

A simplified approach for simulating pollutant transport in small rivers with dead zones using convolution

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Abstract: In the paper an alternative method to solve the one-dimensional advective-diffusive equation describing the pollutants transport in river with dead zones is presented. Because very often transport in a small river can be treated as a 1D issue, then instead of numerical solution of the advection-diffusion equation an equivalent approach based on the convolution technique can be used. Consequently, for a given impulse response function the numerical calculations are required to compute a convolution only. The impulse response function is obtained as an analytical solution of the linear advection-diffusion equation for the Dirac delta function imposed as the boundary condition at the upstream end. Therefore, it represents the Gauss distribution and consequently, this approach is unreliable when the dead zones occur. To reproduce an asymmetric distribution of concentration along the channel axis an approximation of analytical impulse response function using the asymmetric Gumbel distribution is proposed. This approach valid for solution of the transport equation with constant coefficients is extended for piecewise constant coefficients. Convolution approach does not produce any numerical dissipation and dispersion errors typically generated by the methods based on the finite difference technique. Validation of the method using the results of field measurements confirmed its effectiveness.

Keywords: 1D pollution transport; Dead zones; Convolution; Impulse response function.

1 INTRODUCTION

Despite ongoing progress in the construction of sewage treatment plants, various anthropogenic substances dissolved in water are still being discharged into rivers and streams. Many of them being harmful to the aquatic environment are considered as the pollutants. As the pollutant transport in watercourses is a common phenomenon, then it is important to have appropriate tools for modeling this process. There are several advanced 3D mathematical models, which can be used in the rivers with complex riverbeds. This approach can be found, for example, in the paper by Ouro et al. (2018), whereas implementations of 3D contaminant transport equations are available even in the form of ready-made computer software (see for instance Deltares, 2011). However, complex models require large amounts of data and significant computational effort. For this reason, the 1D models are still interesting because they can be easily implemented for small watercourses. On the other hand, they should provide results of appropriate quality. Such a tool for small watercourses with the dead zones is proposed in this article.

Consider the simplest partial differential equation describing the 1D transport of non-degradable pollutant in open channel valid in the far-field, where the solute is completely-mixed in the channel cross-section (Cunge et al., 1980, Rutherford, 1994):

$$\frac{\partial C}{\partial t} + \frac{Q}{A} \frac{\partial C}{\partial x} - \frac{1}{A} \frac{\partial C}{\partial x} \left(A \cdot D \frac{\partial C}{\partial x} \right) = 0 \quad (1)$$

where t is time, x is spatial coordinate, C is concentration, Q is flow rate, A is cross-sectional area of channel, D is coefficient related to the longitudinal dispersion.

In open channel hydraulics, very often Eq. (1) is called the advection-dispersion transport equation, whereas the factor D is called the longitudinal dispersion coefficient. This name can be

misleading because in hydromechanics the term “dispersion” has also another physical meaning related to the wave propagation (Fletcher, 1991). Note that the solution to Eq. (1) has the form of a propagating wave. The dispersion coefficient appears during the accuracy analysis of the numerical solution of Eq. (1) using the modified equation approach. It is related to the 3rd order derivative, while the D factor is related to the 2nd order derivative (see Eq. (1)). Since in this work the term “dispersion” is used in both senses therefore, to avoid misinterpretation Eq. (1) will be called the advection-diffusion equation and the coefficient D - the coefficient of effective diffusion (Hervouet, 2007). However, it should be remembered that this coefficient is related to the process of averaging flow velocity and concentration. First, the 3D advection-diffusion equation, valid for laminar flow, is adapted for turbulent flow. For this purpose, the Reynolds approach is used. Therefore, the instantaneous values of velocities and concentration are expressed as the sum of their time-averaged values and random fluctuations. The products of velocity and concentration fluctuations are expressed using the formulas analogous to Fick's law. This brings the turbulent mass diffusion coefficients (the components of turbulent diffusivity tensor) into the equation. As one can see, they result from fluctuations of the advection velocities. Next, the 3D advection-diffusion equation is reduced to a 1D one via averaging flow velocity and concentration over channel cross-section. Note that the term “dispersion coefficient” introduced while averaging process results from nonuniform distribution of the advective velocity and concentration over channel cross-section. Consequently, one can assume that in fact mass transfer of pollutants is caused by advection and diffusion only.

There are three main reasons for the possible discrepancy between observed and calculated concentrations of pollutants using Eq. (1). The first reason is related to its numerical solution when the advective transport dominates over the diffusive transport. It is well known that the truncation error introduced

during the approximation of the 1st order derivatives involved in Eq. (1) can change the amplitude and phase celerity of the waves representing an exact solution of equation (Fletcher, 1991). Usually, numerical methods used to solve Eq. (1) can generate numerical dissipation and dispersion. As the result a strong smoothing or spurious oscillations very often can be observed in the solution. Only in particular cases, usually when advective Courant number is equal to 1, certain methods ensure the exact solution of linear advection-diffusion equation (Eq. 1). Unfortunately, these cases have no significant role in practice, because the calculations are always carried-out for the Courant number different than unity. As the finite difference method bases on the Taylor series expansion of involved function, a truncation error, greater or smaller, occurs always. To improve the accuracy of numerical solution, this error should be reduced. In the last decades many algorithms, using the finite differences, the finite elements or the finite volume method have been proposed to solve the 1D advective-diffusive equation (Eq. 1) (see, for instance, Cunge et al., 1980; Fletcher, 1991; Runkel and Chapra, 1993; LeVeque, 2002; Szymkiewicz, 2010; Szymkiewicz and Gąsiorowski, 2021). It should be stressed that the widespread use of the 1D pollution transport equation results from the availability of ready-made software as the HEC-RAS (2016) and MIKE 11 (2021) packages. It is worth adding that there are also a significant number of analytical solutions of the advection-diffusion equation describing the transport of pollutants in a river, which are of practical importance. They can be found, among others, in the following books and papers: Fischer et al. (1979), De Smedt et al. (2005), Jaiswal et al. (2011), Mazaheri et al. (2013), van Genuchten et al. (2013a, 2013b). Examples of the use of analytical solutions of pollutant transport equations to analyze very practical engineering problems are presented, for instance, by Řiha et al. (2023) and Velisková et al. (2023). Of course, analytical solutions do not generate numerical errors.

