

## OXIGEN DISPERSION MODELLING IN THE WATER TRANSPORT PIPES

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*În literatura de specialitate se întâlnesc multiple exemple de cazuri în care se contează pe dispersia și transferul de masă al unui gaz într-un lichid în regimul turbulent de curgere. Astfel, asemenea aplicații apar în procesele de oxigenare, ozonizare, clorinare în care se injectează un gaz direct în conducta de transport a masei apoase. Acest procedeu are ca rezultat reducerea costurilor de realizare a stațiilor de tratare și epurare a apelor uzate.*

*In literature we meet numerous examples in which the dispersion and mass transfer of gas into a liquid mass are two important coefficients. This applications appear in the oxygenation processes, ozonization, chlorination in which the gas is injected directly in the water transport pipe. This method has an important impact over reduction of design costs of waster water treatment plants.*

**Keywords:** concentration, dispersion, modelling, simulation

### Introduction

In nature and industry it does not exist, in true mean of the notion, homogeneous and isotropic fluid, only for pure water and some liquids with high purity from chemical industry.

The presence of different phases in fluid medium modifies its proprieties and it is hard to appreciate the boundaries inside of which the mechanics principles and laws are valid. The results obtained by the applications of mechanics laws of homogenous fluids, most of time, are not in concordance with the experimental reality due to dispersed substances in the fluid medium.

### 1. Theoretic models for the diffusion and dispersion of oxygen in water field.

The mass transfer phenomenon permits the general study of processes dynamic characteristics. Transfer processes can be mathematically modelled with idealized models.

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**Oxygen transfer from gas into water.** We consider a gas particle situated in water. Considering the liquid film theory, a thin layer,  $\delta$ , is formed at the gas - liquid interface. The molecular diffusion phenomenon takes place in this interface. The process is developed at small speed.

For smaller values of the ratio between air particle beam thickness,  $\delta$ , and the oxygen concentration flux in normal direction at the contact surface between air particle volume and water phase, the relation is:

$$q_m = D\mu \left( -\frac{dC}{dx} \right) \quad (1)$$

where:  $-dC/dx$  is the concentration gradient after the normal direction at water-air separation surface.

The transfer equation for the mass transfer in permanent flow, without chemical reaction between the constituents and unidirectional flow, becomes:

$$\frac{d}{dx} \left[ -D_\mu \frac{dC}{dx} \right] = 0 \quad (2)$$

for  $x = 0$ ;  $C = C_s$  and  $x = \delta$ ,  $C = C$ , boundaries conditions.

$$\xrightarrow{\int} q_m = \frac{D_\mu}{\delta} (C_s - C) \quad (3)$$

If we consider the mass specific flux:

$$q_m = K_L (C_s - C) \quad (4)$$

then the mass transfer coefficient is:

$$K_L = \frac{D_\mu}{\delta} \quad (5)$$

This mass transfer coefficient expression corresponds to double fluid model in gas-lift installation.

If diffusion coefficient is constant, the mass transfer equation becomes:

$$D_\mu \frac{d^2 C}{dx^2} - kC = 0 \quad (6)$$

The plug flow model with axial dispersion is the theoretical model applied in our study.

For the non-ideal situation we determined the experimental characteristics of reactor hydraulics and mixing conditions. For the exemplification we consider the plug flow longitudinal dispersion model. In this case the reacting substances are mixed in the longitudinal direction due to the gradient concentrations, dispersion and turbulent diffusion. The flow concentration along  $Ox$  axis, is:

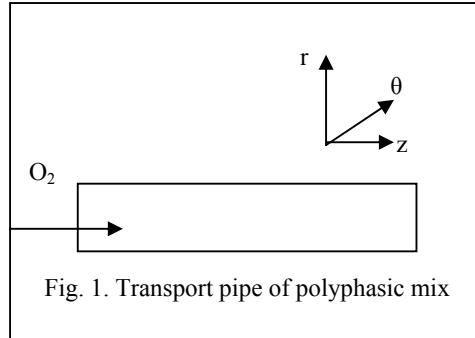
$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} = D_d \frac{\partial^2 C}{\partial x^2} + r(C) \quad (7)$$

in which  $u$  is the longitudinal water speed,  $D_d$  is the axial dispersion coefficient given by  $D_d = D_\mu + \varepsilon_d$ , where  $\varepsilon_d$  is the turbulent dispersion coefficient determined experimentally for each case.

