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Approximated Boundary Conditions of the Equation of Diffusion

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Abstract

The paper focuses on boundary conditions in mathematical physics equations. These equations describe the processes of pollutants' migration. The emphasis is put on the influence of boundary conditions' approximation on the solution of one-dimensional advection-dispersion equation. Analytical and numerical solutions were used as a basis for the theoretical consideration.

The research included the following methods: 'distant boundary' method, rejection of diffusion flux in the boundary profile, rejection of 'the near field' and solution of mass or energy balance equation.

The research afforded possibilities for quantitative and qualitative identification of the influence of boundary conditions' approximation methods on the equation solution inside domain. The derived formulas made it possible to estimate the margin of error introduced by the simplified method. The formulas were presented in the form of nomograms.

1. Introduction

In general, the following variables describe the process of migration of pollutants (Sawicki 1998):

- velocity,
- pressure,
- density,
- temperature,
- and concentration of dissolved matter of each pollutant.

The problem of pollutants transport in water is fully formulated in the mathematical physics sense when three main conditions are fulfilled (Godunov 1975):

- the process is described by the proper equation (or system of equations),
- the domain of solution and its property is defined,

– the boundary and initial conditions are defined.

The problem is well posed when it can be solved for any initial and boundary data that belong to a certain class and when the solution is unique and depends continuously on boundary conditions. This means that the function, which is a solution of a differential equation, satisfies this equation in the considered domain as well as the defined conditions on the domain boundary. The initial conditions occur in the equations that describe unsteady processes. They include information concerning function in the domain at the initial moment. The boundary conditions include information concerning the function in demand on the boundary of a domain. Three basic forms can express these conditions: it can be the value of this function (Dirichlet condition); that normal to the boundary a derivative of this function may be given (Neumann condition) or a relation between the value of the function and its normal derivative (Hankel condition).

The demand of the solution existence in the majority of physical equations is fulfilled for situations that are described by conservation equations (Godunov 1975). The condition of the univocal nature of solution depends on the proper definition of boundary conditions that are defined in different ways for particular types of equations.

In many cases the determination of boundary conditions is very difficult or even impossible. In these cases we may distinguish two ways of proceeding:

1) the approximation of real conditions;
2) the substitution of inaccessible real conditions (which are very often part of the solution) by reduced models or by formally different, but technically equivalent conditions.

2. Equation of Pollutants Transport

If we consider a one-dimensional model, which is natural in the case of rivers and channels, the unsteady transport of mass or energy in one-dimensional flux of constant average velocity ($|\mathbf{u}| = \text{const} = u$) and constant depth ($h = \text{const}$) can be described by an advection-dispersion equation. If we reject source terms and assume dynamic passivity of the process, the transport equation may then have the following form (Puzyrewski, Sawicki 2000):

$$\frac{\partial \overline{C}_j}{\partial t} + u\frac{\partial \overline{C}_j}{\partial x} = \frac{\partial}{\partial x}\left[(D_j + D_T + K_L)\frac{\partial \overline{C}_j}{\partial x}\right], \tag{1}$$

$$\frac{\partial \overline{T}}{\partial t} + u\frac{\partial \overline{T}}{\partial x} = \frac{\partial}{\partial x}\left[(D_W + D_{WT} + K_L)\frac{\partial \overline{T}}{\partial x}\right], \tag{2}$$

where:

x, t – space and time variable,
C_j – mass concentration of j dissolved matter,
T – temperature,
u – average velocity of advection,
D_j – diffusion coefficient of j dissolved matter,
D_W – coefficient of temperature distribution,
D_{WT} – coefficient of turbulent diffusion,
K_L – coefficient of dispersion.

Comparing equations (1) and (2) we notice that they are formally identical, irrespective of the physical meaning of the dependent variable in the transport equation (concentration of j dissolved matter or temperature). In this paper a general scalar f and effective coefficient of diffusion process D_e are used. The D_e coefficient describes the total intensive of molecular diffusion, turbulent diffusion and dispersion:

$$D_e = D_j + D_T + K_L \quad \text{or} \quad D_e = D_W + D_{WT} + K_L. \tag{3}$$

Effective coefficient (3) joins the processes the nature of which is the same (phenomena of turbulent diffusion and dispersion are analogous to the full with phenomenon of molecular diffusion).

