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ANDRZEJ BIELSKI*

MODELLING OF MASS TRANSPORT IN WATERCOURSES AT UNSTEADY STATES

In terms of quality particularly difficult to describe are processes of mass exchange between different phases (e.g., atmospheric air–water, water–river sediment, water–algae, etc.). Whitman's model is most often used to describe the mass transport processes through the phase boundary. Theoretical analysis of the mass transfer process through the phase boundary showed that in unsteady states, the calculation results obtained from Whitman's model differ from the results obtained using the accurate diffusion model. These differences are due to the fact that concentration profiles in the direction of diffusion process change in time. Assumptions for Whitman's model do not include changes in the concentration distribution over time. Therefore, the correction factor was introduced to Whitman's model. The correction factor is defined as a parameter that multiplies a concentration derivative over time in the mass transport model. The correction factor can be used to estimate the effective diffusion coefficient of the substance that permeates from the aqueous phase to the sediment. The correction factor improves the degree of fit of the mass transport model to the measurement data. It can be used to estimate the effective turbulent diffusion coefficient from water phase to the sediment phase.

1. INTRODUCTION

Complex models of mass propagation in water environment describe rates of substance transformation as well as rates of their interactions with other components of the environment. Such models enable one to explain, in a more precise way, actual nature of processes as well as to calculate with more accuracy the quantity of substance in a definite place and time. All the models require numerical values of some parameters to be identified; more elaborate models require more parameters to be known. Identification of the numerical values of the parameters is usually not easy. In most cases, both specific field investigations and laboratory tests are required. Some

*Cracow University of Technology, Department of Environmental Engineering, ul. Warszawska 24, 31-155 Cracow, Poland; e-mail: abielski@riad.usk.pk.edu.pl

investigations and tests allow identifying just one parameter while in the case of other parameters, simultaneous determination of several numerical values is required.

If biochemical, chemical and physical process rates are considered in mass transport models, appropriate kinetic equations have to be developed. Since the mass transport model for unsteady states (flows varying in time) is very complicated, it is recommended kinetic equations to remain rather simple. It should be noted though that too extensive simplification may result in poor model accuracy. Particularly demanding, in terms of good qualitative description, are processes of mass exchange between different phases (e.g.: atmospheric air–water, water–river sediment, water–algae, etc.).

Whitman's model has been most frequently used in description of mass transport through a phase boundary [1–7]. Theoretical analysis of mass transport through a phase boundary showed that in unsteady states the final results obtained from this model may occasionally considerably differ from the results obtained using diffusion models [8–12]. The differences may be explained by the fact that concentration profiles directed along diffusion vary in time. Since the assumptions of Whitman's model do not consider changes in distribution of concentration in time, an attempt to improve Whitman's model has been made The correction factor can be defined as a parameter that multiplies the concentration derivative with respect to time in the mass transport model [10, 12]. The correction factor to Whitman's model may be used to estimate the efficient diffusion coefficient of the substance that is transferred from water to a sediment phase [8, 9, 11, 12].

The element of the mass transport model, featuring the Whitman's model correction factor, is the only element of the mass transport model that may delay advective movement of the transported mass.

2. MASS TRANSPORT MODEL

To describe mass transport in water environment in unsteady states, two systems of equations were used, related to flows and flux of the transported mass. Time dependent flows Q and water level elevations H in a water bed were described with de Saint-Venant's equations, comprising:

- Continuity equation [13–21].

$$\frac{\partial A}{\partial t}+\frac{\partial Q}{\partial x}=q_L \tag{1}$$

- Momentum balance equations [13–21].

$$\frac{\partial V}{\partial t}+V\frac{\partial V}{\partial x}=g\left(-\frac{\partial H}{\partial x}-S_f\right)+(U-V)\frac{q_L}{A} \tag{2}$$

Equations (1) and (2) make de Saint-Venant's equations system. In the following discussion, it was assumed that the aerial flow is perpendicular to the river axis, thus $U = 0$).

