

MATHEMATICAL SIMULATION OF AERATION AND DIFFUSION PROCESSES IN THE AIR-WATER INTERFACE

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Abstract. This paper deals with problem of water aeration. Water aeration is important factor that influences process of open water self-purification. Aeration first of all depends on purely physical diffusion process taking place in the interface between air and water. Specific of the character of these processes was discussed. Also attention was paid to the features and behavior of air and water bubbles created in the falling water turbulence flow. The final goal of this paper was to describe these processes mathematically. Mathematical simulation kinetic equations describing air and water bubbles adsorption and desorption processes were proposed. The results show good coincidence with experimental data obtained by independent researchers.

Keywords: aeration simulation, solar radiation, interface, air-water, diffusion, algae.

1. Introduction

The processes taking place in the air-water interface are important from many points of view and first of all from point of view of environmental engineering including physical, chemical and mechanical investigation. Among these processes open water self purification process takes important role. Human activity highly influences natural processes. With the continuous extension of manufacturing activities, the anthropogenic factor exerts an increasing impact on global environment, including both air and water pollution. The challenge we face is to evaluate and determine the maximal anthropogenic stress that the environment, i.e. water and atmosphere, can still be subjected to the level it can resist through self-purification (Vaideliene 2007a). Such an objective can't be achieved without investigation of the pure physical processes, which take place in interfaces between open water and atmosphere as well as between separate deep water layers. Both interfaces are of significant importance for the water quality of open water bodies. Usually those interfaces are considered separately one from another. Some researchers (Gulliver 1990; Higbie 1935; Danckwerts 1951; Donelan 2002; Yeghiazarian *et al.* 2009; McNeil 2004; Kim 1999; Perez-Buerto *et al.* 2000; Yang 2007) specify that physical processes at the open water-air interfaces are stronger determinants of water quality than those taking place in deep water. Therefore the consideration of the present paper is focused on the open water-air interface. The abovementioned physical phenomena are fully determined by diffusion-based proc-

esses such as aeration and reaeration or evaporation and adsorption processes (Picard and Davoust 2006; Margaret 2004; Zuev *et al.* 2001; Koval *et al.* 2006; Gulbiniene *et al.* 2008; Li *et al.* 2009; Berthier and Davoust 2003; Davoust and Picard 2005). Moreover, those processes can be regarded as separate cases of diffusion itself, where the character of processes rate is determined by ambient properties and their boundary conditions. Investigation and evaluation of those properties and boundaries conditions in various specific cases obviously is a pure physical problem. Only under investigation of this problem related to diffusion process and its mathematical description can be achieved the right solution. Determined significant dependences between the processes parameters allow to simulate the process mathematically and give practically useful tool for environmental engineering.

All physical processes taking place in the air-water interface are influenced by many factors. One of these factors is solar radiation. It can be treated as part of total cumulative radiation because the open water surface usually is affected not only with direct solar radiation but also with energy of atmospheric scattered solar radiation and both medians, air and water, own radiation. Part of direct solar radiation reflects from the interface (Perez-Buerto 2000), the other part refracts and penetrates into the water where it is absorbed. The amount of reflected and refracted radiations depends on both – water and atmosphere properties such as color (Rajvanski 1981), surface roughness, nebulosity, depth, etc. Different components of solar radiation spectrum differently affect struc-

ture and state of mediums on both sides of air-water interface. The radiation of short waves stimulates growth of algae and increase dissolved oxygen in water (Donelan and Wanninkhof 2002; Yeghiazarian *et al.* 2009; McNeil and Stuart 2004; Perez-Buerto *et al.* 2000). Long waves' solar radiation heats water and changes thermal conditions of diffusion process.

Second of the most important factors making influence on diffusion processes is mass transfer over the weirs and through the hydropower plants turbines. This process should be regarded as a common natural physical phenomenon like it is common for mass transfer through the air-water interface in natural water reservoirs (lakes and dams) and streams (rivers). Exclusive feature of water falling from weirs or forcing through hydropower plants turbines is so cold "white water" phenomenon. This water consists of air and water bubbles mixed together in the water surface. Both these factors stimulate oxygen diffusion into water.

