POLLUTANT DISPERSION MODELLING IN NATURAL STREAMS

Liviu Valentin BALANESCU[1], Catalina Raluca MOCANU[2], Dan ROBESCU[3]

The industrialization and urbanization has determined the disposal of different pollutant substances in different hydrographical basins. Designing a new mathematical model system for pollutant transport in aquatic medium and the evaluation of pollutants agents flood routing and estimation the impact over the environment and human health are strongly recommended. At international level exists a series of programmable software's, based on numerical simulation of experimental dates that can model the pollution effect over the environment. All this programs has been developed in unidirectional and bidirectional plans and they can not predict the real conditions of the pollutant wave. For mathematical modelling of pollutant propagation, event evolution prediction and environmental impact estimation are necessary a great number of informational instruments. The study of pollutants dispersion in the fluid medium has direct implications in the environmental rehabilitation.

Keywords: pollutant discharge, dispersion, mathematical modelling, numerical simulation, natural stream.

1. Introduction

In this paper authors propose a new approach in the study of pollutant dispersion near an accidental discharge point. The pollutant dispersion has been studied in ANSYS software in different discharge conditions. Mathematical models are frequently used for quantitative description. These have multiple input and output equations and model characteristics description.

The theoretical model will permit the numerical simulation of pollutant wave evolution in aquatic medium in receptor basin. After theoretic model calibration, this will be easily used to create a national informational system for water quality monitoring in agreement with European directives.

[1] Lect. PhD student, Police Academy "Alexandru Ioan Cuza" Fire Officers Faculty, Bucharest, Romania
[2] SR III PhD.Eng. ,Environment Equipments Department, National Research and Development Institute for Gas Turbines – COMOTI Bucharest, Romania
[3] Prof., Power Engineering Faculty, University "Politehnica" of Bucharest, Romania

2. Mathematical Equations for the pollutant dispersion

To create the mathematic model of pollutant dispersion into a natural stream the solutions fields of the two phases – water and pollutant – are consider identical. The volume and mass fraction are $y_2 = 0$. A single pressure field it is considering for the two phases of the biphasic model, ($_1$ for water and $_2$ for pollutant).

$$\overline{u_{i1}} = \overline{u_{i2}} = \overline{u_i} \tag{1}$$

$$k_1 = k_2 = k \tag{2}$$

$$\varepsilon_1 = \varepsilon_2 = \varepsilon \tag{3}$$

in which, u_i is the velocity along the stream flow, k is the turbulent kinetic energy and ε is the turbulent kinetic energy dissipation factor.

- ✓ **Continuity equations:**

$$\frac{\partial}{\partial t}(r_1\rho_{01}) + \frac{\partial}{\partial x_j}\left(r_1\rho_{01}\overline{u_j}\right) = 0 \tag{4}$$

$$\frac{\partial}{\partial t}(r_2\rho_{02}) + \frac{\partial}{\partial x_j}\left(r_2\rho_{02}\overline{u_j}\right) = 0 \tag{5}$$

r is the fluid volume fraction, ρ is the fluid density,

- ✓ **Quantity movement equations**

$$\begin{aligned}
&\frac{\partial}{\partial t}[(r_1\rho_{01} + r_2\rho_{02})\overline{U_i}] + \frac{\partial}{\partial x_j}[(r_1\rho_{01} + r_2\rho_{02})\overline{U_i}\,\overline{U_j}] = \\
&= -\frac{\partial \overline{P^{**}}}{\partial x_i} + \frac{\partial}{\partial x_j}\left[((r_1\mu_1 + r_2\mu_2) + (r_1\mu_{t1} + r_2\mu_{t2}))\left(\frac{\partial \overline{U_i}}{\partial x_j} + \frac{\partial \overline{U_j}}{\partial x_i}\right)\right] - \\
&- r_1\rho_{01}\beta_1\left(\overline{T} - T_{01}\right)g_i - r_2\rho_{02}\beta_2\left(\overline{T} - T_{02}\right)g_i + \\
&+ r_1\rho_{01}\alpha_1\left(\overline{Y_1} - Y_{01}\right)g_i + [(r_1\rho_{01} + r_2\rho_{02}) - \rho_0^*]g_i
\end{aligned} \tag{6}$$

In which

$$-\frac{\partial \overline{P^{**}}}{\partial x_i} = -\frac{\partial \overline{P}}{\partial x_i} + \rho_0^* g_i - \frac{2}{3}\frac{\partial}{\partial x_i}[(r_1\rho_{01} + r_2\rho_{02})k] \tag{7}$$

μ is the viscosity, μ_t is the turbulent viscosity, P^{**} is the average pressure, β is the coefficient for the thermal expansion, $\overline{T}$ is the average temperature, T_{0i} is the reference temperature (depends on ρ_{0i}), $\overline{Y_1}$ is the pollutant average mass fraction,

Y_{0i} is the reference mass fraction (depends on ρ_{0i}), ρ_0^* is the reference volume mass and g_i is the gravitational acceleration.