3. Motion resistance equations (Manning's equations) [14, 15, 17, 22, 23]:

$$S_f = \frac{V|V|x_n^2}{R_h^{4/3}} \tag{3}$$

Time dependent concentrations c and absorption and/or adsorption a have been described through the system of equations consisting of:

- Mass balance equation for water (mobile) phase [10, 11]:

$$\left(1-\frac{D}{h}a_2\right)\frac{\partial c}{\partial t}+V\frac{\partial c}{\partial x}=\frac{1}{A}\cdot\frac{\partial}{\partial x}\left(E_x A\frac{\partial c}{\partial x}\right)+\frac{q_L}{A}\left(c_d-c\right)-\frac{K}{h}\left(c-c^*\right)-k_c c \tag{4}$$

- Mass balance equation for the sediment (stationary) phase [10, 11]:

$$\frac{\partial a}{\partial t}=\frac{K}{L_0}\left(c-c^*\right)-\frac{D}{L_0}a_2\frac{\partial c}{\partial t}-k_r a \tag{5}$$

- Equilibrium equation (Henry's isotherm) [10, 11, 4, 1]:

$$a = \Gamma c^* \tag{6}$$

In Equations (4) and (5), the coefficient a_2 is the correction factor to Whitman's model [8–12].

Harmonic analysis of the diffusion equation shows that for a sinusoidal change of the concentration at the water/sediment phase boundary [8, 12].

$$a_2 = -\frac{1}{\omega}\sqrt{\frac{\sqrt{k_r^2+\omega^2}}{D}}\sin\left(\gamma_M\right) \tag{7}$$

where:

$$\gamma_M = \frac{1}{2}\operatorname{arctg}\left(\frac{\omega}{k_r}\right) \tag{8}$$

Equation (7) may also be used in the case of impulse-type changes of concentration; the wave period (T) is equal to impulse duration.

In the case of random changes of concentration, the coefficient a_2 may also be used in Eq. (4). As was presented elsewhere [10, 11], the correction factor to Whitman's model is equivalent to the factor related to adsorption/absorption processes proceeding at an infinitely high rate through equilibrium states or – in the case of periodic fluctuations of concentration – the value of the factor is valid for the factor related to adsorption/absorption processes proceeding partially at the infinitely high rate.

Therefore, such a correction factor enables simultaneous considering processes of adsorption/absorption proceeding at a finite and infinitely high rate in the mass transport model.

3. APPLICATION OF THE MASS TRANSPORT MODEL

At unsteady state conditions, in order to perform simulation of transport of pollutants that undergo chemical or biochemical transformations including adsorption/adsorption processes, it is necessary to solve the system of equations: (1)–(6). The system was solved numerically through a specially customized computer program. Equations (1) and (2) were integrated with a four-point two-weight numeric scheme (Fig. 1) [24], while Eqs. (4) and (5) with an explicit schemes with a second order accuracy, after decomposition of advection-diffusion process into two separate processes: advection and diffusion. The program enabled one to determine time distribution of: *c*, *a*, *Q*, and *H* along the water body as well as their distribution within a particular river cross-section, and, finally, determination of model parameters based on the measured data. The values of the unknown parameters were coordinates of the minimum sum of squares of deviations between the values measured and calculated from the models. Minimization of the sum of squared deviations was performed by the simplex methods by Nelder–Meade [25–27].

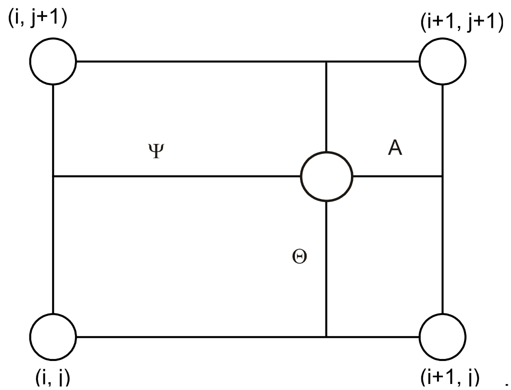

Fig. 1 Mesh points (*x*, *t*): *i* – index related to coordinate $x = i \cdot \Delta x$, *j* – index related to coordinate $t = j\Delta t$, *A* – intermediate mesh point).