The plug flow model is applied in oxygenation equipments, in the ozonation pipe installations, for water oxygenation at medium and deep injection, in wastewater processes (chlorination, flocculation etc).

## 2. Mathematical modelling

We consider a circular pipe through which a homogeneous fluid (clean water) flows. We will study the oxygen mass transfer from gas into liquid along the transport pipe. The boundary conditions at constituents phases interface must respect the conservative and continuity principles.



We watch the oxygen transferred variation from gas into water along the transports pipe.

We consider the mass transfer equation in cylindrical coordinates:

$$\frac{\partial C}{\partial t} + v_r \frac{\partial C}{\partial r} + v_\theta \frac{\partial C}{\partial \theta} + v_z \frac{\partial C}{\partial z} = D \left[ \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial C}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 C}{\partial \theta^2} + \frac{\partial^2 C}{\partial z^2} \right] + S_r \quad (8)$$

In the following hypothesis:

- Unidirectional flow  $- v_z \neq 0, v_\theta = v_r = 0$ ;
- Flow permanent regime  $- \frac{\partial \vec{v}}{\partial t} = 0$ ;
- Stationary regime  $- \frac{\partial C}{\partial t} = 0$ ;
- Constant diffusion coefficient;
- The concentration variation  $C$  with  $\theta$  is neglected (the pipe diameter is much smaller than its length), and
- Axial symmetric movement.

Equation (8) is completed with the movement equation in cylindrical coordinates, equation Navier - Stokes:

$$\frac{\partial v_r}{\partial t} + v_r \frac{\partial v_r}{\partial r} + \frac{v_\theta}{r} \frac{\partial v_r}{\partial \theta} - \frac{v_\theta^2}{r} + v_z \frac{\partial v_r}{\partial z} = -\frac{1}{\rho} \frac{\partial p}{\partial r} + \nu \left[ \frac{\partial}{\partial r} \left( \frac{1}{r} \frac{\partial}{\partial r} (r v_r) \right) + \frac{1}{r^2} \frac{\partial^2 v_r}{\partial \theta^2} - \frac{2}{r^2} \frac{\partial v_\theta}{\partial \theta} + \frac{\partial^2 v_r}{\partial z^2} \right] + g_r \quad (9)$$

$$\frac{\partial v_\theta}{\partial t} + v_r \frac{\partial v_\theta}{\partial r} + \frac{v_\theta}{r} \frac{\partial v_\theta}{\partial \theta} + \frac{v_r v_\theta}{r} + v_z \frac{\partial v_\theta}{\partial z} = -\frac{1}{\rho r} \frac{\partial p}{\partial \theta} + \nu \left[ \frac{\partial}{\partial r} \left( \frac{1}{r} \frac{\partial}{\partial r} (r v_\theta) \right) + \frac{1}{r^2} \frac{\partial^2 v_\theta}{\partial \theta^2} + \frac{2}{r^2} \frac{\partial v_r}{\partial \theta} + \frac{\partial^2 v_\theta}{\partial z^2} \right] + g_\theta \quad (10)$$

$$\frac{\partial v_z}{\partial t} + v_r \frac{\partial v_z}{\partial r} + \frac{v_\theta}{r} \frac{\partial v_z}{\partial \theta} + v_z \frac{\partial v_z}{\partial z} = -\frac{1}{\rho} \frac{\partial p}{\partial z} + \nu \left[ \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial v_z}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 v_z}{\partial \theta^2} + \frac{\partial^2 v_z}{\partial z^2} \right] + g_z \quad (11)$$

in witch:

$\rho$  – the density of newtonian fluid, constant;

$\nu$  – viscosity of newtonian fluid, constant;

$p$  – pressure;

$v_r, v_\theta, v_z$  – the speed components along  $r, \theta, z$ ;

$g_r, g_\theta, g_z$  – the mass force along  $r, \theta, z$ .