- ✓ **Mass fraction of the pollutant equation**

$$\frac{\partial}{\partial t}\left(r_1\rho_{01}\overline{Y_1}\right)+\frac{\partial}{\partial x_j}\left(r_1\rho_{01}\overline{Y_1}\overline{U_{j1}}\right)=\frac{\partial}{\partial x_j}\left(r_1(\Gamma_{Y1}+\frac{\mu_{t1}}{\sigma_Y})\frac{\partial\overline{Y_1}}{\partial x_j}\right)-r_1\overline{S\left(\overline{Y_1}+y_1\right)} \quad (8)$$

Γ_{Y1} is the coefficient for the turbulent mass diffusion, σ_Y is the turbulent Schmidt number, S is source and y is the turbulent fluctuation of the pollutant mass fraction.

- ✓ **Additional equation**

$$r_1+r_2=1 \quad (9)$$

- ✓ **$k\varepsilon$ model equations**

$$\mu_{t1}=C_\mu\rho_{01}\frac{k^2}{\varepsilon}\ ; \qquad \mu_{t2}=C_\mu\rho_{02}\frac{k^2}{\varepsilon} \quad (10)$$

C_μ – semi empiric coefficient (C_μ = 0,09)

$$\begin{aligned}&\frac{\partial}{\partial t}[(r_1\rho_{01}+r_2\rho_{02})k]+\frac{\partial}{\partial x_j}[(r_1\rho_{01}+r_2\rho_{02})k_1\overline{U_j}]=\\&=\frac{\partial}{\partial x_j}\left((r_1\frac{\mu_{t1}}{\sigma_k}+r_2\frac{\mu_{t2}}{\sigma_k})\frac{\partial k}{\partial x_j}\right)+\tilde{P}_1+\tilde{G}_1-(r_1\rho_{01}+r_2\rho_{02})\varepsilon\end{aligned} \quad (11)$$

$$\begin{aligned}&\frac{\partial}{\partial t}[(r_1\rho_{01}+r_2\rho_{02})\varepsilon]+\frac{\partial}{\partial x_j}[(r_1\rho_{01}+r_2\rho_{02})\varepsilon_1\overline{U_j}]=\\&=\frac{\partial}{\partial x_j}\left((r_1\frac{\mu_{t1}}{\sigma_\varepsilon}+r_2\frac{\mu_{t2}}{\sigma_\varepsilon})\frac{\partial\varepsilon}{\partial x_j}\right)+C_{1\varepsilon}\frac{\varepsilon}{k_1}(\tilde{P}+C_{3\varepsilon}\tilde{G})-C_{2\varepsilon}(r_1\rho_{01}+r_2\rho_{02})\frac{\varepsilon^2}{k}\end{aligned} \quad (12)$$

with:

$$\tilde{P}=[(r_1\mu_{t1}+r_2\mu_{t2})]\frac{\partial\overline{U_i}}{\partial x_j}\left(\frac{\partial\overline{U_i}}{\partial x_j}+\frac{\partial\overline{U_j}}{\partial x_i}\right) \quad (13)$$

$$\tilde{G}=[r_1\frac{\mu_{t1}}{\sigma_T}\beta_1+r_2\frac{\mu_{t2}}{\sigma_T}\beta_2]g_j\frac{\partial\overline{T}}{\partial x_j}-r_1\frac{\mu_{t1}}{\sigma_Y}\alpha_1 g_j\frac{\partial\overline{Y_1}}{\partial x_j} \quad (14)$$

In which: $\tilde{P}$ is the turbulent kinetic energy evolution factor due to the turbulence and average speed gradient interaction; C_μ = 0,09; σ_k = 1,0 ; σ_ε = 1,3 ; $C_{1\varepsilon}$ = 1,44; $C_{2\varepsilon}$ = 1,92; $C_{3\varepsilon}$ = 0. If r_1 = 1 (r_2 = 0) in water are present only the aqueous phase parameters and the above equations are solved for the aqueous phase flow. If r_2 = 1 the equation are solved for the pollutant flow only. All the equation can be written as a general convection – dispersion equation with the variable *Φ*:

$$\underbrace{\frac{\partial(\rho\Phi)}{\partial t}+\frac{\partial}{\partial x_j}\left(\rho\Phi\overline{U_j}\right)}_{1}=\underbrace{\frac{\partial}{\partial x_j}\left(\Gamma_\Phi\frac{\partial\Phi}{\partial x_j}\right)}_{2}+\underbrace{S_\Phi}_{3} \tag{15}$$

1– the Φ transport through convection;
2– the Φ transport through molecular diffusion and turbulent diffusion;
3–Φ production or destruction factor.

