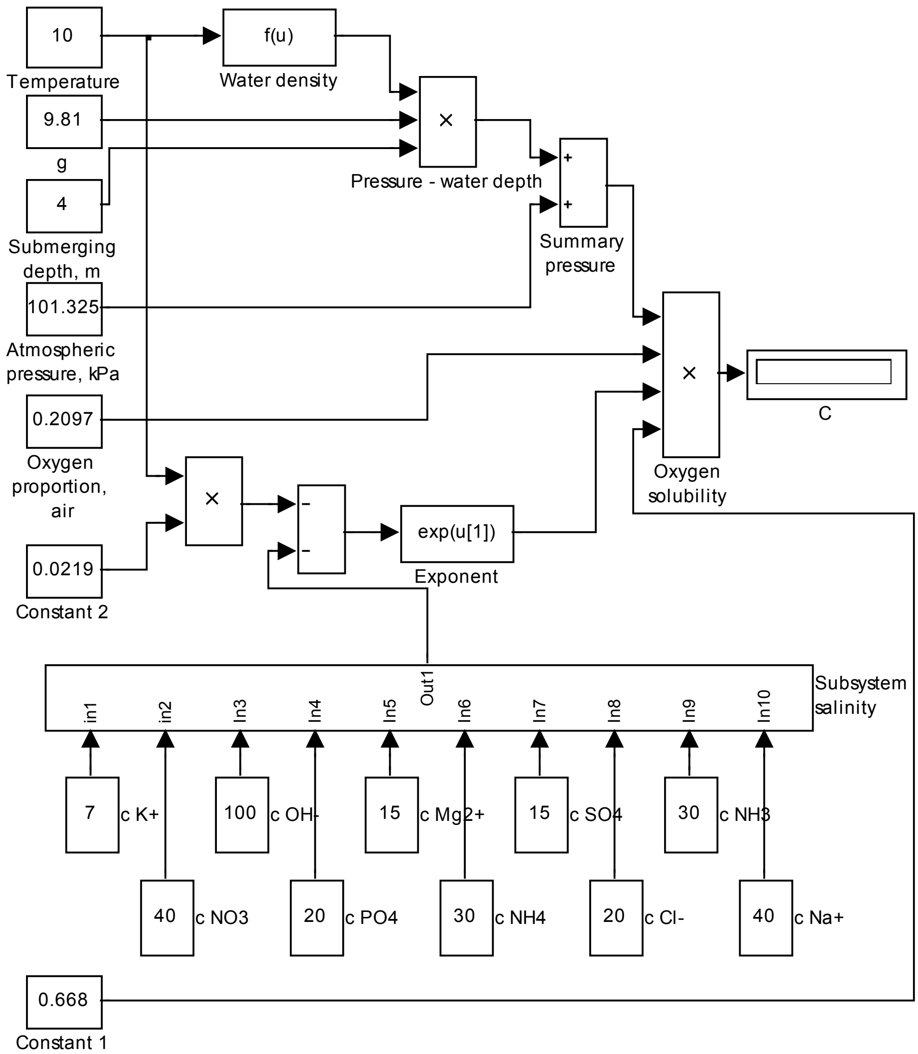

Fig. 1 The virtual model of oxygen solubility

α^x – Bunzen's coefficient for oxygen, $m^3 \cdot mol^{-1}$.

A formula describing Bunzen's coefficient for oxygen was developed using experimental data (Weiss, 1970) and applying nonlinear regression model:

$$\alpha = 4.91 \cdot \exp(-0.0219 \cdot \Theta). \quad (4)$$

Gas pressure impact on gas solubility can be described using a modified formula (Broecker, Peng, 1982; Sawyer, McCarty, 1978):

$$C_1 \cdot p_1^{-1} = C_2 \cdot p_2^{-1}, \quad (5)$$

where

C_1 and C_2 – gas solubility for two different pressures, $g \cdot m^{-3}$;

p_1 and p_2 – gas pressures, Pa.