The measured data presented in [28] were used in calculations. They were obtained during experimental tests carried out at the Colorado River. The experiments were performed with a tracer – rhodamina WT, at unsteady flow conditions [28] along 380.5 km of the river. To maintain unsteady flow conditions, setting culverts at the Glen Canyon Dam was changed.

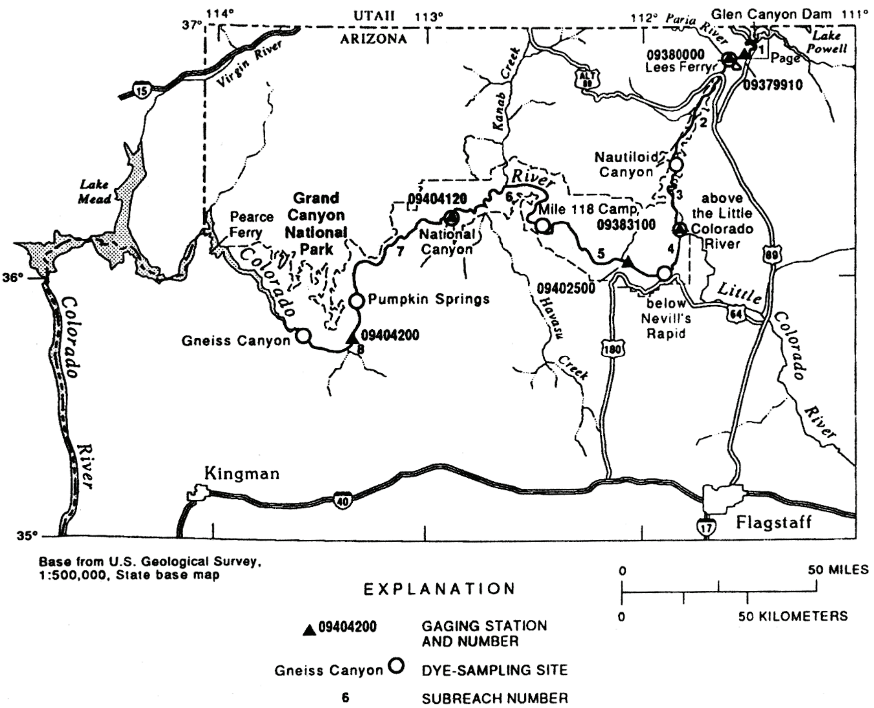

Fig. 2. Map of the Colorado River with marked cross-sections where analysis and measurements were taken

Estimation of parameters of the mass transport model was carried out in two river segments: segment No. 1 from the Nautiloid Canyon cross-section to the Above the Little Colorado River one; segment No. 2, from the Above the Little Colorado River cross-section to the Nevill's Rapid one (Fig. 2).

4. ESTIMATION OF THE MODEL PARAMETERS

4.1. IMPACT OF PARAMETERS OF THE NUMERIC SCHEME ON GOODNESS OF FIT OF THE FLOW MODEL TO MEASURED DATA

Numeric solution of differential equations may more or less differ from the exact solution. Determined coefficients of the model, described with differential equations, should be free from calculation errors, including numerical errors. In the case of the flow model, the value of the motion resistance coefficient was unknown. To minimize numeric errors that can significantly influence its estimation, impact of the parameters: Δx, Δt, Ψ and Θ was investigated on the minimum of Φ function (sum of squared deviations between time dependent calculated Q_{calc} and measured Q_{meas} flows, at the cross-section x = 24 900 m, segment No. 2. Function Φ in this case was minimized with respect to the motion resistance coefficient x_n. Details concerning determination of the parameters have been described elsewhere [29]. The coefficients Ψ and Θ influence both diffusion and numeric dispersion [30]. Numerical diffusion causes the wave attenuation. Numerical dispersion is responsible for the appearance of abnormal oscillations in the course of flow, speed, water depth in the river over time.