The second reason of the possible discrepancy is related to the coefficient D involved in the diffusive term. Note that the interpretation of this coefficient is clear in the case of a 3D transport equation. The situation becomes more complex, when in the case of small rivers and streams the 3D equation is reduced to the 1D or 2D equation (see, for instance, Gualtieri, 2010). Since instead of the actual distribution of the flow velocity and concentration their average values over the cross-section are introduced into the equation, then the averaging effect must be corrected. For this purpose, a diffusion analogy is used. Consequently, the effect of elimination of variable advective transport over the cross-section is described using a diffusive term. However, the value of the coefficient associated with this term does not depend on the properties of water and dissolved pollutant but on the flow velocity and concentration distribution over the channel cross-section. This so-called “the dispersion coefficient” can be considered as “the coefficient of effective diffusion” (Hervouet, 2007). Determining of its value is still a challenge in hydromechanics. More information on the roots of this term is given, for instance, by Cunge et al. (1980) and Rutherford (1994).

The third reason of the possible discrepancy is related to the various types of irregularities occurring in natural channels. These are changes in the shape of cross-sections and the presence of vegetation rooted on the bottom and on the side surfaces of the riverbed. These are the so-called dead zones. Their presence causes the storage of part of the mass of the transported pollutant during the initial phase of its flow. Then the stored mass of pollutant is partly returned to the mainstream. Therefore, the plot of the pollutant concentration in the control cross section

becomes asymmetric. The front of the pollution wave is steeper, while the process of decreasing is longer and may be continued even after the discharge of pollutants to the mainstream has stopped (Rowiński et al., 2004; Sokáč et al., 2018, 2019; Valentine and Wood, 1977, 1979).

The subject of the article are issues related to the two mentioned problems, i.e. the numerical solution of the 1D advection-diffusion equation, which takes into account the presence of dead zones.

Comparison of the observed concentration with the concentration provided by solution of Eq. (1) shows their inconsistency. This was discovered many years ago (Lees et al., 2000; Thackston and Schnelle, 1970), resulting in attempts to improve the mathematical description of the transport process. To increase the accuracy of the simulation results, Eq. (1) was improved by introducing a source term describing the mass exchange between the main-stream and pollutant retention sites and vice versa (Czernuszenko and Rowiński, 1997; Czernuszenko et al., 1998; Rowiński et al., 2004; Runkel, 1998). Consequently, Eq. (1) is combined with an additional equation (Runkel, 1998):

$$\frac{\partial C}{\partial t} + \frac{Q}{A} \frac{\partial C}{\partial x} - \frac{1}{A} \frac{\partial C}{\partial x} \left(A \cdot D \frac{\partial C}{\partial x} \right) = \beta(c - C) \quad (2)$$

$$\frac{\partial c}{\partial t} = \beta \frac{A}{a} (C - c) \quad (3)$$

where c is concentration of pollutant in the dead zones, a is cross-sectional area of the dead zones, and β is a coefficient of mass exchange between mainstream and the dead zones.

Interesting research on the special case of dead zones in a river was performed by Weinbrecht (2004). The studied dead zones are the spaces between groynes constructed in the river bed. The subject of the research was various aspects related to river regulation using groynes, such as their location, groin field geometry and its dimensions, shape of groins, and orientation in relation to the river bank. As a mathematical model of pollutant transport, Weinbrecht (2004) used Eqs. (2, 3).

Another, so called the aggregated dead zone model (ADZ model) belongs to the family of data-based mechanistic models. The concept of this approach was proposed by Young and Lees (1993). In ADZ model, a considered river reach is represented by the numbers of interconnected subreaches. It is assumed that every unit is well mixed. Moreover, the outflow concentration was equal to the cell concentration, and the entrance concentration was equal to the exit concentration of the upstream cell with the time delay. This model has been developed by Chabokpour (2020) to obtain more accurate and effective tool for simulation of pollutant transport in the rivers with dead zones.

Equations (2) describes transport of pollutant in mainstream, whereas Eq. (3) represents mass conservation in the dead zones. They can be treated as an attempt to better describe the transport of pollutants using a 1D mathematical model, although it is known that this process should be considered at least as a 2D problem.

Among the known proposals, it is worth paying attention to the approach proposed by Sokáč et al. (2018, 2019). The authors' idea was to propose relatively simple and reliable method of solution when the dead zones occur. In this approach the analytical solution of the linearized Eq. (1) proposed by Fischer et al. (1979) is replaced by another one, more suitable for asymmetric distribution of concentration. With constant

parameters Eq. (1) can be rewritten as:

$$\frac{\partial C}{\partial t} + U \frac{\partial C}{\partial x} - D \frac{\partial^2 C}{\partial x^2} = 0 \quad (4)$$

where $U = Q/A = \text{const.}$ is cross-sectional average flow velocity and $D = \text{const.}$ is effective coefficient of diffusion. Equation (4) is valid when the non-degradable pollutant is well-mixed over the channel cross-section. If a pollutant of mass M is instantaneously discharged its movement along the channel axis is described by the analytical solution proposed by Fischer et al. (1979):

$$C(x, t) = \frac{M}{2A \cdot (\pi \cdot D^{Ga} \cdot t)^{1/2}} \cdot \exp\left(-\frac{(x - U \cdot t)^2}{4D^{Ga} \cdot t}\right). \quad (5)$$

Equation (5) is based on the Gaussian distribution. For this reason, the symbol D^{Ga} involved in Eq. (5) denotes the effective diffusion coefficient associated with this distribution. As formula (5) generates a solution consistent with the Gauss concentration distribution, it is valid for a channel without dead zones. Unfortunately, it is unreliable in the presence of dead zones. Consequently, a river with dead zones requires a change in the mathematical model. The idea of replacing the solution of the system of Eqs. (2, 3) with the solution of Eq. (4) presented by Fischer et al. (1974), has been proposed by Sokáč et al. (2018). To obtain the effect of solution's asymmetry caused by the dead zones, Sokáč et al. (2018) proposed a modification of the Fischer's solution. The modification consists in replacing the Gaussian distribution with an asymmetric Gumbel distribution. After performing the appropriate transformation, Sokáč et al. (2018) obtained the formula alternative to Eq. (5):

$$C(x, t) = \frac{M}{A \cdot (D^{Gu} \cdot t)^{1/2}} \cdot \exp\left(\frac{x - U \cdot t}{(D^{Gu} \cdot t)^{1/2}} - \exp\left(\frac{x - U \cdot t}{(D^{Gu} \cdot t)^{1/2}}\right)\right) \quad (6)$$

where D^{Gu} is the coefficient of effective diffusion related to the Gumbel distribution. Equation (6) is not an analytical solution to the advection-diffusion equation (4). It only replaces Eq. (5) being its solution (Sokáč et al., 2018). Note that D^{Gu} is the only parameter in Eq. (6) ensuring that the calculation result matches the observations. For this reason, it cannot be identified with the D^{Ga} coefficient appearing in Eq. (5). Nevertheless, a significant improvement of the solution accuracy was shown by Sokáč et al. (2018). The better properties of the unsymmetrical distribution over the Gaussian distribution were also confirmed by Velisková et al. (2023), who used it to solve the inverse problem of pollutant spread in a complex network of open channels.