In general, taking the above denotation into consideration, we can write the one-dimensional equation of mass or energy transport as follows:

$$\frac{\partial f}{\partial t} + u\frac{\partial f}{\partial x} = \frac{\partial}{\partial x}\left[D_e \frac{\partial f}{\partial x}\right], \tag{4}$$

where:

f – mass concentration of j dissolved matter or temperature,
D_e – effective coefficient of transport.

Additionally, if coefficient D_e = const, equation (4) will have the following form:

$$\frac{\partial f}{\partial t} + u\frac{\partial f}{\partial x} = D_e \frac{\partial^2 f}{\partial x^2}. \tag{5}$$

3. Formulating of Pollutants Transport Problem

Initial conditions, a very important element of each unsteady technical problem, describe the values of the unknown function (or certain quantity of such functions) in the initial moment ($t = t_0$, often $t_0 = 0$):

$$f_p = f(x, t = t_0). \tag{6}$$

Boundary conditions determine the influence of surroundings on the considered system (Rutherford 1994). For equations of parabolic type (5), in the one-dimensional case, when the unknown function f is defined along the segment L:

$$\text{from } x = x_p \text{ to } x = x_k = x_p + L, \tag{7}$$

one boundary condition on each boundary point should be given (Fig. 1):

- on the "first" boundary point ("left", "inflow"),
- on the "last" boundary point ("right", "outflow").

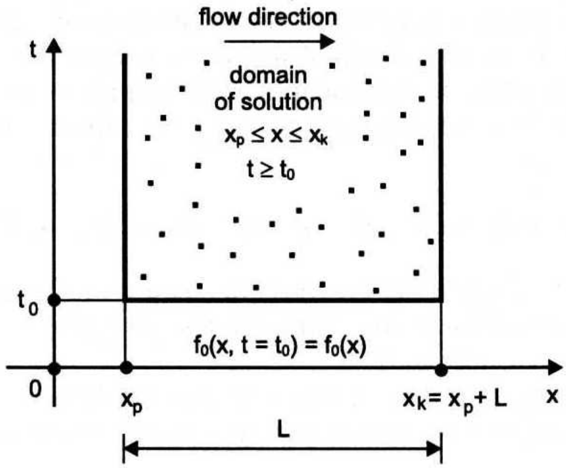

Fig. 1. Method of formulating of boundary conditions for parabolic equation

The advection equation ($D_e = 0$) requires one boundary condition, only for the initial value of coordinate $x = x_p$ (Fig. 2):

$$f_o = f(x = x_p, t). \tag{8}$$

3.1. Possibilities of Defining the Initial Condition

The initial condition usually has a simple mathematical form. But in practice, its description is quite difficult. This problem appears when elements describing the considered process are influenced by permanent space modification. However in many cases the initial state is constant (so-called "background") and only the disturbance, varying in time, is the object of description. Such situations occur very often in the considered problems, related to pollutants transport, and for this reason the constant concentration of dissolved matter was accepted as initial condition in this paper (Fig. 3):

$$f_p = C_{ip} = \text{const.} \tag{9}$$

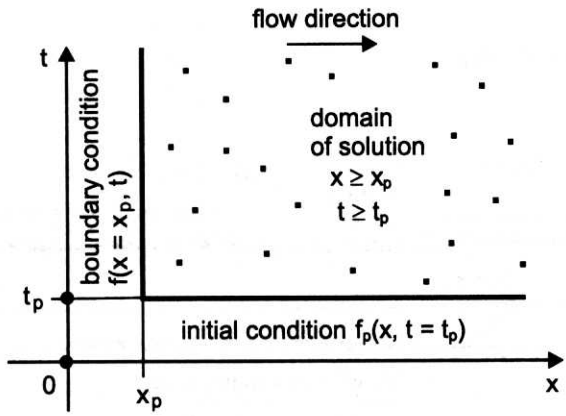

Fig. 2. Boundary conditions for advection equation ($u > 0$)

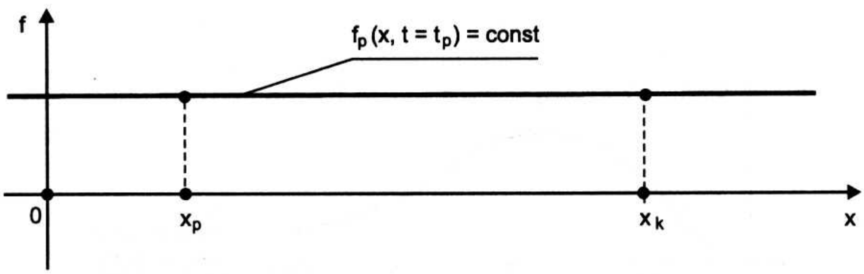

Fig. 3. Initial condition in considered problem

The same assumption can be accepted for the temperature

$$f_p = T_p = \text{ const.} \tag{10}$$

3.2. Possibilities of Defining the "Inflow" Boundary Condition

In the case of migration of dissolved matter ($f = C_i$) and thermal energy ($f = T$), the change of the function f on the boundary will practically always be the result of injection of a certain load of mass or energy. As a rule, this border will have the character of an "inflow" boundary (because the injected load has to "flow into" the system).

