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Environment Pollution Modeling on the Base of Quick Computing Models

Purpose. Development of a fast calculation models for determining zones of ground waters and air chemical pollution during the emission of chemically hazardous substances from anthropogenic sources of pollution. To model the process of passive impurity transfer in ground waters and in atmospheric air, the G. Marchuk model is used, which takes into account the speed and direction of the flow, the intensity of the emission of chemically hazardous substances, and atmospheric diffusion (dispersion in round waters). **Methodology.** The process of ground waters and air pollution modeling is based on the numerical integration of the mass transfer equation (G. Marchuk model). Two numerical models were built. One numerical model was built to simulate ground waters pollution. Another numerical model was built to simulate air pollution. The construction of a numerical models of the impurity propagation process was carried out by splitting of the mass transfer equation (G. Marchuk model). Then a variable-triangular finite-difference decomposition schemes were used for numerical integration. The unknown value of the concentration of a chemically hazardous substance is carried out using explicit formulas. A set of applied programs has been developed based on the constructed numerical models. **Findings.** A set of applied programs has been developed based on the constructed numerical models. The results of numerical calculations are presented, showing the efficiency of the proposed numerical models. **Originality.** Proposed numerical models of mass transfer allow to compute quickly the areas of chemical air pollution due to the emission of toxic substances from anthropogenic sources of pollution. **Practical value.** Based on the proposed numerical models, a computer code has been developed. The developed models and computer code make it possible to estimate the size and intensity of environmental pollution, and can be used in solving the problem of assessing the negative impact on the ground waters and air from different sources. The results of numerical calculations show the operability of the proposed models.

Key words: ground waters pollution; air pollution; landfills; emergency release; mathematical model; numerical simulation

Introduction

Landfills for solid construction waste are long-term sources of environmental pollution. Almost every country has a significant number of such landfills. These sources has intensive negative effect on the ground waters and air pollution (Fig. 1).

Therefore, considerable attention is paid to the problem of assessing the impact of landfills for solid household waste on the environment, the emission of hazardous substances from landfills [2–6, 8, 9] and the problems of reducing the negative impact on the environment [6].

Fig. 1. Fire sources at the landfill [https://opentv.media/v-dnepropetrovskoj-oblasti-sejchas-gorit-poligon-bytovyh-othodov-foto]

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Fig. 2. Accidental emission at the enterprise [https://24tv.ua/avariya_na_fukusimi_1_fakti_pro_motoroshnu_katastrofu_v_yaponiyi_n1185905]

Another problem in the field of environmental safety is atmospheric air pollution during extreme situations at enterprises (Fig.2). Powerful emissions of chemically hazardous substances into the air during such extreme situations lead to large-scale environmental pollution. Therefore, it is very important for practice to have mathematical models for predicting environmental pollution during emergency emissions at enterprises.

Analysis of recent research. Problem of environment pollution is of great interest. Pollution may be caused by industrial emissions, accidental emissions, inflow of toxic pollutants from landfills to ground waters, etc. Many tools were developed to predict atmosphere pollution in case of different emissions. These tools may be divided in some groups:

1. Simplified mathematical models – are used for quick prediction of atmosphere pollution at industrial sites (for example, Berlyand's model). As a rule these are empirical models which do not demand detail information about the atmosphere conditions or source of emission.

2. Gauss models – are widely used for atmosphere pollution prediction. The models are semi-empirical. These models allow to obtain important information for stead- state emissions from different sources. Some well-known commercial codes were developed on the basis of Gauss models (for example, AERMOD).

3. Analytical models which can be used for steady state emissions or accidental emissions.

4. Numerical models which are based on numerical integration of mass transfer equation [1, 2, 4–10].

5. CFD models which are based on numerical integration of Fluid Dynamics models and equation of Mass Transfer. Some well - known commercial codes were developed on the basis of these models (For example, ANSYS Fluent, MODFLOW).

But the problem of quick computing mathematical models development for air pollution problems is still exist. Engineers need «diagnostic» models which allow to predict quickly air pollution using standard input information.

Purpose

Development of quick computing mathematical models to be used in applied calculations of ground waters and atmosphere pollution problems.