Equation (6) is valid for a long channel obtained with initial conditions equal to zero and for the boundary condition at the upstream end in the form of an instantaneous pulse of pollutants having mass M . This is a serious limitation of the method's capabilities. Since the approach proposed by Sokáč et al. (2018) turned out to be an effective alternative tool for the boundary condition in the form of contamination impulse having mass M , it seems worth developing it for an arbitrary boundary condition imposed at the upstream channel end. For this purpose, instead of the analytical solution of the advection-diffusion equation proposed by Fischer et al. (1979) and developed by Sokáč et al. (2018), an exact solution corresponding to the boundary condition at the upstream end in the form of the Dirac delta function can be used. Such approach makes it possible to solve

the transport equation for any boundary condition imposed at the upstream end. It can be developed also for flow with variable velocity. Both issues are a subject of this paper.

2 METHODS

In the case of Eq. (1) it is possible to apply another form of its analytical solution than the one proposed by Fischer et al. (1979) and next developed by Sokáč et al. (2018). It is an alternative description of 1D transport of pollutant based on an exact solution of linear advective-diffusive equation (4) with constant coefficients. This solution obtained for the Dirac delta function (Mc Quarrie, 2003) imposed at the upstream end, has the form of convolution.

2.1 Alternative description of 1D transport of pollutants

Consider Eq. (1) linearized to the form of Eq. (4). Its solution for an infinite channel and instantaneous plane source uniformly distributed at $t = 0$ and $x = 0$ over the wetted cross-section is a Gaussian distribution of concentration as a function of space coordinate x , whereas the concentration distribution at the fixed time t is a normal density function. If concentration C is normalized by the total mass of pollutant discharged into the channel, it fulfils the following condition (Czernuszenko and Rowiński, 1997):

$$\int_0^\infty U \cdot C(x, t) \cdot dt = 1 \quad \text{at any } x > 0 \quad (7)$$

where $C(x, t)$ is a Gaussian distribution concentration. Let us select a cross-section with coordinate $x_1 > 0$, in which concentration is described by the function $C_1(t)$. Condition (7) will take the form:

$$\int_0^\infty U \cdot C_1(t) \cdot dt = \int_0^\infty U \cdot \frac{1}{2(\pi \cdot D^{Ga} \cdot t)^{1/2}} \cdot \exp\left(-\frac{(U \cdot t - x_1)^2}{4D^{Ga} \cdot t}\right) \cdot dt = 1. \quad (8)$$

On the other hand, assume that the introduced mass of pollution has the form of the Dirac delta function $\delta(t)$, which is defined as follows (Mc Quarrie, 2003):

$$\delta(t - \tau) = \begin{cases} \infty & \text{for } t = \tau \\ 0 & \text{for } t \neq \tau \end{cases}, \quad \int_0^{+\infty} \delta(t) \cdot dt = 1. \quad (9a, b)$$

This implies that the introduced mass is equal to $M = 1$. Therefore, one can assume that the concentration C normalized by the total mass of pollutant discharged into the channel and condition (8) is valid.

Let us consider a river reach between cross-sections $x = 0$ and $x = x_1$, i.e. with length x_1 , as a dynamic system which transforms the function $C(0, t) = C_0(t)$ into function $C(x_1, t) = C_1(t)$ for $t > 0$. If this system is linear and time invariant, then it can be described by the following convolution (Szymkiewicz, 2010):

$$C_1(t) = C_b(t) + \int_0^t h(\tau) \cdot C_0(t - \tau) \cdot d\tau \quad (10)$$

where $C_0(t)$ is concentration imposed at upstream end ($x = 0$), $C_1(t)$ is computed concentration at the downstream end ($x = x_1$), $C_b(t)$ is component of concentration $C_1(t)$ independent on $C_0(t)$, τ is dummy parameter, and $h(t)$ is the impulse response of system. The function $h(t)$ is an output of system when the input

has the form of unit mass pulse (the Dirac delta function). From Eq. (10) results that $h(t)$ is expressed in units that are the inverse of time units, i.e. in 1/s or 1/h. On the other hand, definition of the Dirac delta function (9) implies that

$$\int_0^{+\infty} h(t) \cdot dt = 1. \quad (11)$$

Knowing the impulse response $h(t)$ one can calculate the function $C_1(t)$ for any value $x_1 > 0$. The required conditions indicate that the impulse response function $h(t)$ for the advection-diffusion equation (4) takes the form of the relationship (8), which is rewritten as follows:

$$h^{Ga}(t) = \frac{U}{2(\pi \cdot D^{Ga} \cdot t)^{1/2}} \cdot \exp\left(-\frac{(U \cdot t - x_1)^2}{4D^{Ga} \cdot t}\right) \quad (12)$$

where $h^{Ga}(t)$ is the impulse response function related to the Gauss distribution. Equation (12) is known as a unit hydrograph for linear diffusive wave proposed by Hyami (Eagleson, 1970).

If a river reach $\langle 0, x_1 \rangle$ is linear and time-invariant, the advective-diffusive transport can be described either by Eq. (4) or by the convolution (10). Both approaches are equivalent. Consequently, instead of solving partial differential equation (Eq. 4) with appropriately imposed initial and boundaries conditions, one can use Eq. (10), in which the definite integral must be calculated numerically. Equations (10) and (12) allow to calculate the function $C_1(t)$ at any cross section $x_1 > 0$ for any function $C_0(t)$ imposed at the upstream end $x = 0$.

