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An approximate method for 1-D simulation of pollution transport in streams with dead zones

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Abstract: Analytical solutions describing the 1D substance transport in streams have many limitations and factors, which determine their accuracy. One of the very important factors is the presence of the transient storage (dead zones), that deform the concentration distribution of the transported substance. For better adaptation to such real conditions, a simple 1D approximation method is presented in this paper. The proposed approximate method is based on the asymmetric probability distribution (Gumbel's distribution) and was verified on three streams in southern Slovakia. Tracer experiments on these streams confirmed the presence of dead zones to various extents, depending mainly on the vegetation extent in each stream. Statistical evaluation confirms that the proposed method approximates the measured concentrations significantly better than methods based upon the Gaussian distribution. The results achieved by this novel method are also comparable with the solution of the 1D advection-diffusion equation (ADE), whereas the proposed method is faster and easier to apply and thus suitable for iterative (inverse) tasks.

Keywords: Environmental hydraulics; River pollution; Hydrodynamic dispersion; Longitudinal dispersion; Dead zones.

INTRODUCTION

The transport of a solute in a stream is usually driven by a combination of advection and dispersion. Both phenomena are related to the characteristics of the streamflow and help to reduce the maximum concentration values in the stream. The main parameter of dispersion is the dispersion coefficient, whose determination plays therefore a key role in studies about the transport of pollutants in streams and water quality modelling (Baek and Seo, 2016; Toprak and Cigizoglu, 2008; van Mazijk, 1996).

Furthermore, solute transport in streams and rivers is strongly related to river characteristics, such as mean flow velocity, velocity distribution, secondary currents and turbulence features. These parameters are mainly determined by the river morphology and the discharge conditions. Most natural channels are characterized by relevant diversity of morphological conditions. In natural channels, changing river width, curvature, bed form, bed material and vegetation are the reason for this diversity. In rivers, which are regulated by man-made constructions, such as spur dikes, groins, stabilized bed and so on, the morphological diversity is often less pronounced and, thus, flow velocities across the stream are more homogeneous.

In natural channels, some of these morphological irregularities, such as small cavities existing in sand or gravel beds, side arms and embayments, bigger obstacles, bank vegetation, uprooted trees can produce recirculating flows which occur on different scales on both the riverbanks and the riverbed. These irregularities act as dead zones for the current flowing in the main stream direction. In regulated rivers, groyne fields are the most important sort of dead zones. Groyne fields can cover large parts of the river significantly affecting its flow field. Dead-water zones or dead zones can be defined as geometrical irregularities existing at the river periphery, within which the mean flow velocity in the main stream direction is approximately equal to zero (or even negative) (Weitbrecht, 2004).

Dead zones significantly modify velocity profiles in the main channel as well as they are affecting dispersive mass transport within the river. They collect and separate part of the solute from the main current. Subsequently the solute is being slowly released and incorporated back to the main current in the stream. Even the hyporheic exchanges between the surface waters and the adjacent/underlying groundwater may affect the transport of solutes with the long-time tailing behaviour in the time-concentration curves (Tonina, 2012).

Thus, in recent years exchange processes between the main stream and its dead zones were increasingly studied, mostly using experimental laboratory and field works (Brevis et al., 2006; Engelhardt et al., 2004; Jamieson and Gaskin, 2007; Kimura and Hosoda, 1997; Kurzke et al., 2002; Muto et al., 2000; Sukhodolov, 2014; Uijttewaal, 1999, 2005; Uijttewaal et al., 2001; Weitbrecht and Jirka, 2001; Weitbrecht et al., 2008; Yossef and de Vriend, 2011). Also, computational methods were widely carried out to investigate hydrodynamics in channels with dead zones of different type and shape (Gualtieri, 2008, 2010; McCoy, 2008; McCoy et al., 2006; Weitbrecht, 2004).

Mathematical solution of the dispersion in streams with dead zones has been extensively described (De Smedt, 2006, 2007; De Smedt et al., 2005; Runkel, 1998) as well as the effect of the vegetation in stream (Shucksmith et al., 2010) (Shucksmith et al., 2011), (Murphy et al., 2007). However, the majority of these solutions are complicated, regarding the mathematical apparatus and their numerical application (Czernuszenko et al., 1998; Davis and Atkinson, 2000; De Smedt, 2006; De Smedt et al., 2005). Code programming is quite difficult and longer computing time is required, especially in cases where many simulations are needed. On the other hand, based on the nature of analytical solutions, the superposition principle can be applied. Based on this, the analytical solutions can be widely applied in engineering practice including their ability to simulate various types of pollution inputs (continuous, discontinuous, steady, unsteady etc.) as well as other specific pollution types, e.g. turbidity (Wang et al., 2017).

The goal of this paper is to provide a simple mathematical method, which would allow quick and easy one-dimensional modelling of the dispersion process in streams with influence of dead zones. Our effort was oriented to find a mathematical approximation formula of the dispersion process with focus on instantaneous injection. This formula was verified on tracer experiments data measured on three streams (channels) in southern Slovakia, where a significant presence of the dead zones was found (Malá Nitra, Šúrsky and Malina streams).

DEAD ZONES EFFECT ON MASS TRANSPORT IN RIVERS

The classical Dead-Zone-Model

Following a tracer cloud from the source until it is spread over the entire river cross-section, three stages of mixing can be distinguished (Rutherford, 1994). In the *near-field* mixing is dominated by buoyancy and momentum forces that are determined by the effluent, so transport phenomena must be considered as 3D problems. In the *mid-field* the tracer mass is already mixed over the river depth, so transport phenomena can be treated as depth-averaged 2D problems. The sum of the above mixing zone is also termed as *advective length*. In the *far-field*, the tracer mass is well-mixed over the entire river cross-section, so transport phenomena are often studied as cross-sectional 1D problem. Also, in the far-field the skewness of the tracer distribution in the longitudinal direction slowly vanishes. Therefore, in the far-field, solute transport is usually analyzed by using the classical 1D advection-dispersion equation (ADE), where the main problem is to apply a reasonable value of the longitudinal dispersion coefficient. The general form of the ADE is (Socolofsky and Jirka, 2005)

$$\frac{\partial C}{\partial t} + v_x \frac{\partial C}{\partial x} = D_x \left(\frac{\partial^2 C}{\partial x^2} \right) + M_s \qquad (1)$$

where t is the time (s), C is the concentration of a substance (kg m^{-3}), D_x is the dispersion coefficient in the longitudinal direction (m^2 s^{-1}), v_x is the velocity of water flow in x (longitudinal) direction of flow (m s^{-1}), M_s is a function representing the sources of pollution (kg m^{-3} s^{-1}), x is the spatial coordinate – distance (m).