The goal of this paper is to determine weirs or hydropower plants and solar radiation influence on oxygen diffusion processes taking place in open water reservoirs' air-water interface and develop mathematical model describing these processes with evaluation of solar radiation influence.

2. Material and methods

2.1. Solar radiation interaction with material in the air-water interface

Water surface and deeper layers of open water reservoirs are affected by biological, physical, chemical, gas convection, evaporation and condensation processes. Usually these processes were treated as processes not affected by solar radiation. Many authors (Zuev *et al.* 2001; Kowal *et al.* 2006; Berthier and Davoust 2003; Davoust and Picard 2005; Vaidelienė *et al.* 2009; Tsoukala and Moutzouris 2008) investigating diffusion processes in air-water interface neglect influence of solar radiation.

However, oxygen and pollutants diffusion processes are highly dependent on solar radiation influence. Some physical processes taking place in the air-water interface also in the deeper water layers are described mathematically (Susilowati *et al.* 2004; Obernosterer *et al.* 2008), but without evaluating solar radiation influence. The idea of this paper is to estimate this influence.

As can be seen from figure 1 diagram, all processes taken place in the air-water interface according to chosen approach of investigation can be divided into two types of processes: non-radiation mass transfer processes and processes affected by solar radiation. We focus our work on the second type of processes.

First of all there is a sense of total solar radiation to divide into short waves (visible and ultraviolet range) and long waves (infrared range) spectra (Sedlar 2009). Both spectra partly reflect from the air-water interface and partly refract into water according to Snell's law, therefore only part of total incident energy penetrates into water and interacts with it.

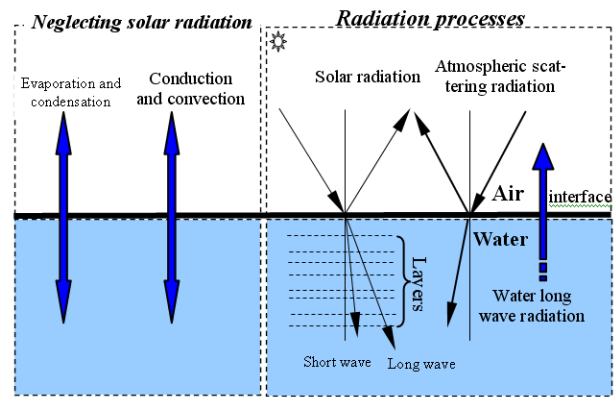


Fig 1. Schematic diagram of processes in air-water interface

Reflected and refracted energy depends on many factors: intensity of solar radiation, radiation beam incident angle (Morel 1991), chemical composition, depth of water, velocity of wind, year season, daily hour, etc (Picard and Davoust 2006; Hutson and Hauger 2002). We separated water's under layer into small layers which refractive index and properties can be treated as being uniform (Fig1).

Total flux of solar radiation incident upon water surface can be written as:

$$R = R_{direct} + R_{difus} + Q_{short}^{in} - Q_{short}^{out} + Q_{long}^{in} - Q_{long}^{out}, \quad (1)$$

where R_{direct} – direct solar radiation, R_{difus} – diffusive solar radiation, $Q_{short}^{in}, Q_{short}^{out}$ – incoming and outgoing short wave radiation fluxes; $Q_{long}^{in}, Q_{long}^{out}$ – incoming and outgoing long wave radiation fluxes.

Incoming short wave radiation activity depends on sun declination angle, solar constant, day time and latitude of location. Clouds distribute part of solar radiation and absorb the other part (Wang and Yee 2009). At some sky clouds reflect and absorb 65% of solar radiation. Ultraviolet and visible wave's range with wave length from 300 nm to 780 nm penetrates into water. Intensity of penetrated light changes according to Lambert-Beer law:

$$I_z = I_0 e^{-kz}, \quad (2)$$

where I_z – intensity of solar light, z – depth of the water, I_0 – intensity, when $z = 0$, k – attenuation constant (about 0,15 in the clear water). Solar short wave radiation activates photosynthesis reaction below air-water interface.

Above mentioned wavelength's range has enough energy to stimulate growth of algae, therefore usually it is named as a photo synthetically active radiation. Light's attenuation with its going through layers as well as nutrients and temperature (Meier *et al.* 2003) highly influences growth of algae. Light's parameters (intensity and wave length range) determine not only rate of algae growth but also its species.