Tacking in consideration the flow phenomenon and introducing the gas in the system the diffusion equation is completed with additional terms witch show the intensity of the source.

The mass source intensity is function of divers parameters such as substance concentration, hydrodynamic flow conditions, temperature etc.

In a first approximation we neglect the source  $S_r$   
 $C$  – oxygen concentration, [mgO<sub>2</sub>/l]

$$v_r \frac{\partial C}{\partial z} = D \frac{\partial^2 C}{\partial z^2} \quad (12)$$

From analytical integration;

$$\Rightarrow v_z C = D \frac{\partial C}{\partial z} + k \Rightarrow \quad (13)$$

I.  $k=0$ :

$$v_z C = D \frac{\partial C}{\partial z} \Rightarrow \frac{v_z}{D} dz = \frac{dC}{C} \Rightarrow \ln \frac{C}{C_0} = \frac{v_z}{D} (z - z_0) \Rightarrow C = C_0 \exp \left[ \frac{v_z}{D} (z - z_0) \right] \quad (14)$$

II.  $k=ct \neq 0$

### 3. Numerical integration

Through numerical integration we obtain the distribution of oxygen concentration from air into water. The movement of macroscopic fluids mass realizes the convective transport/transfer of properties.

FlexPDE (A Flexible Solution System for Partial Differential Equations) program realised the numeric integration of equation.

We study four integration cases for different values of molecular diffusivity  $D$ , at the constant  $k$  ( $k=0$ ;  $k=k$ ;  $k=k*C$ ;  $k=k*C^2$ ) and at different lengths of the pipe.

In FlexPDE we modelled the oxygen dispersion equation in water mass into a circular pipe. In the pipe exists a turbulent flow:

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial r} + w \frac{\partial C}{\partial z} = D \left[ \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial C}{\partial r} \right) + \frac{\partial^2 C}{\partial z^2} \right] \quad (15)$$

The FlexPDE solutions for our hypothesis:

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TITLE      'unidirectional stationary diffusion along x axis, k=k' {the problem
           identification}
VARIABLES  {system variables}      c
           u
DEFINITIONS {parameter definitions}
           D=0.5 {axial dispersion coefficient}
           k=1.5
           a=10 {length of aerated basin}
           b=1 {depth of aeration basin}
           i=1
           hour=60*60
           day=hour*24
INITIAL VALUES c=0.9
               u=1
EQUATIONS   dt(c)+u*dy(c)=D*[dxx(c)+1/y*dy(y*dy(c))]+k
               u=i*(y/b)
BOUNDARIES  region 1
               start(0,0)
               value(c)=0.9 {Dirichlet condition}
               line to (a,0)
               line to (a,b)
               line to (0,b)

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natural(c)=0 {Neuman condition – the concentration flux is zero by
walls of aerated basin}
line to finish
TIME {if time dependent} 0 to 50*day by 10
MONITORS {show progress} for cycle=50
    contour(c) as "concentration"
    vector(u) as "flow velocity"
    contour(u) as "flow speed"
PLOTS {save result displays} for t=day by day to 10*day
    by 10*day to 50*day
    contour(c) as "concentration"
    contour(u) as "flow speed"
    contour(c) zoom(a/2,0,b,b) as „c”
END