However, many field studies demonstrated that the ADE predictions often do not fit well with the observed tracer concentrations from instantaneous spills. Two discrepancies were observed (Weitbrecht, 2004). First, the tracer concentration curve shows a sharp front and a long tailing. Second, in natural channels, the average velocity of the solute is always somewhat lower than the average water velocity of the river. This can be explained by the exchange processes between the main flow in the channel and the dead-water zones existing at its periphery – the solute cloud is retarded by boundary trapping. Due to momentum exchange across the interface with the main channel, flow patterns inside the dead zones are characterized by recirculating flows which occur on different scales and exhibit flow velocity in the main stream direction close to zero. Therefore, the most important effect of dead zones on mass transport in rivers is the storage of some amount of the contaminants or nutrients being transported by the main stream inside the dead zones, i.e. some mass of solutes is trapped in the dead zones and later, after an average storage time T_{DZ}, is released back into the main flow. The storage time depends on the strength of the exchange processes occurring between the main stream and the dead zones, which are mostly due to turbulent mixing in the lateral or in the vertical direction, if the dead zone is at the riverbanks or at the riverbed, respectively (Muto et al., 2000; Weitbrecht, 2004).

In a channel without dead zones, the average transport velocity of a tracer cloud that is completely mixed over the river cross-section equals the mean flow velocity. If dead zones are present, the part of the tracer cloud trapped in the dead zones is retarded in comparison with the part of tracer cloud travelling in the main stream with the mean flow velocity. In this case, the transport velocity of the tracer cloud is lower than the average flow velocity. Also, dead zones produce an increased stretching of a passing tracer cloud, which means that the longitudinal dispersion is enhanced. These results in a tail of the contaminants cloud longer than that predicted by the ADE (Czernuszenko et al., 1998) and the length of the tail depends on the exchange between the main flow and the dead zones. This could be explained by two processes (Weitbrecht, 2004). First, dead zones modify the transverse profile of flow velocity in the main channel and increase lateral turbulent mixing, which are the determining parameters for longitudinal dispersion. It is well known that transverse mixing is important in determining the rate of longitudinal mixing because it tends to control the exchange between regions of different longitudinal velocity. Particularly, transverse mixing and longitudinal mixing are inversely proportional. A strong transverse mixing tends to erase the effect of differential longitudinal advection and pollutants particles migrate across the velocity profile so fast that they essentially all move at the mean speed of the flow, causing only a weak longitudinal spreading. On the other hand, a weak transverse mixing implies a long time for differential advection to take effect, so the pollutants patch is highly distorted while it diffuses moderately in the transverse direction and longitudinal mixing is large (Cushman-Roisin, 2012). Second, the tracer cloud is stretched because solute parcels are trapped within the dead zones and only later released back into the main channel. The temporary accumulation of the transported substance commonly causes deformation of the concentration distribution curve (van Mazijk and Veling, 2005). The substance is released later and more slowly, giving rise to the steep front of the concentration distribution curve, followed by "long tail" (Fig. 1). Both processes result in longitudinal dispersion process character, which leads to lower peak levels of tracer concentration, but also to a longer period of time. Finally, these processes are strongly related to the geomorphological conditions of the dead zones. Obviously, if the stream cross-section is not regular, Fick's law cannot be applied even after a long period, since the concentration distribution due to large irregularities of the stream bed will never be a Gaussian (Davis et al., 2000; Nordin and Troutman, 1980).

Therefore, models accounting for the dead zones effects were proposed to be applied in rivers where there is a relevant presence of dead zones. The basic idea of the dead-zone model (DZM) is to distinguish two zones within the cross-section of a river, the main stream and the dead-zone. In the main stream the mass transport is governed by advection in the longitudinal direction, longitudinal shear due to the velocity distribution and transverse turbulent diffusion. Thus, the transport processes in the main stream can be modeled under well mixed conditions using the 1D ADE. In the dead zone, since velocity in the main stream direction is close to zero, transverse turbulent diffusion across the interface between the dead zone and the main stream is the dominant mechanism, which leads to momentum and mass exchange processes. Assuming that in the dead zone the

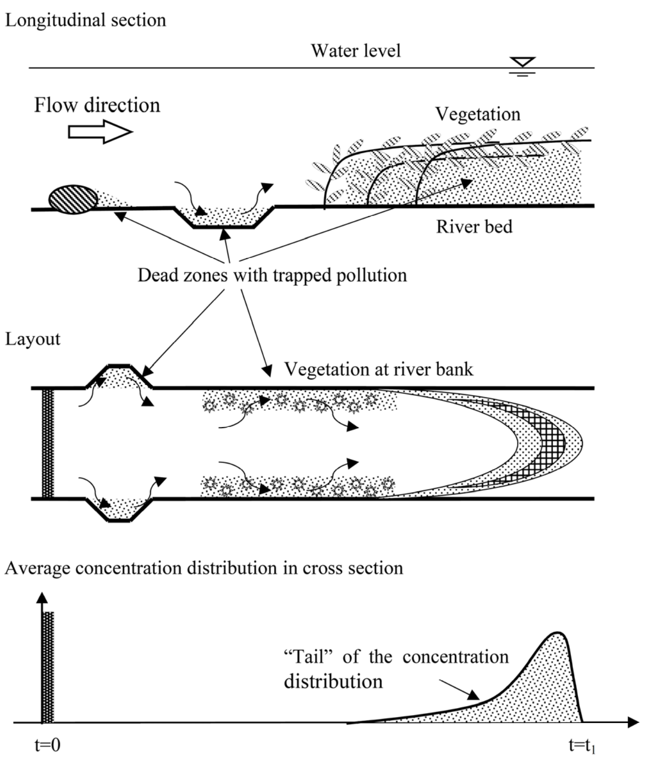

Fig. 1. Scheme of the "dead zones" effects on pollution transport in a stream.

solute concentration is uniform, mass exchange between the dead zone and the main stream is proportional to the difference of the averaged concentration in the dead zone and in the main channel (Chanson, 2004; De Smedt et al., 2005; Jirka, 2004; Jirka et al., 2004; Rowiński et al., 2004; Valentine and Wood 1979). To set up the DZM, conservation of mass for the main stream and the dead-zone should be considered (Czernuszenko and Rowinski, 1997; De Smedt et al., 2005; Nordin and Troutman, 1980):

$$\frac{\partial C}{\partial t} = D_x \left(\frac{\partial^2 C}{\partial x^2} \right) - v_x \frac{\partial C}{\partial x} - m\left(C - C_s\right) + M_s \tag{2}$$

$$n \frac{\partial C_s}{\partial t} = m\left(C - C_s\right) \tag{3}$$

where C_s is the concentration of the substance in the storage zone (kg m^{-3}), m is the mass exchange coefficient between the main stream and the storage zone (s^{-1}), n is the ratio between the storage zone and the main stream cross-sectional area (–). If m or n becomes zero, Eq. (2) reduces to Eq. (1). The set of Eq. (2) and Eq. (3) was also used for developing the OTIS software (Runkel, 1998).