Vertical wave's spectral distribution and its attenuation are related to absorption processes because photosynthetic biota, suspended particles and dissolved compounds change layer's properties.

2.2. Algae grow influence on diffusion process

Exclusive role in the diffusion processes plays algae. Algae being biologically active material interact with short waves' solar radiation and determine oxygen and dioxide diffusion process (Vaidelienė and Mihailov 2008; Vaidelienė, 2007; Vaidelienė *et al.* 2008) run and its results.

The algae's place in the sequence of oxygen/dioxide diffusion into water processes influenced by solar radiation can be seen from figure 2.

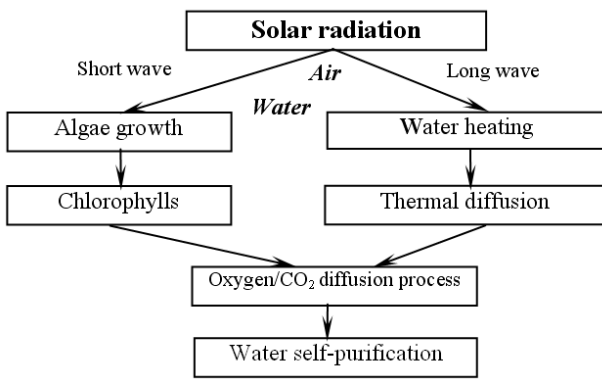
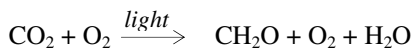


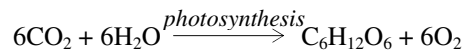
Fig 2. Sequence of oxygen/dioxide diffusion into water processes influenced by solar radiation

Algae situated in the open water reservoirs take part in process of photosynthesis (O'Connor *et al.* 1983; Martin *et al.* 2003; Vrugt *et al.* 2003; Vaidelienė 2007; Pelletier and Chapra 2006). Like all plants having chlorophyll due to solar radiation algae produces oxygen:

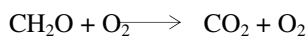


were CH_2O – new cells,

or



Process of photosynthesis depends on solar radiation, therefore photosynthesis presents only at light time. In cases of not sufficient light and at nighttime, algae use oxygen for reactions of catabolism (for respiration):



Concentration of oxygen (O_2) dissolved in water decreases and concentration of dioxide (CO_2) increases. In this case process of absorption and desorption in one water layer influence processes in adjacent layers.

Diffusion, taking place due to photosynthesis and algae respiration, can be described with these equations:

$$\left\{ \begin{array}{l} \frac{\partial C_{O_2}^{(1)}}{\partial t} = \chi_{12} C_{O_2}^{(1)} - \chi_{21} C_{CO_2}^{(1)} - w_{12} C_{O_2}^{(1)} + v_s C_{CO_2}^{(2)} \\ \frac{\partial C_{CO_2}^{(1)}}{\partial t} = \chi_{21} C_{CO_2}^{(1)} - \chi_{12} C_{O_2}^{(1)} - w_{21} C_{CO_2}^{(1)} + v_s C_{O_2}^{(2)} \\ \frac{\partial C_{O_2}}{\partial t} = D^* \frac{\partial^2 C_{O_2}}{\partial z^2} + v_x \frac{\partial C_{O_2}}{\partial z} \\ \frac{\partial C_{CO_2}}{\partial t} = D^* \frac{\partial^2 C_{CO_2}}{\partial z^2} + v_x \frac{\partial C_{CO_2}}{\partial z} \end{array} \right. \quad (3)$$

where C_{CO_2} – concentration of CO_2 , C_{O_2} – concentration of dissolved oxygen, t – time. $\chi_{12} = \alpha_{12} i_{O_2}$; $\chi_{21} = \alpha_{21} i_{CO_2}$. Coefficients α_{12} and α_{21} are O_2 and CO_2 absorption sticking to the surface coefficients respectively, which range from 0 to 1, i_{O_2} – oxygen flux produced by photosynthesis, i_{CO_2} – CO_2 flux produced by respiration by algae, w_{12} – desorption rate of O_2 particles $w_{12} = (1 - \alpha_{12}) i_{H_2O}$ $w_{21} = (1 - \alpha_{21}) i_{air}$ – desorption rate of CO_2 particles. v_s – desorption rate of all particles. $v_s = w_{21} C_{CO_2}^{(1)} + w_{12} C_{O_2}^{(1)}$, $v_x = \chi_{12} C_{H_2O} + \chi_{21} C_{air}$, D^* – diffusion coefficient.