The graph of the function $h^{Ga}(t)$ obtained for $U = 0.30$ m/s, $x_1 = 1000$ m, and $D^{Ga} = 1.0$ m²/s is shown in Fig. 1. An impulse response function is always positive ($h^{Ga}(t) \geq 0$ for $t > 0$) and it has a single peak. For time t tending to infinity ($t \rightarrow \infty$) the impulse response function tends to zero ($h^{Ga}(t) \rightarrow 0$). For very small values of the impulse response function, i.e. when $h^{Ga}(t) \leq \varepsilon$, where ε is a small positive number representing a tolerance for convergence, the product under the convolution (10) $h(\tau) \cdot C_0(t-\tau)$ is close to zero and has no effect on the convolution value. For this reason, one can introduce memory p of river reach system (see Fig. 1). It defines "length of the past" from which the pollutant concentration is taken into account. Otherwise, information about concentration at the upstream end that is distant in time from the current time t has no influence on the information about concentration at the downstream end at a given time t . Taking into account the definition of memory p , Eq. (10) can be rewritten as follows:

$$C_1(t) = C_b(t) + \int_0^p h(\tau) \cdot C_0(t-\tau) \cdot d\tau \quad (13)$$

where p is memory of river reach system. Consequently, time of calculations is shortened and the required computer memory is reduced. As for the $C_b(t)$ term, it must be known. However, in further analysis presented in this paper $C_b(t) = 0$ is assumed.

When $D^{Ga} \rightarrow 0$ the function $h^{Ga}(t)$ given by Eq. (12) tends to the Dirac delta function, i.e. $h^{Ga}(t) \rightarrow \delta(t-x/U)$. This ensures pure translation of any concentration distribution with flow velocity U . Consequently, any concentration distribution imposed as the boundary condition at the upstream end travels along channel axis without any shape deformation.

It should be noted that there is an important difference between application of the numerically solved the partial differential transport equations and the use of a convolution transport

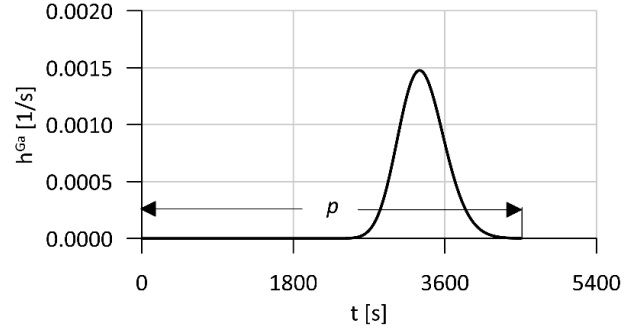


Fig. 1. Impulse response function calculated after Eq. (8) for $x = 1000$ m, $U = 0.30$ m/s and $D = 1.0$ m²/s.

description. Instead of solving Eqs. (2, 3) using the finite differences or elements method, the integral (13) must be calculated numerically. For a system bounded by two neighboring cross-sections 1 and 2 the rectangular method of integration provides the formula:

$$C_k^{(2)} = \Delta\tau \cdot \sum_{i=1}^{P} (h_i^{(1-2)} \cdot C_{k-i+1}^{(1)}) \quad (\text{for } k = 1, 2, 3, \dots) \quad (14)$$

where $C^{(1)}$ is concentration in the upstream cross-section, $C^{(2)}$ is concentration in the downstream cross-section, $h_i^{(1-2)}$ is the impulse response function of the river reach between cross-section 1 and 2, k is index of time step, $P = p/\Delta\tau + 1$ is the discrete memory, $\Delta\tau$ is stepsize used for numerical calculation of convolution integral.

To show how the described approach works, consider the following example. Assume that in a straight long channel a steady uniform flow takes place. The flow velocity equal to $U = 0.30$ m/s is constant over a 4000 m long channel reach. The following initial and boundary conditions are imposed:

$$C(x, 0) = 0 \text{ for } 0 \leq x \leq 4000 \text{ m,}$$

$$C(0, t) = C_1(t) = \begin{cases} 0 & \text{for } t < 600 \text{ s} \\ 1 & \text{for } 600 \text{ s} \leq t \leq 1800 \text{ s} \\ 0 & \text{for } t > 1800 \text{ s} \end{cases}$$

As one can see, in this case a rectangular distribution of concentration travels along x axis. This is a very strong test for numerical solution. The function $C_2(t)$ at the point $x_1 = 3000$ m was calculated for two values of effective diffusion coefficient: $D = 0.0005$ m²·s⁻¹ and $D = 1.0$ m²·s⁻¹ with the stepsize equal to $\Delta\tau = 10$ s. The results are presented in Fig. 2. The obtained solutions are close to the exact ones. In the solution of the advection-diffusion equation, the initial rectangular concentration distribution moves along the channel axis without shape deformation. Even though the effective diffusion coefficient is very small ($D^{Ga} = 0.0005$ m²/s), there are no spurious oscillations in the solution.

The error related to the trapezoidal rule used for integration of the $h^{Ga}(t)$ function is not large on condition that the value of used stepsize $\Delta\tau$ is sufficiently small. It should be noted that the shape of the $h^{Ga}(t)$ function depends on the value of the effective diffusion coefficient D^{Ga} . The higher its value, the longer time interval over which the $h^{Ga}(t)$ function spans. Condition (11) was assumed as a measure of compliance with the principle of mass conservation. Numerical integration of the impulse response function $h^{Ga}(t)$ carried out using the trapezoidal formula showed that the approximate value of the integral (11) calculated for $D^{Ga} = 0.0005$ m²/s and $\Delta\tau = 20$ s is equal to $\int_0^p h^{Ga}(\tau) \cdot d\tau = 1.008$.

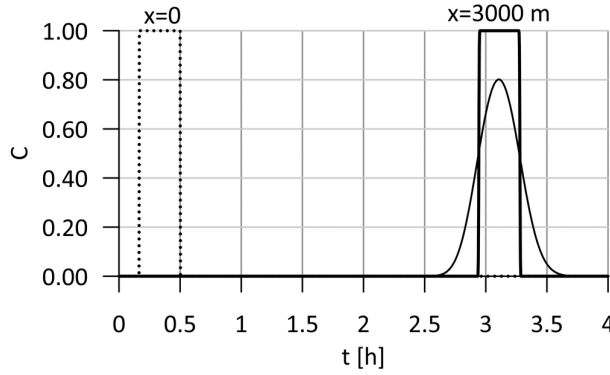


Fig. 2. Concentration imposed at the upstream end (dotted line) and computed at cross section $x = 3000$ m using Eqs. (7) and (8) with $D = 1.0$ m²/s (thin line) and $D = 0.0005$ m²/s (thick line).