Methodology

In this paper, we will consider an express models for assessing the areas of chemical pollution of ground waters and atmospheric air. Therefore, the prediction of pollution areas in ground waters is carried out on the basis of a 2D model of the transport of impurities (planning model, G. Marchuk's model) [1, 2, 8]:

$$\frac{\partial S}{\partial t}+\frac{\partial uS}{\partial x}+\frac{\partial vS}{\partial y}=\frac{\partial}{\partial x}\left(\mu_x\frac{\partial S}{\partial x}\right)+\frac{\partial}{\partial y}\left(\mu_y\frac{\partial S}{\partial y}\right)+$$

$$+\sum_{i=1}^{N}Q_i\,\delta\left(x-x_i\right)\left(y-y_i\right),\,, \quad (1)$$

where S is the average (by transfer height) value of the concentration of a chemically hazardous substance; u, v – components of the speed vector in the projection on the x, y coordinate axes, respectively; x_i, y_i – Cartesian coordinates of the i-th source of emission of a chemically hazardous substance at the facility; t – time, s; μ_x, μ_y – dispersion coefficients; $\delta\left(x_i, y_i\right)$ – Dirac delta function, which is used to specify the location of the pollutant release in the model. The emission intensity of a chemically hazardous substance is equal to Q.

For equation (1), the following boundary conditions are implemented:

1. At *t* = 0, the impurity concentration in the study area is given.

2. At the boundaries where the flow enters the study area, the condition S is set = S1, where S1 is the known concentration of the impurity.

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3. At the boundaries where the flow leaves the study area is given $\frac{\partial S}{\partial n}=0$, where n is the unit vector normal to the boundary.

To simulate air pollution, Eq. (1) is also used and in this case: μ_x, μ_y – are diffusion coefficients.

For numerical integration of the transport equation for ground waters pollution problems the following splitting for Eq. (1) was used:

$$\frac{\partial S}{\partial t}+\frac{\partial uS}{\partial x}=\frac{\partial}{\partial x}\left(\mu_x\frac{\partial S}{\partial x}\right), \quad (2)$$

$$\frac{\partial S}{\partial t}+\frac{\partial vS}{\partial y}=\frac{\partial}{\partial y}\left(\mu_y\frac{\partial S}{\partial y}\right), \quad (3)$$

$$\frac{\partial S}{\partial t}=\sum_{i=1}^{N}Q_{S_i}(t)\delta(x-x_i)(y-y_i) . \quad (4)$$

For the numerical solution of equation (2), the following two-step splitting scheme is used:

– the first step uses the dependency:

$$S_{i,j}^{n+\frac{1}{2}}=S_{i,j}^{n}-\Delta t\frac{u_{i+1,j}^{+}S_{i,j}^{n+\frac{1}{2}}-u_{i,j}^{+}S_{i-1,j}^{n+\frac{1}{2}}}{\Delta x}+$$

$$+\Delta t\mu_x\frac{-S_{i,j}^{n+\frac{1}{2}}-S_{i-1,j}^{n+\frac{1}{2}}}{2\Delta x^2}+\Delta t\mu_x\frac{-S_{i,j}^{n}+S_{i+1,j}^{n}}{2\Delta x^2},$$

– in the second step, the dependency is used:

$$S_{i,j}^{n+1}=S_{i,j}^{n+\frac{1}{2}}-\Delta t\frac{u_{i+1,j}^{-}S_{i+1,j}^{n+1}-u_{i,j}^{-}S_{i,j}^{n+1}}{\Delta x}+$$

$$+\Delta t\mu_x\frac{-S_{i,j}^{n+\frac{1}{2}}+S_{i-1,j}^{n+\frac{1}{2}}}{2\Delta x^2}+\Delta t\mu_x\frac{-S_{i,j}^{n+1}+S_{i+1,j}^{n+1}}{2\Delta x^2},$$

where $u^{+}=\frac{u+|u|}{2}, u^{-}=\frac{u-|u|}{2}$

For the numerical solution of equation (3), the following two-step splitting scheme is used:

– the first step uses the dependency:

$$S_{i,j}^{n+\frac{1}{2}}=S_{i,j}^{n}-\Delta t\frac{v_{i,j+1}^{+}S_{i,j}^{n+\frac{1}{2}}-v_{i,j}^{+}S_{i,j-1}^{n+\frac{1}{2}}}{\Delta y}+$$

$$+\Delta t\mu_y\frac{-S_{i,j}^{n+\frac{1}{2}}+S_{i,j-1}^{n+\frac{1}{2}}}{2\Delta y^2}+\Delta t\mu_y\frac{-S_{i,j}^{n}+S_{i,j+1}^{n}}{2\Delta y^2},$$