2.3. Structural development of air and water dynamic mixing under conditions of falling water

After wears the water has falling stream or jet shape. As known, under these conditions the local (singular) aeration is taking place and the air bubbles are entrained into the water due to jet impact to the water pool or a stream. It results in air-water bubbles mixing near air-water interface (Fig3).

1978 McKeogh first proved that jet's conditions at moment of air entrainment can be described as a function of jet's turbulence (McKeogh 1978). For the certain profile of falling jet, the initial velocity of air entrainment increases with decreasing turbulence of jet (Vaidelienė *et al.* 2009).

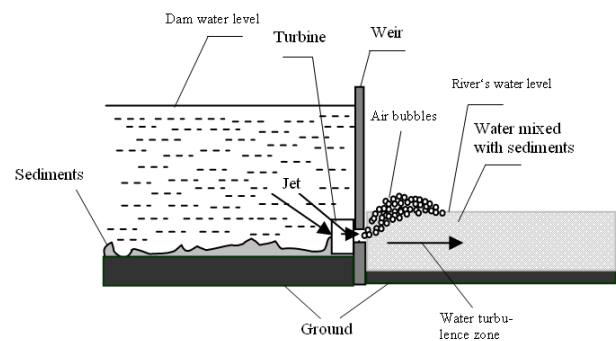


Fig 3. Air and water bubbles mixing below hydropower turbine

Turbulent air bubbles diffusion appears under falling down jet conditions. This process also is known as advective diffusion (Gonzalez and Chanson 2008), (Kucukali, Chanson 2008), (Van Der Geld and Kuerten 2009), (Luu Li-Hua and Forterre 2009). This term denotes the movement of air bubbles from domains with higher spatial gas concentration to domains with lower concentration. The mixing of bubbles stimulates this process.

2.4. Equations of air bubbles diffusion in the open channel

As known, the supercritical flows induce a visual impression of “white water”. Such flows appear in the channels where the turbulence is sufficient for air bubbles entraining into the flow.

As it is shown in Fig 4 two fluxes come from air-water interface to the water surface: water droplets flux and air bubbles flux. The following expressions of kinetic equations we suggest as suitable for use in this case:

$$\left\{ \begin{array}{l} \frac{\partial C_{H_2O}}{\partial t} = \chi_{12} C_{H_2O} - \chi_{21} C_{air} \\ \frac{\partial C_{air}}{\partial t} = -\chi_{12} C_{air} + \chi_{21} C_{H_2O} \end{array} \right. \quad (4)$$

where C_{H_2O} – concentration of water droplets, C_{air} – concentration of air bubbles, t – time. χ_{12} and χ_{21} are adsorption rates of water droplets and air bubbles, respectively, which are expressed as $\chi_{12} = \alpha_{12} i_{H_2O}$, $\chi_{21} = \alpha_{21} i_{air}$, where α_{12} and α_{21} are sticking coefficients of water droplets and air bubbles to the surface respectively, which range from 0 to 1 and i_{H_2O} and i_{air} are the relative fluxes of water droplets and air bubbles to the surface, respectively.

Solution of differential equations (4), gives the following dependences:

$$\left. \begin{array}{l} C_{H_2O} = \frac{\chi_{12} + \chi_{21} e^{-(\chi_{12} + \chi_{21})t}}{\chi_{12} + \chi_{21}} C_{H_2O}(0) - \frac{\chi_{12} (e^{-(\chi_{12} + \chi_{21})t} - 1)}{\chi_{12} + \chi_{21}} C_{air}(0) \\ C_{air} = -\frac{\chi_{21} (e^{-(\chi_{12} + \chi_{21})t} - 1)}{\chi_{12} + \chi_{21}} C_{H_2O}(0) + \frac{\chi_{21} + \chi_{12} e^{-(\chi_{12} + \chi_{21})t}}{\chi_{12} + \chi_{21}} C_{air}(0) \end{array} \right\} \quad (5)$$