This means that the error associated with determining the function $h(t)$ does not exceed 1%. To reduce this error the stepsize $\Delta\tau$ used for integration should be reduced. However, for $D^{Ga} = 1.0$ m²/s, a stepsize $\Delta\tau$ of up to 360 s ensures very good fulfillment of condition (11), because $\int_0^p h^{Ga}(\tau) \cdot d\tau = 1.0$. This means that for both values of the diffusion coefficient D^{Ga} , the principle of the mass conservation of the pollutant dissolved in water is perfectly satisfied.

Interesting information is provided by the Péclet number. This dimensionless number defined as follows:

$$P = U \cdot \Delta x / D^{Ga}. \quad (15)$$

defines the relationship between advective and diffusive part in transport equation (Fletcher, 1991). For $U = 0.30$ m/s, $\Delta x = 3000$ m and $D^{Ga} = 0.0005$ m²/s it is equal to $P = 1\,800\,000$, whereas for $D^{Ga} = 1.0$ m²/s one obtains $P = 900$. Therefore, in both cases transport of pollutant is dominated by advection.

The presented results show that the lack of numerical diffusion and dispersion, typical for the finite difference technique, is the main feature of the convolution approach. Consequently, the provided solution it is not artificially smoothed and not affected by the spurious oscillations. Additionally, the numerical diffusion generated by the method of solution can interfere with the process of identifying the diffusion coefficient D^{Ga} , particularly when the numerical diffusion is not estimated.

2.2 Approximation of the impulse response function for a river reach with dead zones

Formula (12) generates a solution with a Gaussian concentration distribution. As previously stated, the presence of dead zones requires a change in the mathematical model. Sokáč et al. (2018) replaced the Gaussian distribution with the asymmetric Gumbel one. After performing the appropriate transformation, Sokáč et al. (2018) obtained the formula (6). As stated earlier, this equation is not an analytical solution to the advection-diffusion equation (Eq. 4). It is an approximation of the solution (5). However, it improves the solution results when the dead zones exist. Since the proposed approach turned out to be an effective tool for solution with the boundary condition in the form of the contamination pulse having mass M , it seems worth developing it for any boundary condition imposed at the upstream channel end. To this end the convolution approach described earlier is used.

If the total mass of pollutant discharged into the channel has the form of unit mass pulse, the analytical solution has the following unitary form (Sokáč et al. (2018)):

$$C(x, t) = \frac{1}{(D^{Gu} \cdot t)^{1/2}} \cdot \exp\left(\frac{x - U \cdot t}{(D^{Gu} \cdot t)^{1/2}} - \exp\left(\frac{x - U \cdot t}{(D^{Gu} \cdot t)^{1/2}}\right)\right). \quad (16)$$

Therefore, according to condition (7), for $x = x_1 > 0$, Eq. (16) becomes an impulse response function for the channel reach $\langle 0, x_1 \rangle$:

$$h^{Gu}(t) = \frac{U}{(D^{Gu} \cdot t)^{1/2}} \cdot \exp\left(\frac{x_1 - U \cdot t}{(D^{Gu} \cdot t)^{1/2}} - \exp\left(\frac{x_1 - U \cdot t}{(D^{Gu} \cdot t)^{1/2}}\right)\right) \quad (17)$$

where $h^{Gu}(t)$ is the impulse response function corresponding to the asymmetric Gumbel distribution. Using Eq. (17) one can calculate the convolution (14) for any function imposed at the upstream end $C(0, t) = C_0(t)$. Consequently, concentration at the downstream end $C(x_1, t) = C_1(t)$ for $t > 0$ is provided.

Applying Eq. (17) one must be sure that it meets the principle of mass conservation, i.e. Eq. (11) has to be satisfied. To verify this condition consider a straight channel in which a steady uniform flow takes place. The constant flow velocity equal to $U = 0.30$ m/s is assumed. The function $h^{Gu}(t)$ corresponding to $x = x_1 = 1800$ m is calculated for the value of effective diffusion coefficient ranging from $D^{Gu} = 0.001$ m²·s⁻¹ to $D^{Gu} = 5.0$ m²·s⁻¹. The integral (11) was calculated using the trapezoidal method with the stepsize equal to $\Delta\tau = 10$ s. The obtained results show that its value ranges from 0.998 for $D^{Gu} = 0.001$ m²/s to 1.026 for $D^{Gu} = 5.0$ m²/s. It seems that such differences may be acceptable in numerical calculations. However, it is worth adding that the impulse response function corresponding to a Gaussian distribution $h^{Ga}(t)$ for the above data always provides $\int_0^p h^{Ga}(t) \cdot dt = 1$.

The method presented above dealt with steady uniform flow ($U = \text{const.}$). A more realistic case is steady gradually varied flow when the flow velocity and wetted cross-sectional area change along x axis. During steady gradually varied flow, the discharge along the channel axis may be constant ($Q = \text{const.}$) or variable ($Q = Q(x)$). Such a case of transport is described by Eq. (1) (French, 1985):

$$\frac{\partial C}{\partial t} + U \frac{\partial C}{\partial x} - \frac{1}{A} \frac{\partial}{\partial x} \left(A \cdot D \frac{\partial C}{\partial x} \right) = 0 \quad (18)$$

where $U = U(x) = Q/A(x)$ is cross-sectional average velocity, whereas $A = A(x)$ is area of wetted cross-section. Assuming $D = \text{const.}$ Eq. (18) becomes:

$$\frac{\partial C}{\partial t} + \left(U - \frac{D}{A} \frac{\partial A}{\partial x} \right) \frac{\partial C}{\partial x} - D \frac{\partial^2 C}{\partial x^2} = 0. \quad (19)$$

In this equation the advective celerity varies. To solve Eq. (19) using the presented method, the advective velocity can be locally frozen. To this purpose a channel reach of length L is divided into $N-1$ reaches of length Δx_i as it is done in the finite difference or element method (see Fig. 3). Each channel's reach Δx_i is considered as a dynamic system (Szymkiewicz and