Hypothetically, the DZM problem can be also solved using two-dimensional approach, where the transversal movement of pollution will reflect the effect of dead zones. However, two-dimensional analytic solutions are also complicated and their numerical application is difficult (Djordjevich et al., 2017; Skublics et al., 2016).

In general, besides the basic parameters (stream hydraulic parameters, e.g. discharge, dimensions, flow velocity) and the dispersion coefficient, it is necessary to determine also the size of the dead zone (ratio between the active and dead zone) and the coefficient of the solute transfer between the dead and active zones. These parameters should be determined by model calibration, based on the field tracer experiments. Application of values estimated by analogy with other tracer studies, is problematic and can lead to misleading results.

The solution of Eq. (1) for simplified conditions (instantaneous point source, prismatic streambed, steady and uniform flow) by Socolofsky and Jirka (2005), eventually by Fischer et al. (1979) and Martin and McCutcheon (1998), has the following general mathematical expression:

$$C = \frac{M}{A\sqrt{D_x t}}\ f\left(\frac{x}{\sqrt{D_x t}}\right) = \frac{M}{A}\ p\left(\frac{1}{\sqrt{D_x t}}\ ; \frac{x}{\sqrt{D_x t}}\right) \tag{4}$$

where A is a cross- sectional area of the stream (m^2), M is a pollutant mass (kg), and p are the unknown functions („similarity solution"). The unknown function f (or p) can be determined in two different ways (Socolofsky and Jirka, 2005):

1. Based on experiment derive a curve fit to real data.
2. Solve the Eq. (4) analytically.

Solving analytically the Eq. (4), the one-dimensional analytical solution of the ADE for above mentioned simplified initial and boundary conditions, immediate pollution input implies that the solute particles will be spatially symmetrically spread, following the Gaussian normal distribution, whereas the standard deviation σ is temporally depending. The mathematical solution can be obtained in the form (Fischer et al., 1979)

$$C\left(x,t\right) = \frac{M}{2A\sqrt{\pi D_x t}}\ \exp\left(-\frac{\left(x - \overline{v}_x t\right)^2}{4\ D_x\ t}\right) \tag{5}$$

where $\overline{v}_x$ is the mean flow velocity in a stream.

The proposed approximate model

By comparing Eq. (4) and Eq. (5), it could be seen that the analytical solution of the function p has spatially the form of a Gaussian normal distribution with parameters of normal distribution (e.g. standard deviation σ, etc.). In the often-applied temporal expression form (Eq. (5)), this curve does not have the exact shape of a Gaussian normal distribution, but it has asymmetric form. It is caused by substitution of the standard deviation σ (which is constant in Gaussian distribution) by the time-dependent term $\sqrt{2D_x t}$. Another interpretation could be that the asymmetry is caused by the fixed position of the observer on the stream bank. If the observer moves with the same speed as the water flows, the concentrations distribution from the observer's point of view (spatial distribution) will have symmetrical shape of the Gaussian normal distribution.

Analytical solution of advection – dispersion equation in form of (Eq. (5)) is currently considered as the standard solution, but the validity of this solution is limited to flow without barriers, with the assumption of a symmetrical movement of particles at the front and rear of the cloud in downstream and upstream direction. In real streams, however, this assumption is not always valid: movement of particles is slowed down (retarded) by the accumulation of particles in dead zones of streams.

For this reason, in the case of flow in real conditions with occurrence of dead zones in a stream, it is appropriate to approximate the function p from Eq. (4) not in the form of the Gaussian normal distribution as in (Eq. (5)), but to use different statistical distribution form with asymmetric shape.

Based on our field experiments, we propose as an appropriate approximation of the function p from the Eq. (4) the Gumbel's distribution. This distribution was selected based on our field experiments among other distributions because of its simplicity, asymmetry and ability to good fit with the measured data in streams with dead zones. Of course, other distributions may also be used, but this study examines suitability of this one.

The general equation of the Gumbel's distribution is

$$g = \frac{1}{\xi} e^{-\left(z + e^{-z}\right)} \tag{6}$$

$$z = \frac{x - \mu}{\xi} \tag{7}$$

where g is the distribution probability (density), the parameter μ is the location parameter and the parameter ξ is the scale parameter.

The parameters from the Eq. (6) (considering the Eq. (4)) can be defined as follows:

$$\xi = \sqrt{D_{x,G} t} \tag{8}$$

$$z = \frac{\overline{v}_x t - x}{\sqrt{D_{x,G} t}} \tag{9}$$

where the $D_{x,G}$ is the dispersion coefficient in the longitudinal direction ($m^2\ s^{-1}$), used in the proposed model. To be dimensionally consistent, z is a dimensionless parameter and ξ has the dimension of a length (m).

By substituting parameters from Eq. (8) and Eq. (9) into Eq. (6), the one-dimensional analytical solution has the unitary form:

$$g(x,t) = \frac{1}{\sqrt{D_{x,G} t}} \exp\left[-\frac{\overline{v}_x t - x}{\sqrt{D_{x,G} t}} - \exp\left(-\frac{\overline{v}_x t - x}{\sqrt{D_{x,G} t}}\right)\right] \tag{10}$$

By substituting Eq. (10) to Eq. (4) we get the proposed solution, results are in concentration units (kg m^{-3})

$$c(x,t) = \frac{M}{A\sqrt{D_{x,G} t}} \exp\left[\frac{x - \overline{v}_x t}{\sqrt{D_{x,G} t}} - \exp\left(\frac{x - \overline{v}_x t}{\sqrt{D_{x,G} t}}\right)\right] \tag{11}$$

FIELD MEASUREMENTS

Derived Eq. (11) was verified using the experimental data from three tracer studies in Malá Nitra, Šúrsky and the Malina streams. Tracer experiments were conducted in years 2012–2016.