A formula describing complex impact of air pressure and temperature was created using expressions (3), (4) and (5):

$$C = p_x \cdot A \cdot N_A \cdot \alpha^x \cdot 4.91 \cdot \exp(-0.0219 \cdot \Theta). \quad (6)$$

An expression describing the dependence of the air blower output pressure on temperature and the air diffuser submerging depth, and taking into account the nonlinear dependence of water density on temperature was created:

$$p_h = \rho \cdot g \cdot h = (-0.006 \cdot \Theta^2 + 0.0365 \cdot \Theta + 999.91) \cdot g \cdot h, \quad (7)$$

where

p_h – water pressure in depth h (required air blower pressure), Pa;

ρ – water density, kg·m^{-3};

h – air diffuser submerging depth, m;

g – gravity constant, 9.81 m·s^{-2}.

A mathematic model which describes the interrelation between oxygen solubility in wastewater and the scope of external factors – air pressure, oxygen concentration in air, wastewater salinity and the composition of dissolved iones, wastewater temperature, as well as air diffusers submerging depth - is presented in the formula developed by the authors of the presented research:

$$C_S = C(r_{O_2}, p_a, \Theta, K, c_i, h) = \frac{0.668 \cdot r_{O_2} \cdot \left(p_a + \left(-0.006 \cdot \Theta^2 + 0.0365 \cdot \Theta + 999.91\right) \cdot g \cdot h \cdot 10^{-3}\right)}{\exp\left(\sum K_i c_i + 0.0219 \cdot \Theta\right)}, \tag{8}$$

where

r_{O_2} – proportion of oxygen in the air;

p_a – atmospheric pressure.

Virtual model of oxygen solubility using formula (8) and software package Matlab subprogram Simulink was developed (Fig.1) for further exploration of the dynamic response of the wastewater aerotank.

Main parts of the virtual model are the following:

– \`Temperature\` block allows establishing and change wastewater temperature, ºC;
– \`g\` block sets the gravity constante g=9.81 m·s^{-2};
– \`Submerging depth\` block allows establishing the aeration diffusers submerging depth, m;
– \`Atmospheric pressure\` block sets atmospheric pressure, kPa;
– \`Oxygen proportion\` block sets oxygen proportion in supplied air;
– blocks \`Constant 1\` and \`Constant 2\` introduce constants 0.668 and 0.0219;
– \`Water density\` block provides re-calculation of water density according to the water temperature;
– \`Exponent\` block takes into account the exponential characterictics of the solubility;
– blocks with the indicies \`c..\` present the ionic composition of the waste in the wastewater, g·m^{-3};
– blocks \`Pressure – water depth\`, \`Subsystem salinity\`, \`Summary pressure\` and \`Oxygen solubility\` are used for mathematic operations in order to calculate the oxygen solubility.

Oxygen solubility simulation was provided using data from real WWTS. They were the following:

– wastewater temperature Θ=10˚C;
– aeration diffusers submerging depth h=4m;
– atmospheric pressure 101.325 kPa;
– oxygen proportion in air $r_{O_2} = 0.2097$;
– wastewater ionic composition – c_{K+}=7 g·m^{-3}, c_{OH-}=100 g·m^{-3}, c_{Mg2+}=15 g·m^{-3}, c_{SO42-}=15 g·m^{-3}, c_{PO43-}=20 g·m^{-}, c_{Cl-}=20 g·m^{-3}, c_{Na+}=40 g·m^{-3}, c_{NH3}=30 g·m^{-3}, c_{NH4-}=30 g·m^{-3}, c_{NO3-}=40 g·m^{-3}.

Simulation steps :

– initial conditions were established, and the first simulation provoided;
– the following simulation pattern for further simulations was used:
  1. aeration diffusers submerging depth change – depth increase by 1 m (other parameters the same*Ceteris Paribus(CP*));

Table 1

The results of oxygen solubility simulation

Simulation No.	Condition change	Oxygen solubility change , %
1	Initial conditions	100%
2	Aeration diffusers submerging depth h=5m	106.98%
3	Aeration diffusers submerging depth h=6m	113.95%
4	Wastewater temperature Θ=+15˚C	102.11%
5	Wastewater temperature Θ=+20˚C	91.50%
6	Atmospheric pressure p_g=100.725 kPa	90.92%
7	Atmospheric pressure p_g=100.225 kPa	90.35%
8	Oxygen proportion in air r_{O_2}=0.1997	86.04%
9	Oxygen proportion in air r_{O_2}=0.1897	81.73%
10	Increase in wastewater salinity by +100% (peak load)	78.31%