It was concluded that values of parameters Ψ and Θ should be determined based on the coordinates of points located close to the boundary of stability field (Ψ, Θ) of the numeric scheme to minimize numeric diffusion [29]. At those points, the lowest attenuation of the maximum wave flow occurs. It was found that appropriate values of the parameters are as follows: Δx = 249 m, Δt = 300 s, Ψ = 0.3, Θ = 0.55.

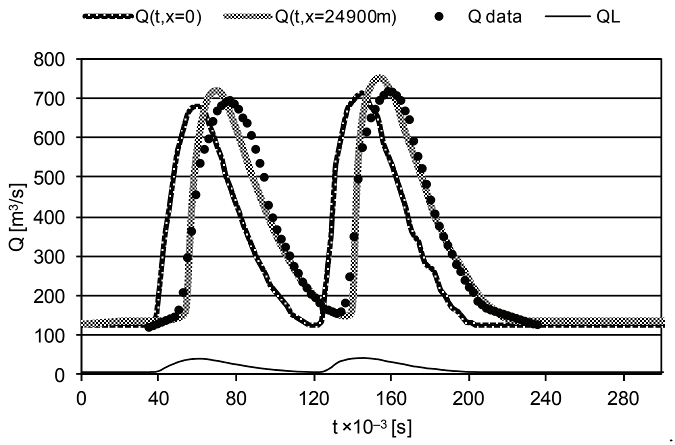

Fig. 3. Time dependences of Q: x = 24 900 m,
segment 2, areal flow q_L, QL – total flow to the segment

Finally, the average absolute fit error, determined for the flow model (segment No. 2) with a real flow q_L established based on the balance of water volume between initial and final cross-sections is ca. 42.99 m^3/s (Fig. 3) at x_n = 0.0856 $s\cdot m^{-1/3}$. The determined values of parameters: Δx, Δt, Ψ and Θ are not the only ones for which calculations may be performed at low diffusion or numerical dispersion.0 An infinite number of such theoretical combinations exist.

4.2. DETERMINATION OF THE COEFFICIENTS OF THE MASS TRANSPORT MODEL AT SEGMENT NO. 2

If the values of the parameters and coefficients for the flow models are known, it is possible to determine the values of the coefficients in the mass transport model in the segment No. 2.

Minimization of the sum of squared deviations Φ_c between the measured and calculated values at the cross-section $x = 24\,900$ m enabled one to determine the mass transport model coefficients: $E_x = 314.62$ m^2/s, $Da_2 = -246.53 \times 10^{-3}$ m, $K = 0.28286 \times 10^{-9}$ m/s. For the model described with the equations: (4)–(6), taking into account the inflow q_L at $c_d = 0$, the following parameter values were assumed: $\Gamma = 1$ m^3/m^3 of the solid state, $L_0 = 1$ m, $k_c = 0$, $k_r = 0$. Figure 4 presents the goodness of fit of the model to the measured data. A very good fit of the model to the actual mass propagation path was obtained. The average absolute error of fit was 0.86 mg/m^3. Calculations were performed at: $\Delta x_{C1} = 249$ m, $\Delta x_{C2} = 300$ m, $\Delta t = 100$ s. Such steps of integration provide sufficiently low numerical diffusion.

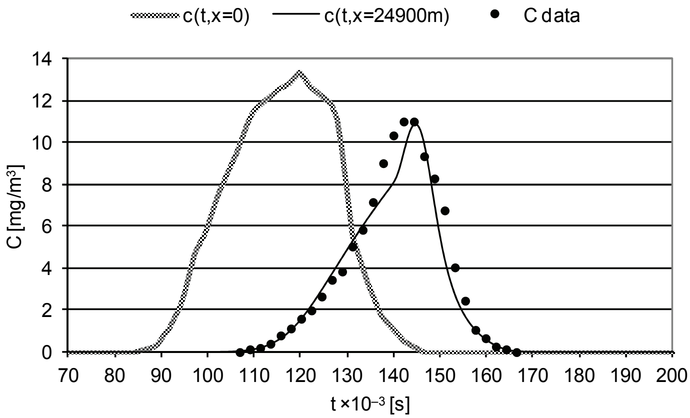

Fig. 4. Time dependences of tracer concentrations at the initial cross-section and at $x = 24\,900$ m (segment No. 2, areal flow q_L)