Test A was performed on a reach of the Malá Nitra stream, located within the village Veľký Kýr (N48.181799°, E18.155373°). The experiments described in this paper were performed in two reaches with lengths of 785 and 1340 metres, respectively. The first reach of the stream was straight, the second was slightly curved in both directions (left & right bend). In these reaches, the channel was at the bed about 4 m wide with a banks height of 2.5 m and a bank slope of approximately 1:2. It should be mentioned that the original prismatic cross section was not fully preserved and its form was modified because of ongoing morphological processes. The discharge in the whole measurements period ranged from 0.138 to 0.553 $m^3\ s^{-1}$, but for the model tests a stable discharge, from 0.230 up to 0.235 $m^3\ s^{-1}$ was used. The hydraulic roughness was determined from field measurements and hydraulic calculations (Limerinos, 1970), leading to a Manning coefficient n = 0.035. Water level slope, determined by geodetic levelling, was found constant and approximately equal to 1.5‰. The shape of the stream can be considered in the examined reach of the stream as a prismatic one. The stream had a width of 5.5 m and a water depth in the range from 0.4 up to 0.6 m. The range of determined longitudinal dispersion coefficient was from 0.5 to 2.5 $m^2\ s^{-1}$.

Test B was performed on straight stream reach of the Šúrsky stream, located close to the village Svätý Jur (Slovakia, N48.232957°, E17.202934°). The field measurements were made in 300 up to 500 m long straight reach with relatively prismatic cross section profile. The stream width was from 4 to 5.5 m, depth was in the range from 0.4 to 0.8 m, flow velocity from 0.21 to 0.36 m s^{-1} and discharge was from 0.38 to 0.43 $m^3\ s^{-1}$. The range of determined longitudinal dispersion coefficient was from 0.63 to 0.98 $m^2\ s^{-1}$.

Test C was performed at the Malina stream, located in the cadastral areas of Lab and Zohor municipalities (N48.334771°, E16.967445°). The experiments were carried out on selected stream reach with a length of 1415 m. It was a straight section of the Malina stream, without significant directional changes.

Originally constructed cross section shape was significantly influenced by vegetation. The measured discharge during the experiments was 0.408 $m^3\ s^{-1}$. The water level slope, specified

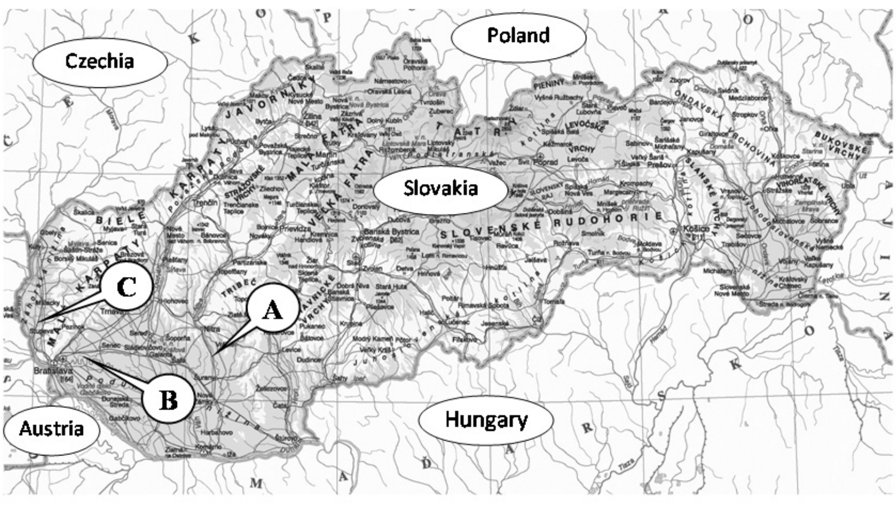

Fig. 2. Map of the field tracer experiments.

by levelling measurements, was about 0.45‰. The stream shape in the examined stream section can be considered prismatic, the width was around 5 m, the average depth was 0.88 m, the determined dispersion coefficient was 0.95 $m^2 s^{-1}$.

In the first two locations, common salt was used as a tracer. Conductivity was measured at the end of examined stream reach and converted to the salt concentration using local specific calibration curve. However, in both cases a linear dependency between conductivity and salt concentration was determined within the ranges of observed concentrations. Because of this it is possible to show graphs in this paper also with conductivity units.

In the test C (Malina stream) the colouring agent – E133 (brilliant blue, food colour) was used and the tracer concentration was measured and determined using field spectrophotometry device.

In all field experiments an instantaneous tracer injection in the centre of the stream width was used. The tracer (common salt, colouring agent) was thoroughly mixed in a barrel with some amount of the water (typically 30–50 litres) and such homogenous mixture was injected to the centre of the stream.

The experiments on the sites A and C (Malá Nitra and Malina stream) were performed in high summer and the vegetation was present in large extent (emergent as well as submerged vegetation). The tracer experiment B (Šúrsky channel) was performed on early spring and the vegetation presence was minimal. The covering of the cross-sectional area of the streams was not exactly determined, just estimated as follows: experiment B – 10%, exp. A – 30%, exp. C – 40% of the cross - stream sectional area was influenced by vegetation (see also Table 4).

RESULTS

During the field measurements, deformations of the concentration distribution at all streams were found. It shows significant presence of dead zones. These zones were formed by the stream beds irregularities as well as by the vegetation along the stream banks and on bed.

Some results from measured data and concentration distribution approximated by Eq. (5) and Eq. (11) are shown for illustration in Figs. 3–7. From the Figures, it is visually clear that the proposed method (Eq. (11)) approximates the measured very well, particularly in the increasing part of the curve.

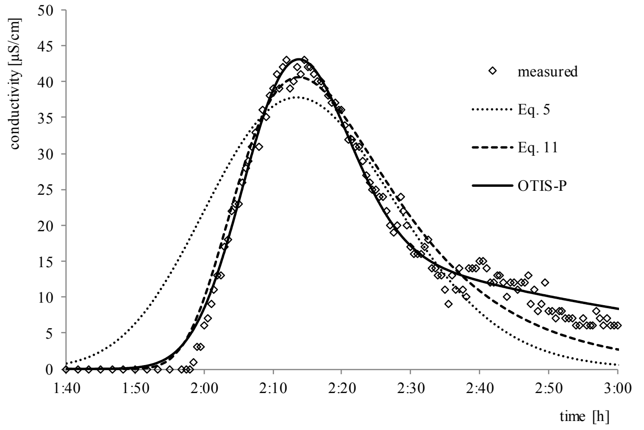

Fig. 3. Comparison of measured and simulated conductivity distribution in the test A - Malá Nitra stream, experiment Nr. 5-V (1340 m).