During adsorption process upper layer gets in contact with air and concentration of air and water bubbles changes. Character of this change describes proposed equations (4). However in eq. (4) the process of water droplets removal from the surface is not involved. Evaluating desorption process the eq. (4) takes the following form:

$$\left\{ \begin{array}{l} \frac{\partial C_{H_2O}^{(1)}}{\partial t} = -w_{12} C_{H_2O}^{(1)} + v_D C_{H_2O}^{(2)} + \chi_{12} C_{H_2O}^{(1)} - \chi_{21} C_{air}^{(1)} \\ \frac{\partial C_{air}^{(1)}}{\partial t} = -w_{21} C_{air}^{(1)} + v_D C_{air}^{(2)} + \chi_{21} C_{air}^{(1)} - \chi_{12} C_{H_2O}^{(1)} \end{array} \right. \quad (6)$$

Where $C_{H_2O,air}^{(1)}$ and $C_{H_2O,air}^{(2)}$ are relative concentrations in first and second monolayer; w_{12} and w_{21} are desorption rates of water droplets and air bubbles, respectively; v_D is the total desorption rate expressed as: $v_D = w_{21} C_{air}^{(1)} + w_{21} C_{H_2O}^{(1)}$.

Two first components of equation (6) describe removal rate of air or water bubbles from the surface monolayer and next two components describe entrapment (adsorption) rate of air or water bubbles. Terms with sign minus give the removal rate of air/water bubbles from the surface monolayer and the terms with sign plus give the entrainment rate of air/water bubbles into the surface monolayer as a result of the entrapment of relocated bubbles and as a result of the arrival of air/water bubbles from the next monolayer.

The monolayer approach of dynamic mixing process was taken. It expresses eq. (6). To solve this equation the variations of surface concentration in second layer must be known. Because of continuous adsorption and desorption the mixing of water and air bubbles between layers takes places. In case when due to entrainment (adsorption) and removal (desorption) air and water particles move from K layer to $K - 1$ or $K + 1$ this concentration rate can be expressed in this way:

$$\left\{ \begin{array}{l} \frac{\partial C_{H_2O}^{(K)}}{\partial t} = v_D (C_{H_2O}^{(K+1)} - C_{H_2O}^{(K)}) + v_A (C_{H_2O}^{(K-1)} - C_{H_2O}^{(K)}) \\ \frac{\partial C_{air}^{(K)}}{\partial t} = v_D (C_{air}^{(K+1)} - C_{air}^{(K)}) + v_A (C_{air}^{(K-1)} - C_{air}^{(K)}) \\ K \geq 2 \end{array} \right. \quad (7)$$

where v_A is the total adsorption rate expressed as: $v_A = \chi_{12} C_{H_2O} + \chi_{21} C_{air}$.

It can be shown that eq. (7) have the form of diffusion equation with moving boundary. After simple mathematical rearrangements eq. (7) can be converted into the following form:

$$\left\{ \begin{array}{l} \frac{\partial C_{air}}{\partial t} = D^* \frac{\partial^2 C_{air}}{\partial x^2} + v_x \frac{\partial C_{air}}{\partial x} \\ \frac{\partial C_{H_2O}}{\partial t} = D^* \frac{\partial^2 C_{H_2O}}{\partial x^2} + v_x \frac{\partial C_{H_2O}}{\partial x} \end{array} \right. \quad (8)$$

where D^* – effective diffusion coefficient, expressed as $D^* = (v_R + v_E) h_0^2$, h_0 – thickness of separate monolayer, surface movement velocity $v_x = h_0 (v_R - v_E)$.

Bubbles exchange between air and water usually takes place in the upper layers. In the case which we investigated the element composition of air and water bubbles was changeable also in lower layers.

3. Results and discussions

Solar radiation can't be neglected has meaning in territories where amount of solar radiation is enough intensive during a year. Let's take a look at solar radiation situation in Lithuania. The information about amounts of solar radiation energy we took from measurements performed by Kaunas and Šilutė meteorological stations. These stations measure direct and scattered solar radiation that reaches horizontal surface of the Earth. Sum of direct and diffusive (scattered) energies compose total solar radiation energy. Scattered energy expressed by percents of direct radiation dependence on solar high over horizon is given in table 1.