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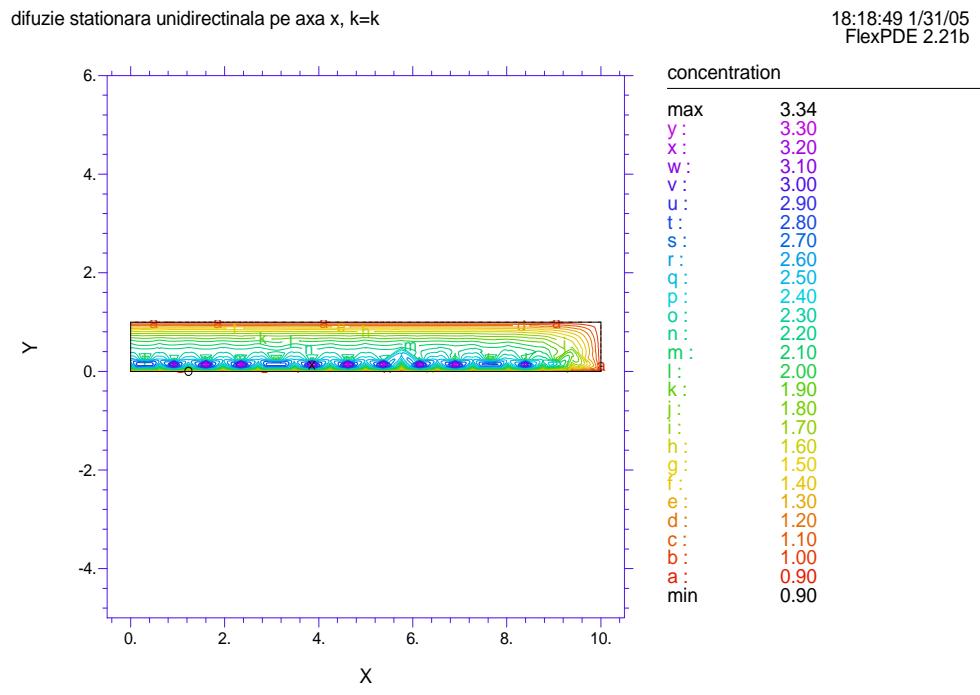


Fig. 2. Oxygen dispersion for  $k = k$

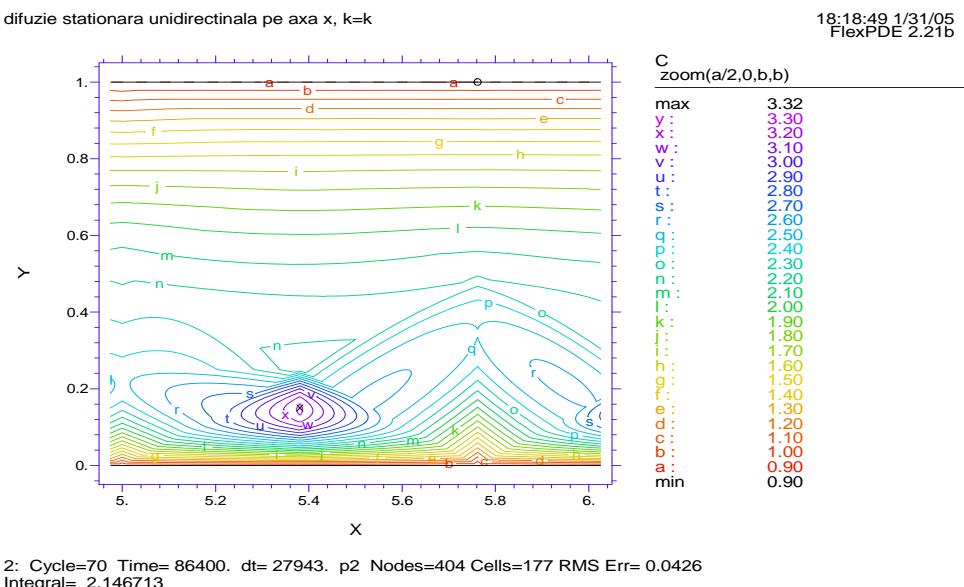


Fig. 3. Oxygen dispersion for  $k = k$  (zoom)