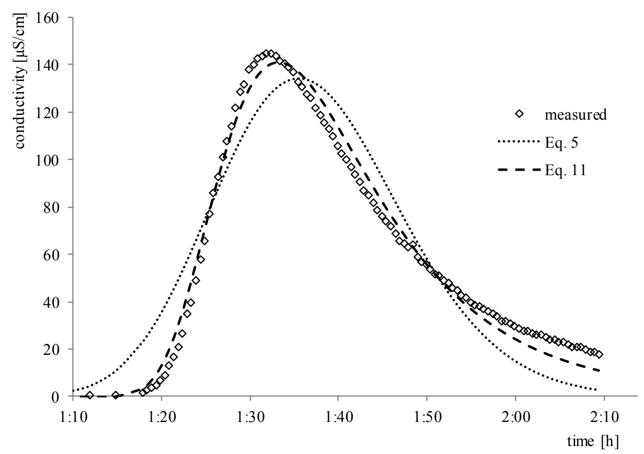

Fig. 4. Comparison of measured and simulated conductivity distribution in the test A - Malá Nitra stream, exp. Nr. 12-III (785 m).

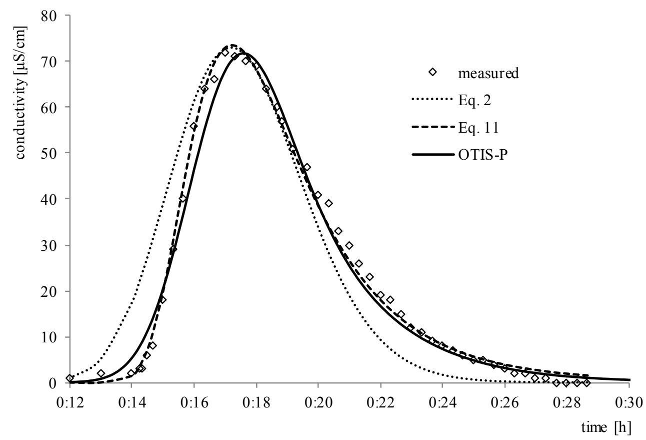

Fig. 5. Comparison of measured and simulated conductivity distribution in the selected profiles on the test B - Šúrsky stream, exp. Nr. 7-II (300 m).

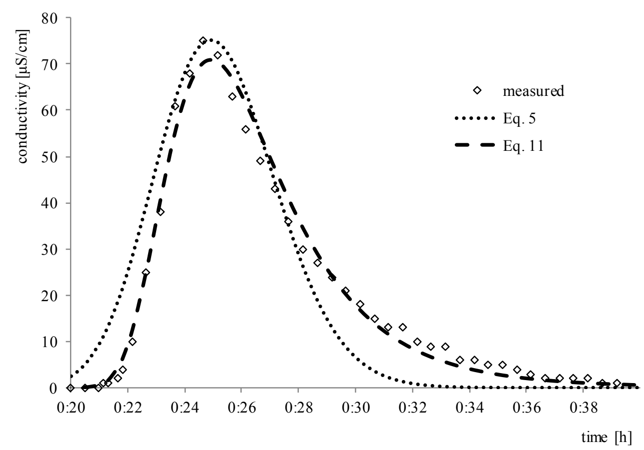

Fig. 6. Comparison of measured and simulated conductivity distribution in the selected profiles on the test B - Šúrsky stream, exp. Nr. 11-II (406 m).

The field tracer experiments performed within the case C (the Malina stream), in addition to standard evaluation of tracer experiments mentioned above, were also evaluated by the OTIS-P software (Runkel, 1998) with optimization of parameters, used in Eq. (2). The optimised parameters were set-up by the OTIS-P software as the following: D_x = 0.0213 m^2 s^{-1}, the storage zone cross-sectional area was A_s = 1.53 m^2, the storage rate exchange coefficient $m = 4.08 \times 10^{-4}$ s^{-1}. A graphical comparison of the results of measured data and approximations (Eq. (5), Eq. (11) and OTIS-P) is presented on Fig. 3, Fig. 5 and Fig. 7.

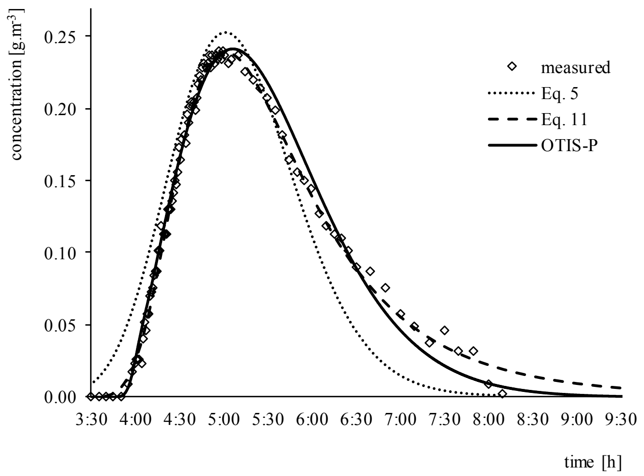

Fig. 7. Comparison of approximation results – test C, the Malina stream (approximation using Eq. (5) and Eq. (11) and the OTIS software).

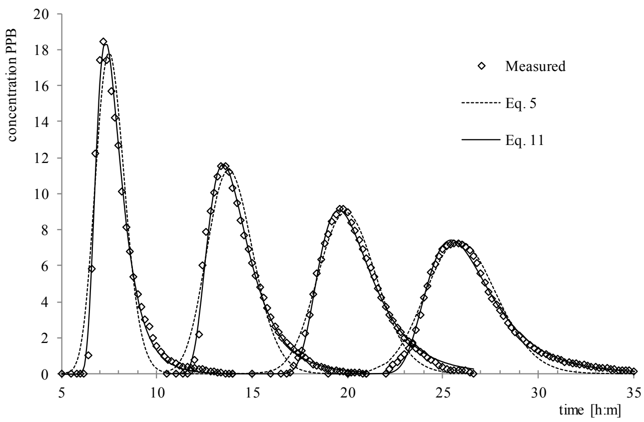

Fig. 8. Comparison between the results of the approximate method and the experimental data – Monocacy River.