Table 1. Diffusive radiation as a percentage part of direct solar radiation as a function of sun height over horizon

Solar height	%I _{solar}	Solar height	%I _{solar}
5	148	50	17,24
10	75,5	55	16,02
15	51,3	60	14,93
20	39,16	65	13,99
25	31,89	70	13,19
30	27,04	75	12,50
35	23,58	80	11,89
40	20,98	85	11,36
45	18,96	90	10,89

Except of diffusive radiation the value of reflected radiation, must be evaluated calculating total radiation that interacts with air and water. Amount of reflected energy depends on properties of water surface: color, roughness, depth, amount of algae on the surface of water. Amount of reflected radiation energy, expressed by percents of direct radiation depicts curves given in figure 4.

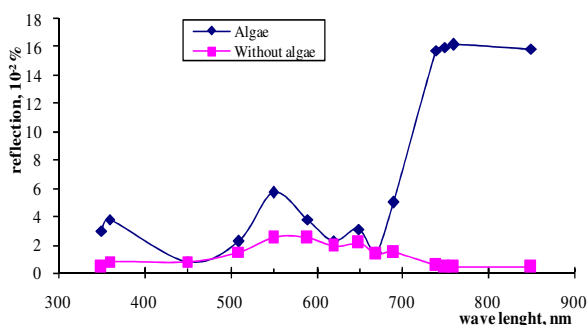


Fig 4. Solar radiation reflection from clear water surface and from surface with great amount of algae

As can be seen from run of curves (Fig 4) clear water surface reflects maximum only 2% of all solar radiation that interacts with water. Green color spectrum has greatest reflection. Water containing algae produce quite dif-

ferent reflection. As can be seen the highest reflection in this case has red color spectrum, which reaches even 16 percents.

Penetrated light usually is absorbed by water. Absorption depends on amount of algae and on its species. Green algae dominate in Lithuanians open water reservoirs, but brown algae presents also. Different algae have different kind of photosynthesis pigments (chlorophyll), which solar energy transforms into chemical energy. Green and brown algae have only so cold a-type chlorophyll pigment. Absorption spectrum of green and brown algae percentage dependence on visible light wave length is given in figure 5.

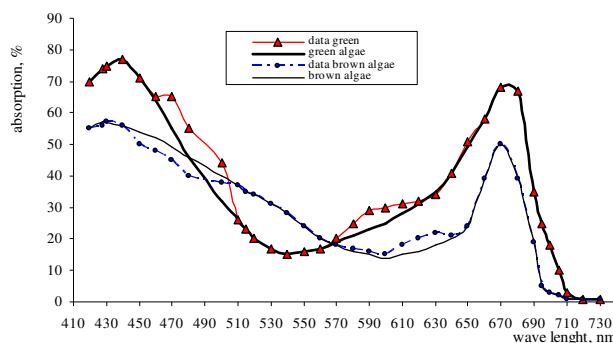


Fig 5. Absorption spectrum of green and brown algae percentage dependence on light wave length

As can be seen from in figure 5 shown light absorption by algae curve has two picks on blue (440 nm) and red (675 nm) color. Dependences were calculated using equations (3) and data of Lithuanians Environment Department measurements. As can be seen from figure 5 green algae have higher absorption as brown algae. Curves calculated according developed mathematical model and measured curves show good coincide.

Algae determine variation of O₂ and CO₂ concentration in the water. Depending on day time, light intensity, year season and temperature they produces O₂ or CO₂, which penetrates into water by diffusion.