Weinerowska, 2005). Assume that over each interval the advective velocity is constant and equal to arithmetic average value taken from the nodes limiting the Δx_i reach. It is defined as:

$$\bar{U}_i = \frac{1}{2} \left[\left(U - \frac{D \partial A}{A \partial x} \right)_{i-1} + \left(U - \frac{D \partial A}{A \partial x} \right)_i \right] \quad (20)$$

where $\bar{U}_i$ is average advective velocity between i and $i+1$ node. Therefore each interval Δx_i ($i = 1, 2, \dots, N-1$) has an impulse response function in the form of Eq. (17) rewritten as:

$$h_i^{(Gu)}(t) = \frac{\bar{U}_i}{2(D^{Gu} \cdot t)^{1/2}} \cdot \exp \left(\frac{\Delta x_i - \bar{U}_i \cdot t}{(D^{Gu} \cdot t)^{1/2}} - \exp \left(\frac{\Delta x_i - \bar{U}_i \cdot t}{(D^{Gu} \cdot t)^{1/2}} \right) \right) \quad (21)$$

Consequently, a channel of length L is divided into $N-1$ systems of length Δx_i in series. An output from preceding system is an input to next one. It should be noted that this approach is similar to the concept used in the ADZ model mentioned earlier (Chabokpour, 2020). In ADZ model, a considered channel is also represented by N channel's reaches Δx_i connected in series.

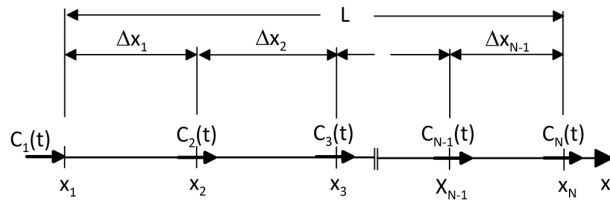


Fig. 3. A channel reach of length L divided into $N-1$ sub-reaches.

3 RESULTS AND DISCUSSION

The procedure of calculation is implemented for steady gradually varied flow and pollutant transport in the Wkra River in Poland, being a tributary of the Vistula River. Pollution concentration measurements were made by Krukowski and Kurzawski (2001). As the marker alcoholic solution of a rhodamine B had been used. It was introduced into a river in the cross-section located at km 131.220. Its concentrations were recorded in 5 cross-sections listed in Table 1. The first cross-section where concentration was measured has been located

600 m below the tracer release point. The average flow velocities and the cross-section areas are also presented in Table 1, whereas the recorded concentrations are displayed in Fig. 4.

Although the measurements were made on a relatively short reach of the river (4180 m), the asymmetric shapes of the observed concentration distributions clearly indicate the presence and influence of the dead zones. In Fig. 4 all concentration curves are asymmetrical. During the passage of a wave of pollutant in a natural riverbed, part of their mass is retained in dead zones from where it returns to the mainstream as the wave is receding. This fact can be checked by mass balance of pollutant dissolved in water and flowing through the subsequent sections. Note that the marker used in field experiments was non-degradable. The results of integrating the concentration curves from Fig. 4 are summarized in Table 2.

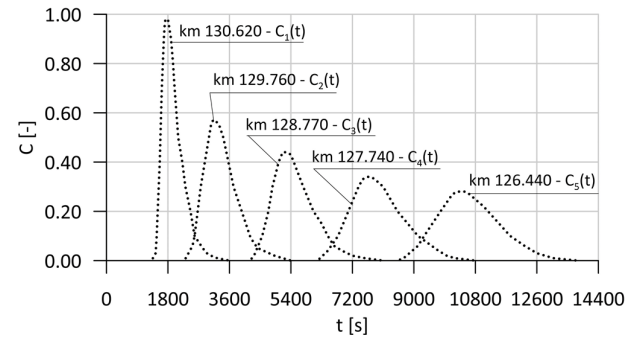


Fig. 4. Measured concentrations of the tracer in selected cross-sections of the Wkra River (Krukowski and Kurzawski, 2001).

The average relative mass of pollutant in 5 sections is equal to 620.82. The difference is therefore from +1.86% to -2.48%. The term “relative mass of a pollutant” is used because the concentration $C(x,t)$ expressed as the ratio of the actual concentration to the maximum concentration is dimensionless and varies from 0 to 1. The measured maximum concentrations ranged from 0.098 kg/m³ in cross-section 1 to 0.028 kg/m³ in cross-section 5.

The values of the relative mass of pollutants flowing through the measurement cross-sections are close to each other. This means that the mass of pollutant retained in the dead zones when the wave is raising was fully returned to the mainstream. The mass balance errors in subsequent river cross-sections are probably the result of unavoidable measurement errors.

Table 1. Hydraulic parameters characterizing the cross-sections of the Wkra River during the measurements (Krukowski and Kurzawski, 2001).

Reach number	Position x [km]	Average flow velocity U [m/s]	Cross-section area A [m ²]	Flow rate Q [m ³ /s]
1	130.620	0.518	8.07	4.18
2	129.760	0.430	9.72	
3	128.770	0.455	9.19	
4	127.740	0.412	10.15	
5	126.440	0.404	10.35	

Table 2. Mass of pollutants flowing through the control cross-sections of the Wkra River.

Index of cross-section	1	2	3	4	5
$\int_0^{t_{\max}} C(\tau) \cdot d\tau$	627.00	628.50	605.40	632.40	610.80

Calculations with the proposed method were carried out for the first system bounded by two control cross-sections located at km 130.620 and km 129.760 (see Fig. 4 and Table 1). Its length was equal to $\Delta x_1 = 860$ m. The boundary condition imposed at the upstream end is the concentration $C_1(t)$ (Fig. 4). The considered system transforms this function into the curve of concentration $C_2(t)$ (km 129.760 in Fig. 4). Numerical tests showed that for the assumed data and for a tolerance for convergence equal to $\varepsilon = 0.000001 \text{ s}^{-1}$ the system memory is ca $p = 4800$ s. Comparison of the measured concentrations in the second cross-section of the Wkra River with the results of calculation provides some interesting insights into the mechanism of pollutant transport. Firstly, pollutants move in the mainstream at a speed higher than the average flow velocity. In order to obtain consistency of the observed and calculated concentration peaks, higher advection velocities should be assumed than those shown in Table 1. For instance, the average flow velocity over river reach of length Δx_1 equal to arithmetic average taken from both system's ends $\bar{U}_1 = (0.518 + 0.430)/2 = 0.474 \text{ m/s}$ had to be increased to 0.668 m/s . This value ensuring consistency of time occurring of both measured and computed concentration peaks in the second cross-section was estimated using recorded concentrations $C_1(t)$ and $C_2(t)$. Knowing the distance between cross-sections 1 and 2 and the lag time of the centers of gravity of both functions $C_1(t)$ and $C_2(t)$, one can calculate the average speed of pollution wave traveling along the channel axis.