Close zone will be formed in the region of the discharge place (Bansal 1971). This is characterized by spatial variability, difficult to describe. However, very often, the size of the close zone is negligible. Further on in this paper a one-dimensional model of mass or energy transport (according to equation (5)) will be considered. The "inflow" point $x = x_p$ will be situated at the beginning of the dispersion zone (distant zone), according to the scheme in Fig. 4.

Another scheme of introduction of initial state disturbance is also possible. A certain load of mass or energy (Fig. 5) is dropped rapidly to any section of the stream of the length e (for $t = t_0$). The section e may be very short and then such

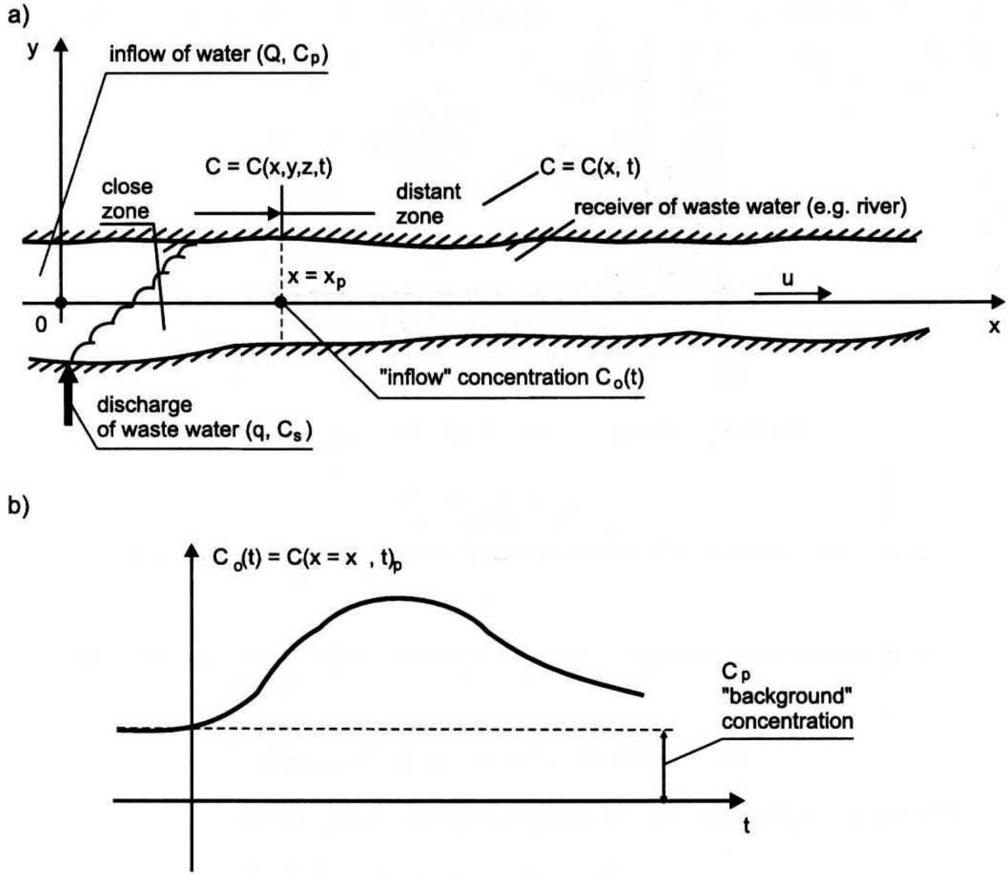

Fig. 4. The rules of defining the "inflow" boundary condition for point drop

a drop may be treated as an impulse (very high concentration of mass or energy on infinitely short distance).