– in the second step, the dependency is used:

$$S_{i,j}^{n+1}=S_{i,j}^{n+\frac{1}{2}}-\Delta t\frac{v_{i,j+1}^{-}S_{i,j+1}^{n+1}-v_{i,j}^{-}S_{i,j}^{n+1}}{\Delta y}+$$

$$+\Delta t\mu_y\frac{-S_{i,j}^{n+\frac{1}{2}}+S_{i,j-1}^{n+\frac{1}{2}}}{2\Delta y^2}+\Delta t\mu_y\frac{-S_{i,j}^{n+1}+S_{i,j+1}^{n+1}}{2\Delta y^2},$$

where $v^{+}=\frac{v+|v|}{2}, v^{-}=\frac{v-|v|}{2}$.

For numerical integration of equation (4), the Euler method is used.

To develop the second numerical model for air pollution modeling, Eq. (1) was split at the difference level (here we use another notation for impurity concentration "C"):

– the first step of splitting (k=1/4):

$$\frac{C_{ij}^{n+k}-C_{ij}^{n}}{\Delta t}+\frac{1}{2}(L_x^{+}C^k+L_y^{+}C^k)+\frac{\sigma}{4}C_{ij}^{k}=$$

$$=\frac{1}{4}(M_{xx}^{+}C^k+M_{xx}^{-}C^k+$$

$$+M_{yy}^{+}C^n+M_{yy}^{-}C^n)+\sum_{l=1}^{N}\frac{Q_l}{4}\delta_l;$$

– the second step of splitting ($k = n$+1/2; $c = n$+1/4):

$$\frac{C_{ij}^{k}-C_{ij}^{c}}{\Delta t}+\frac{1}{2}(L_x^{-}C^k+L_y^{-}C^k)+\frac{\sigma}{4}C_{ij}^{k}=$$

$$=\frac{1}{4}(M_{xx}^{-}C^k+M_{xx}^{+}C^c+$$

$$+M_{yy}^{-}C^k+M_{yy}^{+}C^c)+\sum_{l=1}^{N}\frac{Q_l}{4}\delta_l;$$

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– the second step of splitting ($k = n+3/4$; $c = n+1/2$):

$$\frac{C_{ij}^k - C_{ij}^c}{\Delta t} + \frac{1}{2}(L_x^+ C^k + L_y^- C^k) + \frac{\sigma}{4} C_{ij}^k =$$

$$= \frac{1}{4}(M_{xx}^- C^c + M_{xx}^+ C^k +$$

$$+ M_{yy}^- C^k + M_{yy}^+ C^c) + \sum_{l=1}^{N} \frac{Q_l}{4} \delta_l ;$$

– the fourth step of splitting ($k = n+1$; $c = n+3/4$):

$$\frac{C_{ij}^k - C_{ij}^c}{\Delta t} + \frac{1}{2}(L_x^- C^k + L_y^+ C^k) + \frac{\sigma}{4} C_{ij}^k =$$

$$= \frac{1}{4}(M_{xx}^- C^k + M_{xx}^+ C^c +$$

$$+ M_{yy}^- C^c + M_{yy}^+ C^k) + \sum_{l=1}^{N} \frac{Q}{4} \delta_l .$$

In these expressions L_x, L_y… are difference operators. These operators are described in [1].

Both finite-difference models were coded. For programing of the developed numerical models FORTRAN was used. Computer code includes some SUBROUTINES which perform calculation of each step of splitting for each finite- difference model.

Following input data are used for numerical experiment:

1. information about dimensions of the computational area where the numerical experiment will be carried out;
2. industrial site position (for example, waste landfill position or railway station position where the accidental release may take place);
3. time step;
4. parameters of atmosphere stability, dispersion coefficients, wind speed and wind direction (speed of ground waters flow and direction of this flow);
5. toxic substance emission rate.
6. dimensions and form of emission source.
7. time of emission.

Findings

Based on the developed numerical models, two model problems were solved. The first problem considers the location of a possible landfill near the village and ground waters pollution in case of contaminate inflow from the landfill to ground waters. (Fig. 2).

It is assumed that the ground waters speed was 0.000002 m/s. The HCL emission intensity from the landfill is assumed to be equal to 1 (dimensionless value).

The simulation results are shown in Fig. 3.