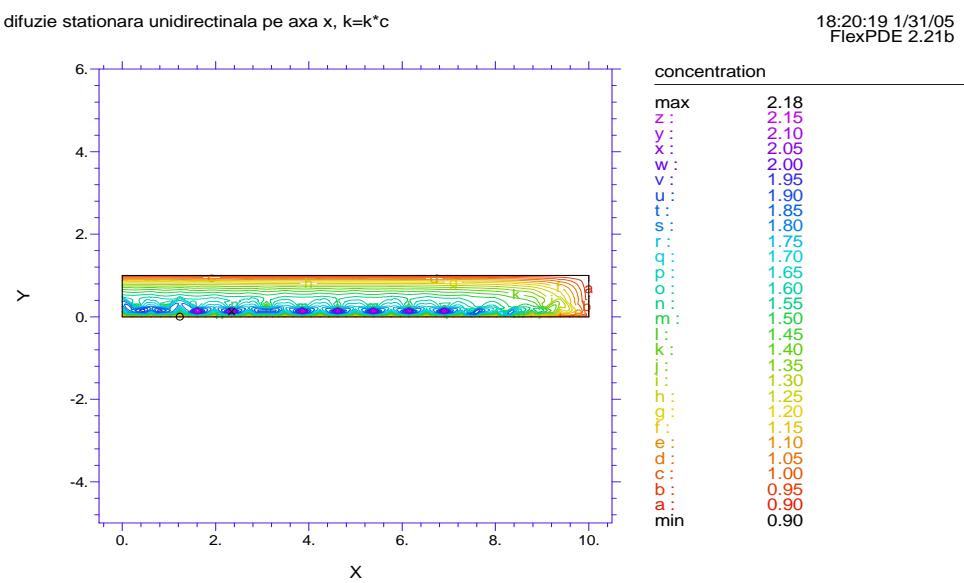


Fig. 4. Oxygen dispersion for  $k = k^*C$

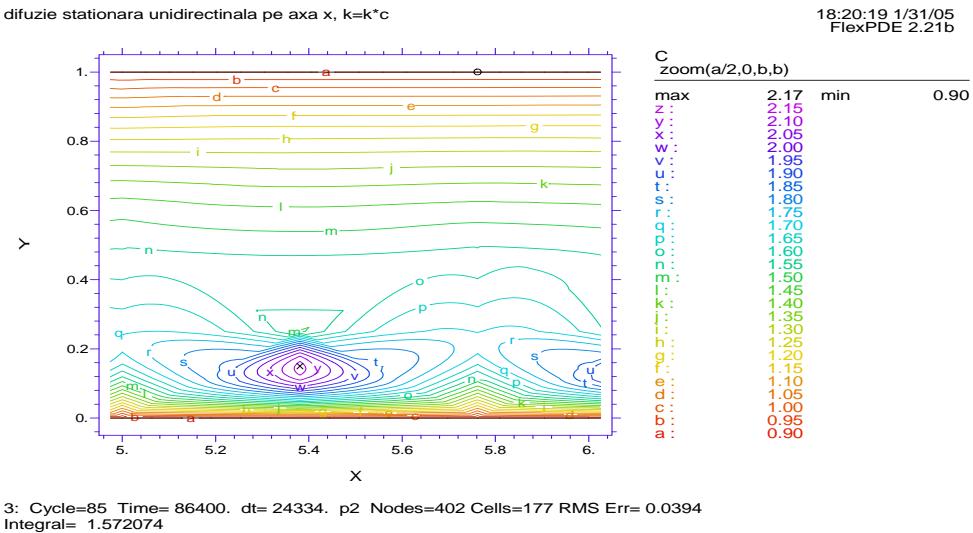


Fig. 5. Oxygen dispersion for  $k = k^*C$  (zoom)

## Conclusions

Due to the mass transfer process the dissolved oxygen concentration may vary in each point of the liquid domain. After the simulations we obtained errors for  $k = 0$  in all models due to the imposed modelling conditions. The flow speed varies between 0 ... 2 m/s, in all types of modelling approaches. The speed flow does not depend on injected oxygen concentration. For different lengths,  $a$ , the oxygen concentration varies with the constant,  $k$ , and the oxygen concentration maximum values is growing from  $k = k$  to  $k = k^*C^2$ . The maximum oxygen concentration, for the same value of  $k$ , does not have a constant evolution for different lengths. This method can be included in the biological treatment by the introduction of a biological element, such as active sludge. This method has been included for the oxygenation or ozonization directly into effluent transport pipes, before the wastewater enters in the treatment plant. This will reduce the exploitations costs, and treatment plant surface.

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