The second factor determining the matching of measurements and calculations is the effective diffusion coefficient D^{Gu} . To evaluate its value more precisely the objective function in the form of the Root Mean Square Error (RMSE) is used:

$$RMSE(D^{Gu}) = \left(\frac{1}{N} \sum_{i=1}^N (C_2(t_i) - \bar{C}_2(t_i))^2 \right)^{1/2} \quad (22)$$

where $C_2(t_i)$ is concentration computed at time t_i , $\bar{C}_2(t_i)$ is concentration measured at time t_i , N is the total number of the compared points. Note that the only parameters involved in Eq. (21) which influences the objective function (22) is the coefficient of effective diffusion for Gumbel distribution D^{Gu} . Therefore, one can try to search such value of D^{Gu} which will minimize the objective function (22). The numerical experiments show that the $RMSE(D^{Gu})$ possesses only one extreme point being its minimum. Unimodal property of the objective function allows to solve the optimization problem about D^{Gu} using simple methods - dividing on three equal parts or dividing using golden number (Press et al., 1992). The best fit was obtained for the diffusion coefficient equal to $D^{Gu} = 30.0 \text{ m}^2/\text{s}$. The results of observations and calculations are shown in Fig. 5. In the same figure the result of calculation using the impulse response function according to the Gaussian distribution is also displayed. This result was obtained for an effective diffusion coefficient much smaller than one used in the case of the Gumbel distribution ($D^{Ga} = 16.0 \text{ m}^2/\text{s}$). Although this value ensured consistency in the culmination of impulse response functions $h^{Gu}(t)$ and $h^{Ga}(t)$ shown in Fig. 6, the calculation results displayed in Fig. 5 are less accurate than in the case of the Gumbel distribution. For instance, the root mean square error is equal to $RMSE = 0.0141$ for the Gumbel distribution, whereas it is equal to 0.0474 for the Gauss distribution. Location of the impulse response function $h^{Ga}(t)$ given by Eq. (12) along time axis for selected cross-section x_1 is determined by the average flow velocity U , whereas its shape is determined by the value of effective diffusion coefficient D^{Ga} .

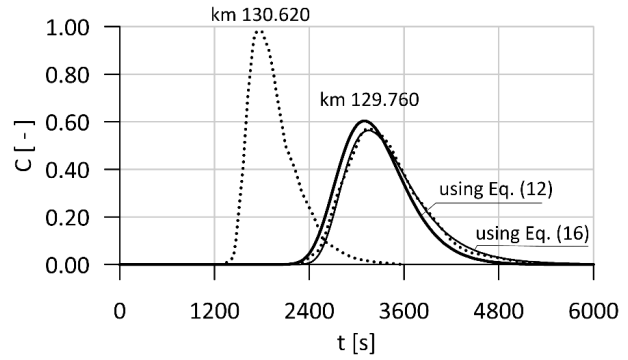


Fig. 5. Measured (dotted lines) as well as computed with Gumbel (thin line) and Gauss (thick line) distribution of concentrations in the second cross-section of the Wkra River.

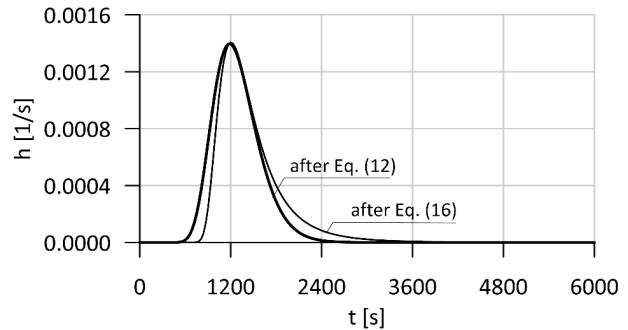


Fig. 6. The impulse response functions calculated for the first river reach Δx_1 according to Eq. (8) (thick line) and Eq. (14) (thin line) with $\Delta t = 30$ s.

For decreasing value of coefficient of effective diffusion the shape of $h^{Ga}(t)$ becomes more and more sharp. However, its integral over time is still equal to 1 (see Eq. 12).

The impulse response function $h^{Gu}(t)$ corresponding to the Gumbel distribution (Eq. 17) is shown in Fig. 6. Comparison of its shape with the shape of the $h^{Ga}(t)$ function described by Eq. (12) confirms that it allows reproducing the effect of dead zones existing in the river. Since the shape of the $h^{Gu}(t)$ function depends on the diffusion coefficient D^{Gu} , its value was assumed to ensure compliance of its peak with the peak of the $h^{Ga}(t)$ function. In this case, this occurs for $D^{Gu} = 30.0 \text{ m}^2/\text{s}$. As the impulse response $h^{Gu}(t)$ is only an approximation of the function $h^{Ga}(t)$ given by Eq. (12), then its integration over time gives a value that is not equal to unity. The difference depends on the assumed value of D^{Gu} diffusion coefficient. For example, $D^{Gu} = 30.0 \text{ m}^2/\text{s}$ causes that the integral $\int_0^p h^{Gu}(\tau) \cdot d\tau$ is equal to 0.9366, whereas for $D^{Gu} = 5.0 \text{ m}^2/\text{s}$ it is equal to 0.9729. The above results indicate that the contaminant mass conservation principle is not satisfied and some mass balance error is generated. As stated by Sokáč et al. (2018), the problem of mass balance error also occurs in the case of Eq. (16) replacing the exact solution proposed by Fischer et al. (1979).