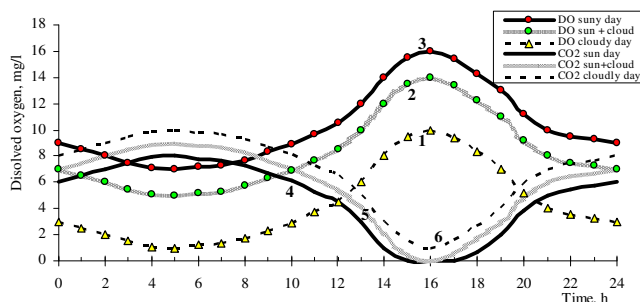


Fig 6. Simulated curves of O₂ and CO₂ concentration

For investigation were used Kaunas hydro plant dam data taken from. Data were received with mean value water temperature 20°C. For simulation were used equations (13). Curves 1, 2, 3 depict amount of dissolved oxygen in mg/l. Curve 1 shows amount of dissolved oxygen on cloudy day. In this case dissolved oxygen maximum concentration (mg/l) was reached at 16 o' clock mean-

while mg/l concentration's maximum was in the sunny day (Fig 6). Thus in the sunny day amount of dissolved oxygen was increased by 6 mg/l. This result can be explained with this fact that algae use oxygen for respiration and produce dioxide in nighttime. The minimal amount of oxygen in the water is at 5 o' clock. As can be seen from figure 6, solar radiation highly influences O₂ and CO₂ concentration in the water. CO₂ concentration variation should be investigated more properly because it has influence on global climate warming.

As figure (3) illustrates, air bubbles are entrained in to the water at the zone of falling water. Size and number of bubbles pooled in to water depends on wear high and on velocity of jet at the moment of jet hit at the surface of water. Jet hit to the water splashes small water bubbles, which mix with the air and makes mixed air-water layers. Air and water bubbles adsorption and desorption processes we simulated with equations (4). For simulation we used experimental data published by (Chanson and Brattberg 2000; Murzyn and Chanson 2009; Toombes and Chanson 2008). These authors obtained experimental data in artificial channel made special for their experiment. They determined concentration of air and water bubbles by means of conductivity measuring in different zones of channel with changing height of weir, flow velocity and horizontal distance from weir till bubbles zone (Fig 3). Determination of bubbles concentration was based on the feature, that conductivity in air burbles zone and in water bubbles zone differences at thousands times.

At the moment of interaction adsorption and desorption processes take place. This process we described with equation (4) and solution of this equation with equation (5). Fig 7 illustrates the solution equations calculated for different initial concentrations according (Chanson and Gonzalez 2005) (Fig 7). Range of initial water bubbles relative concentration we assumed as from 0,01 to 0,3 and air bubbles initial concentration from 0,7 to 0,99 (Fig 7).

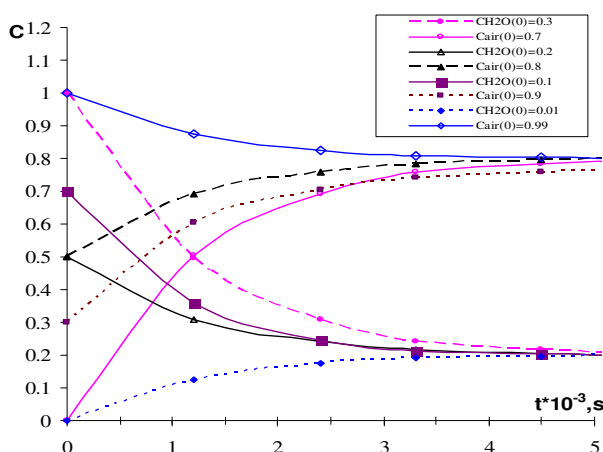


Fig 7. Air and water adsorption curves, with $\alpha_{12}=0.8$, and $\alpha_{21}=0.2$

As can be seen from figure 7, with water and air sticking to the surface probabilistic coefficients respec-

tively $\alpha_{12} = 0.8$ and $\alpha_{21} = 0.2$, air and water bubbles concentration dependence on time changes according exponential law. Asymptotes values of all curves are equal to probabilistic sticking coefficients. The shape of curves depends on initial concentration of air and water bubbles. The curves show sufficient accurate coincidence with experimental data measured by researchers (Chanson and Gonzalez 2005).

4. Conclusions

1. Among many others factors that influences diffusion processes in the open water boundary layers important role plays solar radiation.
2. Water turbulence also influences air bubbles and water droplets mixing, that can be described with diffusion equations.
3. The air bubbles created in the falling water flow stimulate processes of adsorption and desorption.
4. Mathematical simulation of diffusion processes taking place in air-water interface good coincide with dependences obtained from experimental data.
5. Character of solutions of proposed simulation equations developed for air and water bubbles adsorption and desorption processes depends on initial conditions.

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