A very small value of the mass transfer rate constant K (irrelevant from the computational point of view) together with a non-zero value of Da_2 indicates that the absorption/adsorption processes run practically through the equilibrium states. Running the calculations with a sufficiently high K (being equivalent to $Da_2 = 0$) would require very small values of Δx and Δt; it could lead to time consuming and complex computations due to the finite size of the real number representation in the language used for programming.

Dimensional analysis enables one to find a relationship between the dispersion coefficient E_x, the Reynolds number and a geometric similarity module. As a result of the least squared fitting Φ_c, the dispersion coefficient equation in segment No. 2 takes a form:

$$E_x = 19.476\left(VR_h\right)^{1.4888}\left(\frac{A}{hR_h}\right)^{0.40256} \tag{9}$$

or if the water density $\rho = 10^6$ g/m^3 and water viscosity $\mu = 1$ g/(m·s) are assumed, it takes a dimensionless form:

$$\frac{1}{Sc} = 0.022988 Re^{1.4888} \left(\frac{A}{hR_h} \right)^{0.40256} \tag{10}$$

where Sc is the Schmidt number ($Sc = E_x\rho/\mu$), Re – the Reynolds number ($Re = VR_h\rho/\mu$), A – module of geometric similarity ($A/(hR_h)$.

Equation (10) may be transformed into the formula making use of other numbers. After dividing of its both sides by the Reynolds number, the following relationship is obtained:

$$\frac{1}{Sc\ Re} = \frac{1}{Pe} = 0.022988 Re^{0.4888} \left(\frac{A}{hR_h} \right)^{0.40256} \tag{11}$$

where: Pe is the Peclet number ($Pe = VR_h/E_x$); equations based on the Peclet, Reynolds and Schmidt numbers may be found in the literature [31].

In the case when the dispersion coefficient E_x changes its value (Eq. (9)), the following model parameters were obtained: $Da_2 = -225.13 \times 10^{-3}$ m, $K = 0.27011 \times 10^{-8}$ m/s. Like for the constant value of E_x, the value of K remains very small; this means that absorption/adsorption processes run through the equilibrium states. The value of the product Da_2 is almost the same as for the constant dispersion coefficient E_x.

Based on Equation (9), it can be concluded that momentary values of the mass dispersion coefficient may vary in wide ranges from 130 m^2/s to ca. 1100 m^2/s. Increase of both the flow velocity and hydraulic radius R_h (in this case $h \approx R_h$) results in a higher value of the dispersion coefficient in segment No. 2.

4.3. DETERMINATION OF THE COEFFICIENTS IN THE FLOW AND MASS TRANSPORT MODEL IN SEGMENT No. 1

Integration of the flow model in segment No. 1 was performed for the following parameters: $\Delta x = 249$ m, $\Delta t = 300$ s, $\Psi = 0.3$, $\Theta = 0.55$. Minimization of the sum of squared deviations Φ for the flow in the cross-section $x = 40\ 600$ m enabled one to fit the model to the measured values of Q_{meas} and to determine a relationship between the motion resistance coefficient x_n and water depth h:

$$x_n = 0.14364 h^{-0.34755} \tag{12}$$

The average absolute fit error between the flow model and the measured data was small (27.72 m^3/s). A very good fit of an actual flow wave to the model has been obtained (Fig. 5).

Once the values of the flow model coefficients have been determined, the values of the mass transport model coefficients were set. Minimization of the sum of squared deviations Φ_c between the measured and calculated values at the cross-section $x = 40\ 600$ m enabled one to determine the mass transport model coefficients: E_x = 277.31 m^2/s, $Da_2 = -955.00\times10^{-3}$ m (numerical experiments showed that absorption/adsorption processes in segment No. 1 may be approximated with the model of the processes running through the equilibrium states).