To eliminate the mass balance error, the $h^{Gu}(t)$ function must be corrected. This can be done as follows:

- Integrate numerically the function $h^{Gu}(t)$ over the time interval $\langle 0, p \rangle$:

$$\Delta = \Delta t \cdot \sum_{j=1}^{P-1} \frac{(h^{Gu})_j + (h^{Gu})_{j+1}}{2} \quad (23)$$

where Δt is time step, P is discrete memory equal to $P = p/\Delta t + 1$;

- Calculate the correction per unit of ordinate of the function $h_{Gu}(t)$:

$$\Delta h = \frac{1.0 - \Delta}{\Delta t \cdot \sum_{j=1}^P (h^{Gu})_j} \quad (24)$$

- Correct the ordinates of the $h_{Gu}(t)$ function in proportion to their values:

$$(h^{Gu})_j^* = (h^{Gu})_j + \Delta h \cdot (h^{Gu})_j. \quad (25)$$

This correction of the impulse response function ensures the fulfillment of the principle (11) representing conservation of the dissolved pollutant mass.

The approach to simulating pollutant transport discussed above for the first river reach Δx_1 was extended for all considering reaches Δx_i ($i = 2, 3, 4$). It was assumed that the output from the previous system is the input to the next system (see Fig. 3). This assumption is justified because the constant flow rate in the river ($Q = 4.18 \text{ m}^3/\text{s} = \text{const.}$) ensures equality of mass fluxes on both sides of the common cell boundaries. Each pair of neighboring cross-sections delimits a river reach of length Δx_i . In a similar way the advective velocities in the mainstream were corrected for all Δx_i reaches (see Table 3). Note that they are larger than the measured average flow velocity (see Table 1).

At the upstream end ($x_1 = 130.620 \text{ km}$) the boundary condition in the form of curve $C_1(t)$ was imposed (see Fig. 4). Using the convolution (13) the curves representing concentration in the next cross-sections were computed. Similarly to the flow velocity, the coefficients D^{Gu} constant over Δx_i is also assumed. The values of D^{Gu} ensuring compliance of the peaks in subsequent cross-sections are shown in Table 3. The calculated results of the pollutant transport simulation are displayed in Fig. 7.

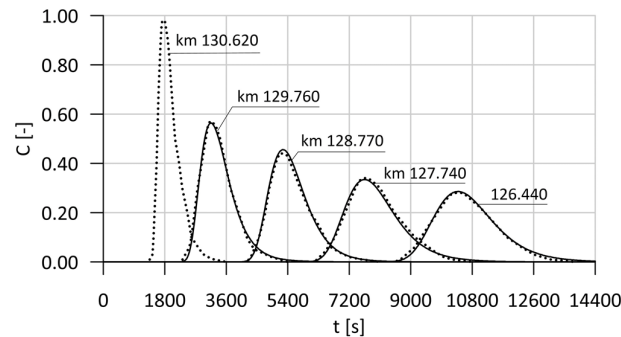


Fig. 7. Concentrations in the control cross-sections of the Wkra River: measured (dotted lines) and computed using Eq. (18) (solid lines).

The accuracy of solution depends not only on the average flow velocities between both ends of each reach Δx_i ($i = 1, 2, \dots, 4$)

and on the coefficients of effective diffusion D^{Gu} , but it is also dependent on the assumed stepsize $\Delta \tau$ used for calculation of the convolution (13). Numerical tests showed that stepsize values of $\Delta \tau$ not exceeding 30 s caused only slight differences in calculation results. The RMSE error values corresponding to the U and D^{Gu} values assumed for the calculations are also presented in Table 3.

Very small values of the RMSE confirm the excellent agreement of the calculation and measurement results visible in Fig. 7. However, note that the effective diffusion coefficient D^{Gu} in the impulse response function corresponding to the Gumbel asymmetric distribution (Eq. (17)) is not identical to the D^{Ga} coefficient involved in Eq. (12), which is the impulse response function corresponding to the Gauss distribution. Equation (17) replaces Eq. (12) and the D^{Gu} coefficient is the only factor influencing the shape of the impulse response function $h^{Gu}(t)$. It replaces influence of several other coefficients involved in Eqs. (2, 3) and describing the impact of dead zones. Consequently, instead of solving an optimization problem in which the optimal values of 6 parameters are sought (Czernuszenko and Rowiński, 1997), in the considered approach only the optimal value of the D^{Gu} coefficient is searched. As shown earlier, in the case of the Wkra River, the value of D^{Gu} is almost twice as high as the value of the D^{Ga} coefficient. This means that, unlike the D^{Ga} coefficient, the D^{Gu} coefficient cannot be treated as a physical parameter characterizing the longitudinal effective diffusion process. However, the calculation results suggest that its value can be related to the D^{Ga} value. Sokáč et al. (2018) propose a mathematical relation of the type $D^{Gu} = f(D^{Ga})$. This makes it possible to determine the D^{Gu} value based on numerous known formulas proposed for estimating the D^{Ga} coefficient.

4 CONCLUSIONS

In the proposed approach a channel reach of length Δx was assumed to be linear and time invariant system which is described by a convolution. The impulse response function of this system is obtained via analytical solution the advection-diffusion equation in a semi-infinite channel for initial condition equal to zero and for boundary condition in the form of a Dirac delta function imposed at the upstream end, which provides an impulse of unit mass. To simulate the advective-diffusive transport in open channel with dead zones this impulse response function, corresponding to the Gaussian distribution, was replaced by the Gumbel asymmetric distribution. In this way it is possible to simulate the transport of pollutants for any boundary condition imposed at the upstream channel's end. However, it turned out that the approximate impulse response function generates an error in the mass balance of the transported pollutant. To eliminate this error a correction of the impulse response function has to be done.

The method does not need any approximation of derivatives. Consequently, it does not produce any numerical diffusion and numerical dispersion leading to artificial damping or spurious

Table 3. Hydraulic parameters characterizing the considered reaches of the Wkra River which ensure satisfying consistency of the measurements and computations.

Reach number	Length Δx_i [km]	Flow velocity in mainstream U [m/s]	Coefficient of effective diffusion D^{Gu} [m ² /s]	RMSE(D^{Gu})
1	0.860	0.668	30.0	0.0141
2	0.990	0.503	8.00	0.0083
3	1.030	0.461	14.00	0.0107
4	1.300	0.509	11.00	0.0072

oscillations, respectively. The approach valid for linear transport equation has been extended to solve the equation with variable velocity. Validation using the results of field experiments showed very high accuracy of obtained solution. This suggests that the proposed approach can be considered as simple and relatively accurate alternative approach to simulating pollutant migration in the small rivers with dead zones.

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Received 2 February 2024
Accepted 8 September 2024