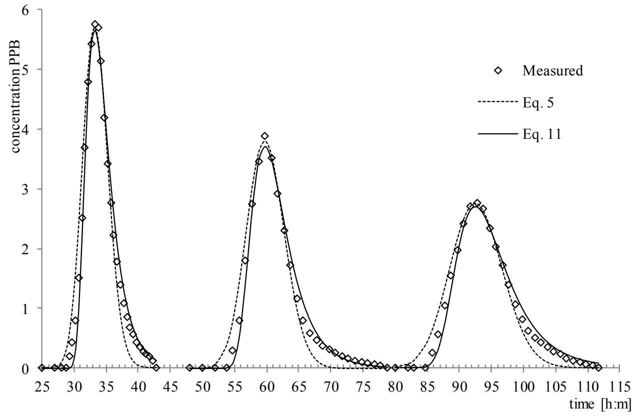

Fig. 9. Comparison between the results of the approximate method and the experimental data – Red River.

As it can be seen on these figures, the approximation with the proposed method according Eq. (11) and OTIS software are quite similar, whereas the approximation with Eq. (5) is less accurate.

The proposed approximate method should be also verified for different ranges of the stream characteristics (longitudinal dispersion coefficient, lengths, travelling times etc.) Such field tracer experiments were not conducted in Slovakia, so the experimental data from (Nordin and Sabol, 1974) collected in the Monocacy and Red Rivers were applied. These data were also used by (Deng and Jung, 2009).

The first tracer dispersion experiment was conducted on June 7, 1968 in the Monocacy River. The four sampling sites were located at 10.30 km, 18.34 km, 26.80 km, and 34.28 km downstream of the tracer injection site. The second field tracer experiment was performed on April 7, 1971 in the Red River. The three sampling sites on the Red River were located at 5.74 km, 75.64 km, and 132.77 km downstream of the tracer injection site. The optimal set of parameters was achieved by the best fit of simulated concentration by the Eq. (5) and Eq. (11), respectively, to the observed concentrations. The input parameters applied in both numerical experiments, as well as those used by (Deng and Jung, 2009), are listed in Table 1.

Table 1. Parameters used in numerical experiments.

Parameter	Unit	River	
		Monocacy River	Red River
$\bar{v}_x$ (Eq. (11)) U (Deng, 2009)	m s^{-1}	0.381 0.37	0.609 0.62
K_s (Deng, 2009)	m^2 s^{-1}	16	40
D_x (average, Eq. (5))	m^2 s^{-1}	27.74	86.20
$D_{x,G}$ (average, Eq. (11))	m^2 s^{-1}	45.44	143.28

Note: K_s is the Fickian dispersion coefficient, calculated by semi empirical method for determination of the Fickian dispersion coefficient, see (Deng and Jung, 2009).

Statistical evaluation

The goodness of fit between measured values and the results from Eq. (5) and Eq. (11) was evaluated by comparing the sum of differences square between the measured and approximated values, i.e.

$$Dif = \sum_{t=t_1}^{t=t_2} \left(\Delta y_t\right)^2 = \sum_{t=t_1}^{t=t_2} \left(y_{m,t} - y_{a,t}\right)^2 \tag{12}$$

where Dif is the sum of differences square, $y_{m,t}$ is the measured value in the time t, $y_{a,t}$ is the approximated value in the time t, t_1 is the measurement start time and t_2 is the measurement end time. The sum of differences square for each measurement and their basic statistical evaluation are presented in Table 2. The model fit shown on Figs. 3–7 was obtained using the built-in nonlinear regression in the standard Excel worksheet (the Solver add-in, using the non-linear GRG algorithm). For the optimization, all physical parameters were taken from the field measurements (velocity, cross-sectional area, the same values of these parameters were used for the OTIS optimization model), the optimized variables were the dispersion coefficient (Eq. (5) and Eq. (11)) as well as the coefficient for the reduction of tracer mass to keep the mass balance. Unfortunately, the optimal parameters dataset for the Eq. (5) (Gaussian) specifies very often the peak time out of the "reasonable" similarity. This means in fact two different values of flow velocity for one field tracer experiment. This can be considered as a non-comparable case and because of this the peak time for each field tracer experiment was fixed.

Suitability of the use of the Gumbel distribution can be assessed by analogy with the goodness of fit test, which is used to verify the conformity of the measured data with the corresponding theoretical distribution. In our case, it was used a procedure analogous to Kolmogorov-Smirnov test (for continuous distributions), using supremum values, defined as it follows:

$$S_n = sup\left|F_n(t) - F(t)\right| \tag{13}$$

where S_n is the supremum, $F_n(t)$ is the normalised value of the cumulative measured concentration, $F(t)$ is the normalised value of the theoretical cumulative (distribution) function. Normalised values in this case means that the values are in the interval <0;1>. The supreme value can be also interpreted as the percentage difference of the measured and modelled distribution value.

The hypothesis H_0 - the measured distribution function is a distribution of the theoretical distribution was tested. In our case the theoretical distributions were according the Eq. (5) and Eq. (11). Hypothesis H_0 is rejected, if $S_n > S_n(\alpha)$, where the $S_n(\alpha)$ is the critical value of the Kolmogorov distribution on the level α.

The critical value of the $S_n(\alpha)$ was defined as it follows:

$$S_{j(\alpha)} \cong \sqrt{\frac{1}{2j}\ln\left(\frac{2}{\alpha}\right)} \tag{14}$$

where j is the number of the measurement points (values), α is the significance level. Results of the statistical evaluation of the results are presented in the Table 2.

DISCUSSION

The above statistical analysis demonstrated that the proposed approximate method (Eq. (11)), if compared with the results from Eq. (5), is much more accurate to reproduce the distribution of the tracer concentration over the time in streams with dead zones. The statistical test of the hypothesis H_0 (the measured distribution function is a distribution of the theoretical distribution), using a high confidence level (α = 0.95), has been confirmed for the Eq. (5) only 4 times (19% of performed measurements), whereas for the Eq. (11) the hypothesis H_0 was confirmed 16 times (76.2%) from total 21 measurements. Other facts that support this statement, are significantly lower supremum values for the proposed method (in average 2.8 times lower) as well as the sum of the squared differences (7.2 times lower).

All the own field experiments were performed with relatively short distances, so the question arises whether it has been achieved the stage of complete transversal and vertical mixing (pollution concentration homogeneity) to meet the assumption of one-dimensional (1D) mixing conditions. Tracer concentrations along the stream width (transversal direction) were measured only in the field experiments in the Malá Nitra stream. A good tracer homogenisation was observed in the distance of 150 m (Velísková et al., 2013). In this experiment the tracer source was placed at the river bank, so for the experiments, presented in this paper (all with stream centre injection) we can assume even smaller mixing length.