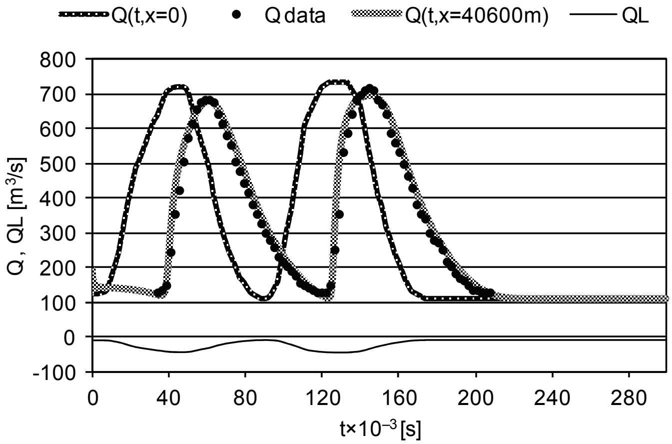

Fig. 5. Time dependences of flow Q (x = 40 600 m, segment No. 1, areal flow q_L, QL – total flow Q_L within the segment)

For the model described with Eqs. (4)–(6), taking into account the inflow $q_L < 0$ at $c_d = c$, the following parameters were assumed: Γ = 1 m^3/m^3 of solid phase, L_0 = 1 m, $k_c = 0$ and $k_r = 0$. The goodness of fit is shown in Fig. 6; it represents a very good fit of the model to the actual path of mass propagation. The average absolute fit error was 0.79 mg/m^3. The calculations were performed for: Δx_{C1} = 249 m, Δx_{C2} = 500 m and Δt = 300 s.

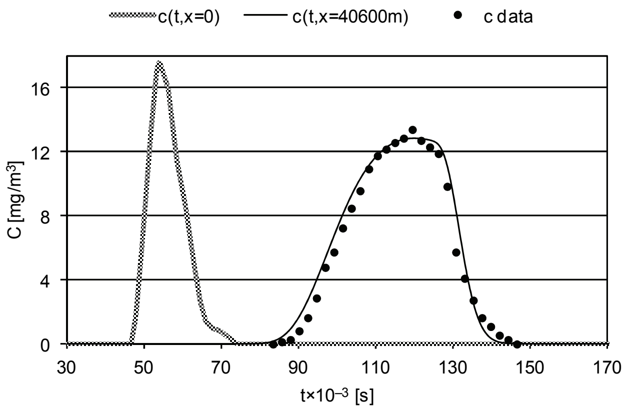

Fig. 6. Time dependences of tracer concentrations at the cross-section x = 40 600 m (segment No. 1, areal flow q_L)

For the segment No. 1, some additional calculations were done for the following integrations steps: Δx_{C1} = 249 m, Δx_{C2} = 500 m and Δt = 50 s. Reduction of the step Δt enabled one to integrate the mass transport model at a rather high mass transfer coefficient K; different model parameters resulted in different effects of the model fit to the measured data (Table 1).

Table 1

Results of estimation of mass transport parameters in segment 1

No.	E_x [m^2/s]	Da_2 [m]	K [m/s]	Mean absolute error [mg/m^3]	Increase of mean absolute error with respect to segment 3 [%]
1	374.61	–0.97027	0	0.75	7.14
2	345.61	0	9.7318×10^{-3}	0.78	8.00
3	300.60	–0.89093	10.877×10^{-5}	0.70	-

In the mass transport model, which uses the parameters from the set Nos. 1 or 2, the average absolute fit error is higher by 7.14% and 8.00%, respectively, if compared with the model employing the correction factor Da_2 to Whitman's model (set No. 3, Table 1). Hence, the correction factor improves significantly the model accuracy.