3. Numerical simulation of pollutants dispersion in natural streams

The above equations are solved with ANSYS software to show the pollutant dispersion in natural streams in different discharge conditions. The first step in model elaboration is the artificial construction of work domain. The model can be an integral or simplify representation of the pollution dispersion phenomena in natural streams.

Depending on the dispersion zone can be defining three distinct models:

- three-dimensional model, this model evaluates the pollutant transport in three directions (depth, sideways and length)
- bidimensional model, the depth dispersion is neglected
- unidimensional model, only the longitudinal dispersion is taken into account.

Fig. 1. The Danube section take into account for the ANSYS simulation of pollutant dispersion

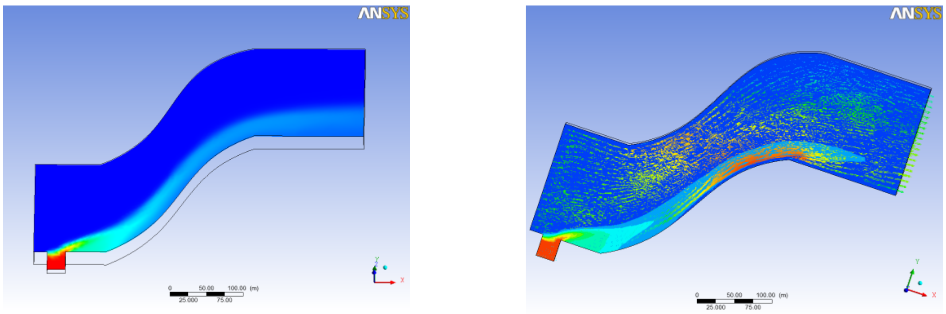

Fig. 2. The sideway pollutant injection. In these figure can be observe the pollutant evolution

along stream. The bank effect can be observed.

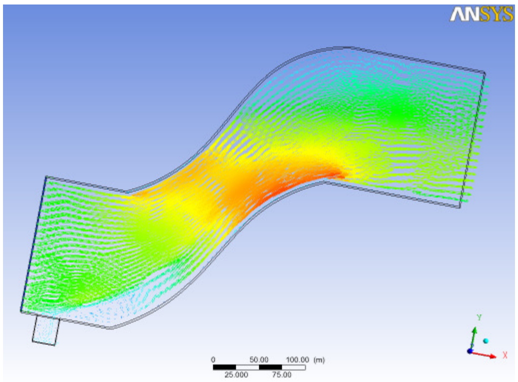

Fig. 3. The velocity stream lines in the work domain.

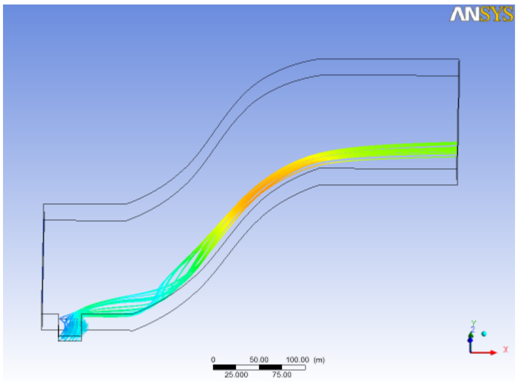

Fig. 4. The pollutant concentration along the work domain.

Fig. 5. The evolution of vectorial speed, density, pressure and pollutant concentration along the work domain.

In figure 5 can be observe that in sideway pollutant injection the parameters evolution is decreasing along the domain, due to river auto-epuration capacity.

6. Conclusions

In this paper the model permit to estimate the river distance that will be polluted in case of accidental pollutant discharge. The spatial and temporal evolution of a pollutant concentration into a natural stream can be observed. The mathematical models and the numerical simulations of pollutants discharge into natural streams offer the possibility to warn the local authorities about the effects of pollutants. The pollutants effects depend on the discharge quantity, discharge position (along the stream, sideway), weather and the ambient temperature.

After the numerical simulation in ANSYS software it was observed that on the distance of 1.5 – 2 kilometres the pollutants dispersion is 80%. The present model can be useful in evaluating the stream pollution or to predict the pollutants effects over aquatic flora and fauna. Predicting the pollutants effects an emergency situation management is realized.

R E F E R E N C E S

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