NUMERICAL SIMULATION OF POLLUTANTS DISPERSION PROCESSES IN DANUBE RIVER

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Abstract: Numerical simulation program FlexPDE achieved in this work possible to estimate the distance that the river will be polluted from the discharge of pollutants and assess the degree of pollution of the river section affected by wave. Basically it is possible to track the time and space of the concentration of pollutants, providing warning of possible effects they may have discharges of pollutants into the Danube, depending on the quantity of substances discharged, coordinates source pollution, rainfall and ambient temperature. As a result of numerical simulations carried out is apparent dispersion of the pollutant concentration, and because of self-purification capacity of the river Danube. The present model can be a useful tool for assessing pollution or pollution prediction could be done to manage situations that arise.

Key words: mathematical modeling, numerical simulations, pollutant dispersion.

Introduction

Using solid modeling computer interaction systems, fluid or gas began in the 80s of last century with the development of personal computer performance. This kind of modeling/simulation has been rightly called Computational Fluid Dynamics (CFD).

The most common CFD codes may be mentioned: FLOW3D, PHOENICS, ANSYS CFX, FIRE, FLUENT, Star CD, CF design, etc. Most codes of this kind are universal and used by engineers to analyze and solve a wide range of problems in industrial sector.

Stage objective is to create finite element for defining the physical process under investigation. Obviously, for creating finite element, develop 2D/3D geometry of the element investigated.

CFD modeling to improve the performance of a system can be divided into four basic steps (fig. 1).

![Fig. 1. Modeling steps CFD.](image)

The process of solving the set of equations can be lengthy depending on the complexity of the problem, the precision of calculation, etc. Calculation results are stored in a separate file or sent directly to post-processing module. Next will be numerically simulate the phenomenon of dispersion of pollutants in natural water courses. This operation is required to determine the environmental impact of an accidental or intentional discharge of a pollutant [1].

Mathematical modelling and numerical simulations

We will present results of numerical simulations carried out in the program Flex PDE – finite element method for solving the partial differential equations. Indicator values are based on BOD5 obtained by monitoring the Danube in 2004 (table 1) in 2 areas: at 375 km from the estuary (Chiciu - the Romanian bank, middle of the Bulgarian bank of the River and Silistra) and 132 km from the estuary (Reni - Ukrainian side, middle of the Romanian bank of the river and Chilia).
To determine the distribution of the dispersion of pollutants in natural water course has been integrated numerically the dispersion equation [2, 3]:

$$\frac{dc}{dt} + u \frac{dc}{dx} + v \frac{dc}{dy} = D_m \left( \frac{d^2c}{dx^2} + \frac{d^2c}{dy^2} \right) + D_{px} \frac{d^2c}{dx^2} + D_{py} \frac{d^2c}{dy^2} - K \cdot c^2$$

(1)


Transposed Flex PDE program [4, 5, 6]:

$$dt(c) + u * dx(c) + v * dy(c) = Dm * dxx(c) + Dm * dyy(c) + dx[Dpx * dx(c)] + dy[Dpy * dy(c)] + K * c^2$$

(2)

For 2D modeling of the dispersion of pollutants in the Danube area we chose a modeling with the following characteristics (fig. 2a, 2b, 2c):
- length = 143 km;
- width = 0.5 km;
- determined pollutant concentration at 375 km from the estuary, left bank (Bulgarian) 2.7 mg/l, the middle of the river 2.4 mg/l and on the right bank (Romanian) 2.1 mg/l.

We made three modeling, based on the following values: speed $u=2$ m/s, molecular dispersion coefficients $D_{px}=2$, $D_{py}=2$ and $D_m=0.155$, $K=0.1$, varying the velocity in 3 situations, such in figures 2a, 2b, 2c (modeling no. 1 – $v = 0$ m/s).

**Fig. 2a.** Graphical representation of the evolution of pollutant concentration.
To highlight the pollutant dispersion in the Danube continues to show a detailed flow at different times of dispersion (fig. 3a, 3b, 3c).
Fig. 3b. Graphical representation of the evolution of pollutant concentration at $t = 100$.

Fig. 3c. Graphical representation of the evolution of pollutant concentration at $t = 400$.

Modeling no. $2 - v = 0.2 \text{ m/s (fig. 4a, 4b, 4c)}$:

Fig. 4a. Graphical representation of the evolution of pollutant concentration.
Fig. 4b. Pollutant concentration profiles in the simulation.

Fig. 4c. Graphical representation of the evolution of pollutant concentration.

Detail of flow at different times of dispersion are given in fig. 5a, 5b, 5c.

Fig. 5a. Graphical representation of the evolution of pollutant concentration at $t = 40$. 
Fig. 5b. Graphical representation of the evolution of pollutant concentration at $t = 100$.

Fig. 5c. Graphical representation of the evolution of pollutant concentration at $t = 400$.

Modeling no. 3 – $v = 0.5$ m/s (fig. 6a, 6b, 6c):

Fig. 6a. Graphical representation of the evolution of pollutant concentration.
**Fig. 6b.** Pollutant concentration profiles in the simulation.

**Fig. 6c.** Graphical representation of the evolution of pollutant concentration.

Details of flow at different times of dispersion are given in fi. 7a, 7b, 7c.

**Fig. 7a.** Graphical representation of the evolution of pollutant concentration at $t = 40$. 

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**Ecoterra, no. 28, 2011**
Fig. 7b. Graphical representation of the evolution of pollutant concentration at t = 100.

Fig. 7c. Graphical representation of the evolution of pollutant concentration at t = 400.

Conclusions

The model developed allows estimating the distance to the river will be polluted from the discharge of pollutants and assessing the degree of pollution of the river section affected by the wave. Basically it is possible to track the time and space of the concentration of pollutants, providing warning of possible effects they may have discharges of pollutants into the Danube, depending on the quantity of substance spilled, contact source pollution, rainfall and ambient temperature. As a result of numerical simulations carried out in the program can be seen Flex PDE dispersion of pollutant concentration and self-purification capacity due to the Danube River. The present model can be a useful tool for assessing pollution or pollution prediction could be done to manage situations that arise.

References

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