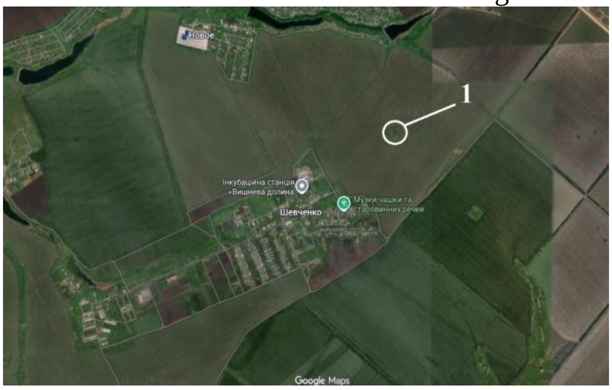

Fig. 3. Location of possible landfill,
(Google Image 2025)

Fig. 4. Contamination zone, HCL concentration:
1 – C = 82 mg/m^3; *2* – C = 61 mg/m^3; *3* – C = 37 mg/m^3

One can see from Fig. 4 that intensive zone of contamination of ground waters is formed near the landfill. This zone can cause contamination of water in wells which are used in the village which is situated near the landfill

Below are the results of solving the second problem – an emergency release at an railway station (fire of oil tank). Wind speed was 8 m/s.

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Fig. 5. Area of contamination, CO concentration:
1 – C = 158 mg/m^3; *2* – C = 96 mg/m^3; *3* – C = 71 mg/m^3

As one can see from Fig.5, large contamination zone is formed near the source of emission.

It took 2 sec to obtain results of numerical experiment. Developed computer code allows to obtain dimensions of contaminated zone and intensity if contamination. Standard input information is used for numerical modeling.

Originality and practical value

Numerical models have been proposed for the operational determination of areas of pollution from anthropogenic sources.

Computer code was developed using FORTRAN. This computer code can be used for operational solution of several applied problems in the field of environmental safety (ground waters and air pollution problems).

Modeling of ground waters and atmosphere pollution is carried out using standard input information. That is important for practical use of developed numerical models. Results of computer experiment are presented as the contamination zones.

Conclusions

1. Quick computing numerical models have been developed for analyze of contamination zones which are formed near different sources of toxic pollutants emission.

2. Fundamental equation of mass transfer (mass conservation law) was used as the basis of numerical model. This equation takes into account wind velocity speed (ground waters speed and direction), it's direction, atmosphere stability, intensity of toxic pollutant emission

3. Developed numerical models can be used for prediction of ground waters and atmosphere pollution in case of release of toxic pollutants from different sites and sources.

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Моделювання забруднення довкілля на базі швидко розрахункових моделей

Мета. Розробка швидко розрахункових моделей для визначення зон хімічного забруднення підземних вод та повітря при емісії хімічно небезпечних речовин від антропогенних джерел забруднення. Для моделювання процесу переносу пасивної домішки в підземних водах та в атмосферному повітрі використовується модель Г. Марчука, що враховує швидкість та напрям руху потоку, інтенсивність емісії хімічно небезпечної речовини, атмосферну дифузію (дисперсію). **Методика.** Процес моделювання забруднення підземних вод, атмосферного повітря базується на чисельному інтегруванні рівняння масопереносу (модель Г. Марчука). Побудова чисельних моделей процесу поширення домішки здійснюється шляхом розщеплення рівняння масопереносу. Далі будуються дві кінцево-різницеві схеми розщеплення. Невідоме значення концентрації хімічно небезпечної речовини визначается за допомогою явних формул, що дозволяє розробити простий алгоритм рішення різницевих рівнянь. **Результати.** Розроблений комплекс прикладних програм на базі побудованих численних моделей. Наведені результати чисельних розрахунків, що показують працездатність запропонованих чисельних моделей. **Наукова новизна.** Запропоновані чисельні моделі масопереносу, що дають можливість швидко розраховувати області хімічного забруднення підземних вод та атмосферного повітря при емісії токсичних речовин від антропогенних джерел забруднення. **Практична значимість.** На базі запропонованих чисельних моделей розроблений комп'ютерний код. Розроблені моделі та комп'ютерний код дають можливість швидко оцінювати розміри та інтенсивність забруднення довкілля, та може бути використани при рішенні двох класів задач по оцінюванню антропогенного впливу на навколишнє середовище від антропогених джерел забруднення.

Ключові слова: забруднення підземних вод, забруднення повітря; полігони відходів; аварійний викид; математична модель; чисельне моделювання

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