Table 2. Comparison of the longitudinal dispersion coefficients values from Eq. (5) and Eq. (11). (α = 0.95).

Site	Experiment Nr.	X distance	D_x Eq. (5)	$D_{x,G}$ Eq. (11)	crit. value $S_n(\alpha)$	S_n Eq. (5)	S_n Eq. (11)	Dif Eq. (5) $\sum(\Delta y)^2$	Dif Eq. (11) $\sum(\Delta y)^2$
Unit		(m)	($m^2\ s^{-1}$)	($m^2\ s^{-1}$)	(–)	(–)	(–)	(–)	(–)
Test A Malá Nitra stream	5-V	1340	1.17	1.56	0.0517	0.1268	0.0622	6288.3	1226.8
	8-IV	785	0.5	0.73	0.0643	0.1024	0.0396	24867.5	2695.6
	8-V	1340	0.6	1.18	0.0533	0.0956	0.0358	5826.0	32.5
	11-III	785	0.67	1.02	0.0623	0.1756	0.0775	31544.1	4524.9
	11-IV	1340	2.5	6.8	0.0374	0.2379	0.0626	998.4	53.3
	12-III	785	0.75	0.86	0.0590	0.1495	0.0557	67609.5	9690.8
	12-IV	1340	0.95	1.96	0.0456	0.0728	0.0219	16150.8	1817.0
Test B Šúrsky stream	1-III	300	0.82	1.10	0.1062	0.0666	0.0402	274.0	46.8
	2-III	300	0.63	0.8	0.1245	0.1092	0.0219	506.4	48.0
	7-II	300	0.64	1.05	0.0872	0.1412	0.0138	4152.3	162.1
	7-III	397	0.74	1.01	0.1114	0.0953	0.0308	1550.7	143.8
	8-II	300	0.7	0.89	0.0930	0.1326	0.0280	3430.3	457.4
	8-III	397	0.74	1.11	0.1046	0.0784	0.0436	933.5	220.1
	9-III	306	0.6	0.74	0.1062	0.1304	0.0465	5445.9	799.8
	10-II	406	0.64	0.77	0.1003	0.1735	0.0629	4486.9	747.2
	10-III	506	0.8	1.15	0.0815	0.1545	0.0575	3845.1	528.7
	11-II	406	0.39	0.77	0.0830	0.1794	0.0350	2826.5	289.9
	11-III	506	0.82	1.11	0.0815	0.1958	0.1035	5973.0	1533.9
	12-II	406	0.45	0.71	0.0900	0.1636	0.0526	3626.5	602.5
	12-III	506	0.98	1.2	0.0788	0.1770	0.0939	4953.3	1331.2
Test C Malina stream	III	1415	0.95	2.41	0.0562	0.0656	0.0305	592.5	69.7
Minimum						0.0656	0.0138	274.0	32.5
Maximum						0.2379	0.1035	67609.5	9690.8
Average						0.1345	0.0484	9327.7	1286.8

Notice: the grey fields in the Table mean that the hypothesis H_0 can be accepted, i.e. the measured values have the assumed theoretical distribution (Eq. (5) or Eq. (11)). Similar comparison of the sum of squared differences between the measured and approximated values *Dif* (see Eq. (12)) was made also in the cases of Monocacy and Red Rivers. In all examined cases the sum of the differences squared using the Eq. (11) was smaller than sum of the differences using Eq. (5). The value of the sum of the differences using Eq. (11) was in the range of 4–40%, compared to the difference sum using Eq. (5).

Table 3. Examples of formulas for mixing length calculation.

Author	Formula	Mixing length for average parameter (m)
(Socolofsky and Jirka, 2005)	$L_{mix} \approx B^2/3h$	13.9
(Fischer et al., 1979)	$L_{mix} \approx 0.1\left(B^2 u / D_T\right)$	75
Yotsukura, N., 1968 – as referred in (Kilpatrick et al., 1970)	$L_{mix} \approx 8.52\left(B^2 u / h\right)$	106.5
(Ruthven, 1971)	$L_{mix} \approx 0.075\left(B^2 u / D_T\right)$	56.25
(Kilpatrick et al., 1970)	$L_{mix} \approx 1.3\left(B^2 u / h\right)$	16.25

Table 4. Dead zones and vegetation parameters in examined streams.

Experimental stream	Estimated vegetation presence	D_x average value	$D_{x,G}$ average value	$D_x / D_{x,G}$ ratio
	(% of the cross-sectional area of the stream, influenced by vegetation)	($m^2\ s^{-1}$)	($m^2\ s^{-1}$)	(–)
A – Malá Nitra	30	1.02	2.02	1.98
B – Šúrsky channel	10	0.69	0.95	1.39
C- Malina	40	0.95	2.41	2.54

Examples of various formulas for estimation of mixing length can be found in Table 3. In this table we also present the mixing lengths for the average parameters of examined streams $B = 5$ m, $u = 0.3$ m s^{-1}, $D_T = 0.01$ m^2 s^{-1}, $h = 0.6$ m.

As can be seen from the Table 3, the mixing length for complete transversal and vertical mixing for the examined streams ranges - with realistic estimation - from 50 up to 100 m. Comparing this length with the lengths of experimental sections, stated in Table 2, the mixing length was about to 7–14% (Malá Nitra stream), 20–30% (Šúrsky stream) and 7% for the Malina stream. This can be considered as an acceptable percentage of the stream section length, in which the measurements were performed.

Similar situation is also in the numerical experiment, described above – the Monocacy and Red Rivers. The experimental reaches in this case have the length of 34.28 km (Monocacy River) and 132.77 km (Red River), so it can be assumed that the mixing length in these cases is really a very small proportion (less than 1–2%) of the total experimental reach length.

An interesting question is, if there is a relationship between the dispersion coefficients, determined by Eq. (5) and Eq. (11) (D_x and $D_{x,G}$). Theoretically, there is no relationship between the both coefficients, but regarding the determined coefficient values of field experiments in Table 2, some relation between both coefficients can be observed. Statistical analysis confirmed significant degree of the correlation between these values, the correlation coefficient was in the range $R^2 = 0.6$ up to $R^2 = 0.9$ (depending of the method used). Assuming a dependency between both coefficients, the value of $D_{x,G}$ could be defined as

$$D_{x,G} = p_{DG}(D_x) \tag{15}$$

where p_{DG} is a function determining the dependency between the values of D_x and $D_{x,G}$.