Table 2

Estimation of parameters of the mass transport model in segment 1 at various integration steps: Δt, Δx_{C1} and Δx_{C2}

No.	Δt [s]	Δx_{C1} [m]	Δx_{C2} [m]	E_x [m^2/s]	Da_2 [m]	K [m/s]	Mean absolute error [mg/m^3]
1	300	249	500	239.53	–0.91452	8.0116×10^{-5}	0.7257
2	50	249	500	300.60	–0.89093	10.877×10^{-5}	0.7047
3	10	249	500	345.34	–0.91517	7.9332×10^{-5}	0.7178
4	50	124.5	250	206.12	–0.88640	10.889×10^{-5}	0.7255
5	10	124.5	250	253.92	–0.87318	13.075×10^{-5}	0.7049

Change of the parameters Δt, Δx_{C1} and Δx_{C2} results in a change of the estimated values of the mass transport model parameters (Table 2). The strongest relative changes, up to about 28.5% of the longitudinal dispersion E_x and the mass transfer rate constant K were observed, if compared to their averaged values. The correction factor Da_2 changed only slightly; its most significant relative change compared to the average was 2.6%. Regardless of considerable changes of E_x and K, the average absolute model error was almost the same and its largest shift from the average was 1.5%. Therefore, at poorly selected parameters: Δt, Δx_{C1} and Δx_{C2}, the values of simultaneously estimated model parameters: E_x, Da_2 and K may not be accurate but the errors of calculated concentrations should be minor. From the above statement it may be concluded that for other rivers of similar flow characteristics and similar mass exchange between the water and sediment, the mass transport model will not be sensitive to its changes of parameters. Obviously, in this case all parameters have to be changed simultaneously, not one by one. During simultaneous changes of all parameters, the effect of an unfavourable change in the value of one parameter is offset by a corresponding change in the value of the other.

For equation (7) at $k_r = 0$ and assuming that the periods of concentration waves in segments: {1, 2} are: {45355, 60733} s, the calculated efficient coefficients of vertical turbulent diffusion ($D = E_z$) in segments: {1, 2} are: $\{2.53 \times 10^{-4}, 1.26 \times 10^{-5}\}$ m^2/s, respectively. In the case of large rivers, the coefficient of vertical turbulent diffusion may be approximated, using equation [32]:

$$\log\left(\frac{E_z}{\nu}\right) = -8.1 + 1.558\log\left(\frac{Vh}{\nu}\right) \tag{13}$$

There are the parameters assumed for both segments: average velocity $V \approx 1$ m/s, water level $h \approx 3$ m, water kinematic viscosity $\nu \approx 1\times10^{-6}$ m^2/s. For such parameter values, the vertical turbulent diffusion coefficient, estimated from Eq. (13) was $E_z = 9.80 \times 10^{-5}$ m^2/s. Its value, calculated from Eq. (13), is similar to the coefficients calculated using Eq. (7). It should be noted that the estimations based on Eq. (7) include also diffusion inside the sediment phase, while the coefficient E_z calculated using Eq. (13) refers to the water phase only.

5. SUMMARY AND CONCLUSIONS

Modelling of transport of pollutants or water natural ingredients is designed to reflect the transport occurring in real conditions; it requires determination of a number of parameters and coefficients. The values of some of them such as: motion resistance coefficient x_n, mass dispersion coefficient E_x can be estimated based on the data on the structure of a watercourse bed, its geometry and nature of the flow. In that case however, even major discrepancies may occur between the actual mass transport and numerical calculations. Therefore, it is recommended to determine the values of the flow model coefficients and mass transport model coefficients, based on measurement data.

Determination of the mass dispersion coefficient based on measurements of tracer concentrations may require application of the mass transport model that takes into account processes accompanying the hydraulic propagation of a tracer. For both organic and inorganic markers strong mass absorption and adsorption in the sediment material should be considered. Both processes can proceed with different intensity. Due to heterogeneity of material of river bed in terms of physical and chemical structure, these processes can run at different rates, depending on the type of material fraction of sediment. Therefore, the mass transport model proposed by the author takes into account these processes running at a finite rate and through the equilibrium states.