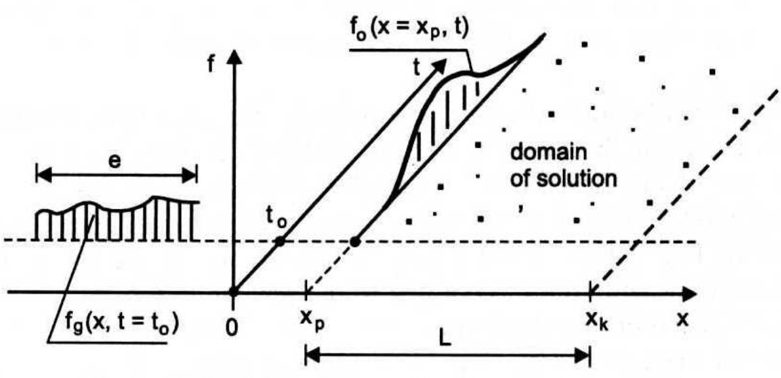

Fig. 5. "Inflow" boundary condition in case of area run-off

The load dropped in this manner will move through section $x = x_p$ (Fig. 5) in the manner described by the function f_0 $(x = x_p, t)$ irrespective of the length of section e. This method is a convenient "in flow" boundary condition.

3.3. Possibilities of Qualifying the "Outflow" Boundary Condition

Formally, it is possible to determine the "outflow" boundary condition in the manner described in the previous chapter, as a function f_k (Dirichlet condition):

$$f_k = f(x = x_k, t). \tag{11}$$

However in the considered case of the advection-diffusion equation, it is practically impossible to formulate the condition of Dirichlet (11) on the "outlet" boundary, as usually the value of the function in the region of the boundary is unknown, and moreover it is the most essential element of the solution in demand. A schematic example of such a situation is presented in Fig. 6, where the "right" boundary of investigated domain is appointed by the river section where the quality of water is of principle significance for users.

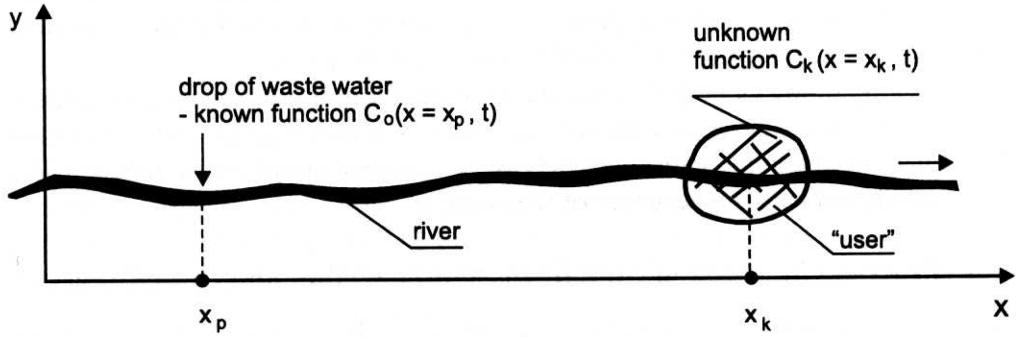

Fig. 6. Practical aspect of "outflow" boundary condition

The possibilities of formulating the Neumann condition for $x = x_k$ are even more limited (Bansal 1971). Analysing this condition in comparison with Fick's law, the normal to boundary derivative of the unknown function is closely connected to the diffusive unit flux of the j component of solution (or respectively with unit flux of convey thermal energy, which results from the Fourier's law). For one-dimensional flow it may be written as follows:

$$\frac{\partial C_j}{\partial x} = -\frac{m_j}{D} \tag{12}$$

and

$$\frac{\partial T}{\partial x} = -\frac{q}{\lambda}. \tag{13}$$

Because of the form of the above relations, the Neumann condition is often commonly called "diffusive flux on the boundary" for advection–diffusion equation. Unfortunately there is no possibility to determine the value of this flux, because it is closely connected with the value of function $f(x,t)$ which we are searching, and there are no physical laws defining $\partial f/\partial x$.

There is yet a third possibility, the boundary condition of the Hankel type (Sawicki 1993):

$$F\left(f,\ \frac{\partial f}{\partial x}\right) = F(x = x_n, t). \tag{14}$$

It can be expressed only in very few special cases. A typical example is an equation expressing equivalence of energy flux conducted in the end section region of a metal bar and of the flux of this energy radiated from the end section of the bar to the environment of the temperature T_z (Sawicki 1993):

$$\frac{\partial T_k}{\partial x} = A\left(T_k^4 - T_z^4\right). \tag{15}$$

There are still several situations for which one may determine the condition of type (15), as for example superficial evaporation of diffused matter (Sawicki 1993), but their application is limited to some specific cases.