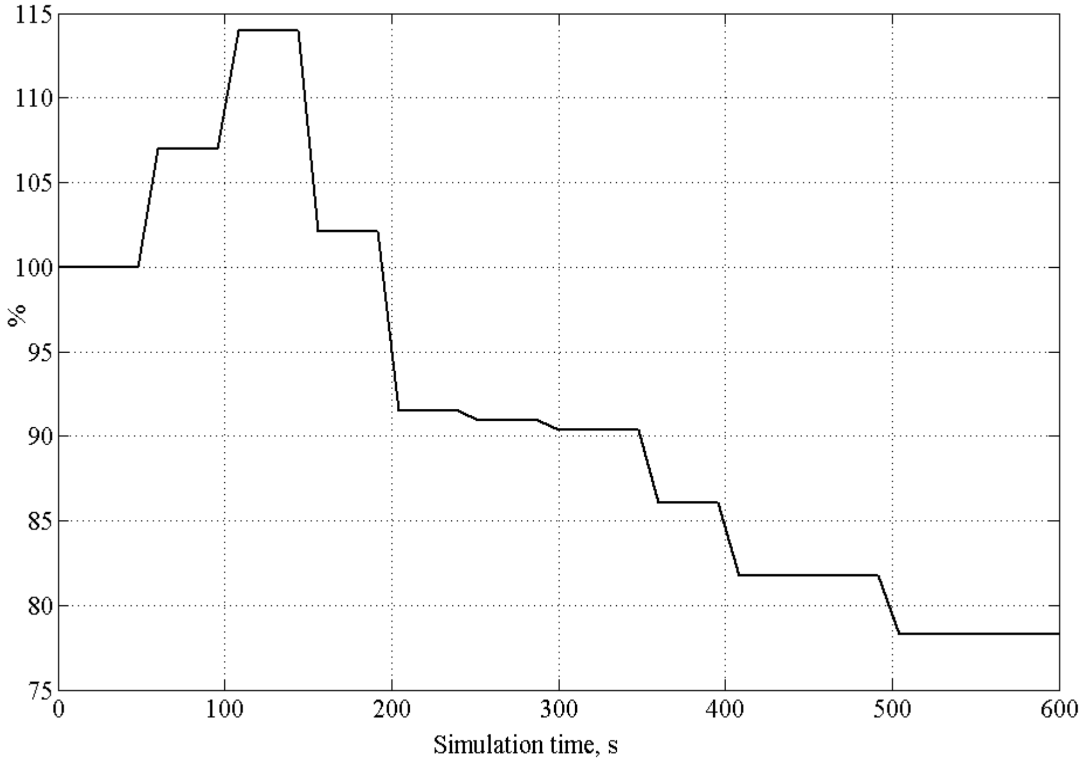

Fig.2 The graph of oxygen solubility simulation results

2. aeration diffusers submerging depth change – depth increase by additional 1 m;
3. wastewater temperature increase by +5˚, Θ=+15˚C, (*CP);*
4. wastewater temperature increase by additional +5˚, Θ=+20˚C, (*CP);*
5. atmospheric pressure decrease by –0.5 kPa (p_g=100.725 kPa);
6. atmospheric pressure decrease by additional –0.5 kPa (p_g=100.225 kPa);
7. oxygen proportion in air decreases by 0.01 (r_{O_2}=0.1997);
8. oxygen proportion in air decreases by aditional 0.01 (r_{O_2}=0.1897);
9. increase in wastewater salinity by +100% (peak load).

Simulation results are presented in Table 1 and Fig. 2.

Conclusions

The analytic expression developed by the authors includes all the important variables influencing oxygen solubility in water. It can be used for the development and design of wastewater aeration control systems.

The virtual model of oxygen solubility developed in Mathlab `Simulink`environment can be used to evaluate the influence of the external factors.

Simulation of the analytic expression shows that different factors differently influence the oxygen solubility – increase in the temperature and salinity is decreasing the solubility, at the same time increase in aeration diffusers submerging depth, atmospheric pressure and oxygen proportion are increasing oxygen solubility.

The analytical model of oxygen solubility in water can be used in wastewater treatment plants in order to develop an improved control system for the aeartion system, which could decrease overall energy consumption of the WWTS.

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