Popular models describing mass transfer in relation to one phase or mass transfer through the phase boundary are based on Whitman's model; they may not be appropriate to describe the processes in unsteady states. Therefore, a correction factor has to be incorporated into the mass transport model due to the rate of concentration change in the liquid phase (aqueous phase). The correction factor to Whitman's model, in the case of periodic changes in concentration, can be used to estimate the efficient turbulent diffusion coefficient from water phase to sediment phase. Application of mass transfer (penetration) models used in steady-state conditions to unsteady states is very limited. Such models can be applied only when concentrations change very slowly over time.

In order to partially eliminate numerical diffusion effects on flow calculations, integration steps and weighting factors should be selected as such, that the ratio of the amplitude dumping coefficients was close to one. In order to determine the step size and possibly the weighting factors, equations may be used that determine participation of numerical dumping in dumping resulting from the exact solutions of a specific differential equation. It is also possible to designate the step size and weighting factors for the wave flow model based on an analysis of maxima of calculation results. In this case, one feature of numerical process is used, which shows that the increase of numerical diffusion is accompanied by reduction of the local maxima of the function being the solution of the wave flow model. The values of the weight parameters Ψ and Θ should be determined based on coordinates of points located close to the boundary of stability field (Ψ, Θ) of the numeric scheme to minimize numeric diffusion [29]. At those points, the lowest attenuation of the maximum wave flow occurs. Determination of Ψ and Θ based on the stability condition for a linear version of flow model does not guarantee the stability of numeric scheme for a non-linear model.

Based on the flow and water level data, a relationship was established between the motion resistance coefficient and water depth in the river.

SYMBOLS

A – surface area, m^2
a – amount of adsorption or absorption, g/m^3 of sorbent
C, c – concentration, g/m^3
c^* – equilibrium concentration, g/m^3
C_d, c_d – concentration in areal flow, g/m^3
Cr – Courant number
D – diffusion coefficient, m^2/s
E_x – longitudinal dispersion coefficient, m^2/s
E_z – coefficient of vertical turbulent diffusion (perpendicular to a solid phase surface), m^2/s
g – acceleration of gravity, J/(mol·K)

h – water depth in a river bed or the average water depth in a river bed, m
H – water level, m
k_r – process rate constant, 1/s
k_c – process rate constant in aqueous phase of the monomolecular first order model, 1/s
K – mass transfer coefficient, 1/s or m/s (depending on the formula used)
L_0 – thickness of the solid phase layer, m
Q – river flow rate, m^3/s
Q_{calc} – calculated flow, m^3/s
Q_{meas} – measured flow, m^3/s
Q_d, Q_L – total area inflow to the river segment, m^3/s
q_L – area inflow, $m^3/(m \cdot s)$
R_h – hydraulic radius, m
S_f – movement resistance, m/m
t – time, s
T – period of a function, s
U – flow velocity component for areal flow $(\vec{U} \parallel \vec{V})$, m/s
V – velocity, m/s
x – linear coordinate (longitudinal for a river), m
x_n – motion resistance coefficient in the Manning's equation, $s/m^{1/3}$

GREEK SYMBOLS

α_M, γ_M – complementary parameters
Γ – adsorption coefficient in Henry's isotherm, m^3 of sorbent/m^3 of liquid
Δt – time step, time difference or time shift, s
Δx – linear coordinate step, m
Φ – sum of squared deviations between measured and calculated size, $(\text{dimension size})^2$
ω – angular velocity, rad/s
μ – dynamic viscosity, $g/(m \cdot s)$
ν – kinematic fluid viscosity, m^2/s
Θ – weighting factor $\Theta \in <0; 1>$
Ψ – weighting factor $\Psi \in <0; 1>$
ρ – density, g/m^3

SUBSCRIPTS

i – number of road coordinate x or relates to the concentration at a phase boundary
j – number of time coordinate t
C – relates to concentration
$C1$ – relates to mass advection
$C2$ – relates to mass dispersion

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