Using statistical approach, focused to find the best theoretical fit between the values given by Eq. (5) and Eq. (11), a simple linear relationship can be obtained

$$D_{x,G} \approx 1.588\, D_x + 0.22 \tag{16}$$

which is valid in the values range of the longitudinal dispersion coefficient D_x from 0.25 up to 2.5 m^2 s^{-1}. Such a relationship was also confirmed by the above mentioned statistical evaluation of the tracer experiments. In our case, both equations were used for approximation of specific measured data and the compliance rate with these data varies, depending on a stream flow character, the dead zone extent and its influence on the dispersion process. The correlation degree between both dispersion coefficients depends on the site conditions (hydraulic conditions, extent and the influence degree of the dead zones) and due the local conditions the multiplication and addition factors in Eq. (16) were slightly different.

As shown in the Table 4, field tracer experiments clearly confirm the dependency between the dead zone parameters and the vegetation extent – increase of the percentage of the stream cross-sectional area, influenced by vegetation caused increase of the longitudinal dispersion coefficients (Gaussian, Eq. (5), as well as Gumbel's - Eq. (11)) and causes increase of the ratio between the longitudinal coefficients. This can be the future base for the expression of the dead zone parameters in proposed solution (Eq. (11)).

It seems that a problem occurs in relation to the analytical solution (Eq. (5)) of the advection dispersion equation (Eq. (1)) and the presented solution (Eq. (11)). Both Eq. (5) and Eq. (11) are solutions of Eq. (1), and this means that this equation can have two (or even more) different solutions.

For this case, it is necessary to point out the reference (Socolofsky and Jirka, 2005). The idea of this study is to provide a theoretical basis and replace the Gaussian form of the function f (or p) in the general similarity solution (Eq. (4)) with a different and asymmetric one that would better correspond with data measured in natural stream. Such function substitution cannot be considered as a solution of the advection – dispersion equation (Eq. (1)) for simplified boundary and initial conditions, but just as a simple approximation, based on the similarity. It is quite clear that such approximation does not explain the dispersion processes in the dead zones and has no specific parameters to characterize the size, residence time or other parameters of the transient storage zones in rivers. The presented approach assumes constant parameters - this is not suitable for the complex simulations of long river reaches. But there is still a possibility to divide the modelled river reach to several branches or sub-reaches with different parameters. The breakthrough curve (output) at the end of previous branch could be used as an input to the next branch, etc.

Results of this study show that proposed approximate method in form of Eq. (11) has better accuracy of concentration distribution in a natural stream with dead zones than the approximation by Eq. (5).

Although nearly all literature sources are based on the application of the Eq. (5) (theory, experiments, coefficients), it can be assumed that proposed approximation by Gumbel distribution will bring significant increase of the accuracy of the dispersion processes simulation in natural stream with dead zones, eventually in case of some special applications with extensive consumption of computer time (e.g. iterative tasks – pollution source localisation).

It is clear that the proposed method requires for practical use careful calibration of the applied dispersion coefficient ($D_{x,G}$), in the ideal case based on in-situ measurements (tracer experiments). On the other hand, each simulation of pollution transport in a stream, based on hydrodynamic approach, needs for correct processing the set of hydraulic parameters, and again in an ideal case this set is based on in-situ measurements.

Simulation without the knowledge of the real conditions and without calibration and verification based on real field experiments, can lead to misleading results. The most frequent cause of this is an inaccurate dispersion coefficient determination, but also neglecting the presence of dead zones, eventually incorrect determination of the dead zones influence. Application of the proposed approximation reduces these inaccuracies in some extent. Furthermore, in some cases it could be hard to detect the presence of dead zones and their extent, even the determination of their parameters can be very difficult. Consequently, the proposed approximation could be useful and helpful for the simulation of pollution spreading in a stream with dead zones without arduous determination of these dead zones parameters. However, it is necessary to mention again that every simulation should be accompanied by the calibration and verification at least in form of one simple tracer experiment.

The use of 1D model approach has its limitations, but we believe that it is still advantageous to use it in the practice also for short reaches. 2D, eventually 3D approach requires much more data – physical dimensions and model boundaries, velocities and dispersion parameters for 2 (or 3) dimensions. Such data are not always available and it can be very difficult, time and money consuming task to collect necessary data.

CONCLUSIONS

In this paper a simple numerical approximate method for one-dimensional simulation of the dispersion of a solute in a stream is introduced. The presented method is suitable especially for streams with significant influence of dead zones, which cause a strong asymmetry in the shape of the concentration distribution curves over the time. Eq. (5) is not fully applicable in such conditions and the differences from measured values are considerable. Similar analytical solutions for streams with occurrence of dead zones, described in literature sources up to now (De Smedt et al., 2005) are clearly mathematically correct and accurate, but these methods are difficult for code programming and computational time, especially in case of inverse tasks solving (iterative tasks, brute force methods).

The proposed method was verified using the experimental data from three tracer field studies. The field experiments were performed at three streams in south Slovakia – Šúrsky channel, Malá Nitra and Malina streams. Evaluation of the field tracer experiments from all streams has shown considerable asymmetry of the concentration distribution, which clearly indicates extensive presence of dead zones in all the streams. The statistical evaluation of the proposed method shows that the (Eq. (11)) is much more accurate for simple approximation of the concentration distribution in streams with dead zones than Eq. (5).

Another verification was performed for rivers with different hydraulic parameters and longer distances, using previously published data (Nordin and Sabol, 1974) for the Monocacy and Red river field tracer experiments. The proposed approximation method (Eq. (11)) was significantly more accurate than the standard method (Eq. (5)) even in this case. The sum of squared difference was in case of the approximate method smaller by 60, up to 96%.

Results of the study confirmed that proposed one-dimensional analytical method approximates the solute concentration distribution very well and is fully applicable in the practice for simple tasks (simulations) of the pollution dispersion in streams. Its advantage is simple programming and computational speed (less computational time is needed). This could be very advantageous for iterative tasks solving, e.g. the inverse task (pollution source localisation). For full application, a simple verification and calibration is sufficient, but it is not necessary to determine the parameters of dead zones, used in Eq. (2). Besides, the estimation of these parameters is quite difficult in practice. Finally, major advantage of the proposed method is the possibility to apply on it the superposition principle (a common feature of all analytical solutions). This allows simulation of various arbitrarily defined pollution inputs into the stream.

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