Summing up, we can say that the exact formulation of the "outflow" boundary condition for the advection-diffusion equation is impossible in general. Hence different types of simplification are necessary. Those simplifications generate the error, which worsens the accuracy of the solution.

4. Practical Methods of Simplified "Outflow" Boundary Conditions

This chapter presents these simplified boundary conditions, which in the author's opinion, may be treated as universally accepted and generally applied.

4.1. "Distant Boundary" Method

This method may be used when the "outflow" section has, at the beginning, constant concentration (or temperature), and more generally – constant value of the unknown function f_t. Very often it is the "background" value, whereas the disturbance of the system's state has the character of a "wave" of which forehead approaches to boundary point $x = x_k$ only after a certain time has passed. To this moment we may accept the Dirichlet boundary condition:

$$f_k(x = x_k, t) = f_t. \tag{16}$$

At this stage it is accepted that the final coordinate of domain is defined by value $x = x_{k1}$ (Fig. 7).

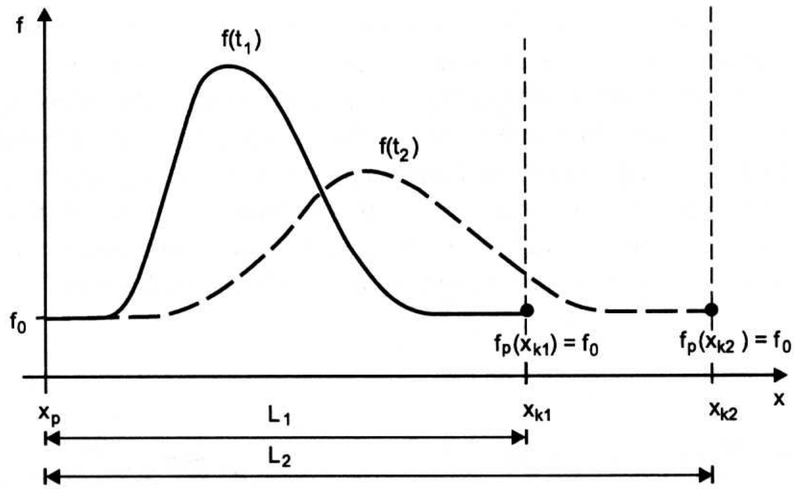

Fig. 7. Scheme explaining "distant boundary" method

When (after a certain time $t_1$has passed) the "wave" forehead of concentration or temperature approaches in section x_{k1}, the boundary is transferred to point x_{k2}. This operation permits removal of the boundary condition from oncoming changes of function f (Fig. 7). In this manner the domain of solution is lengthened.

This method affords the possibility to express precisely the condition on "outflow" boundary only in a special case – before the "wave" front of disturbances. This method is useless in simulations of real processes, when variability of concentration appears in the domain. It is caused by continuous changes inside the domain and boundary points. The use of this method leads to the extension of domain and influences the scale of the task. It can be easily noticed that this method leads, in a short time, to increasing the number of problems connected with time of calculations and with the quantity of the necessary computer memory.

4.2. Neglecting of Diffusive Term in the "Outflow" Section of the Stream

The second method tested in this paper consists of the omission of the diffusive term in the "outflow" section of the stream. It is a basic manner of approximate qualification of an unknown boundary condition. It may be written as follows:

$$\left.\frac{\partial f}{\partial x}\right|_{x=x_k} = 0. \tag{17}$$

Interpretation of this method is taken from the estimation of particular terms of the transport equation in dimensionless form. Taking into consideration the real values of effective transport coefficients it may be stated that the advective term is much more important than the diffusive one (at least on the short section of the stream). We may suspect that the omission of the diffusive flux along the last section dx will not introduce a serious error. This estimation is intelligible by intuition. However, so far, an error that is generated by assumption (17), has not been an object of research. Mathematical interpretation of the above approximation is the following. The value of flux $\partial f/\partial x$ is interpreted as an inclination of the tangent to the diagram of the function $f(x,t)$ (Fig. 8). In general the angle α differs from zero and changes in time. If we assume the lack of diffusive flux (that is, if we make the assumption $\partial f/\partial x = 0$) we extort orthogonality of tangent to function f in relation to the transverse section in the end sector.

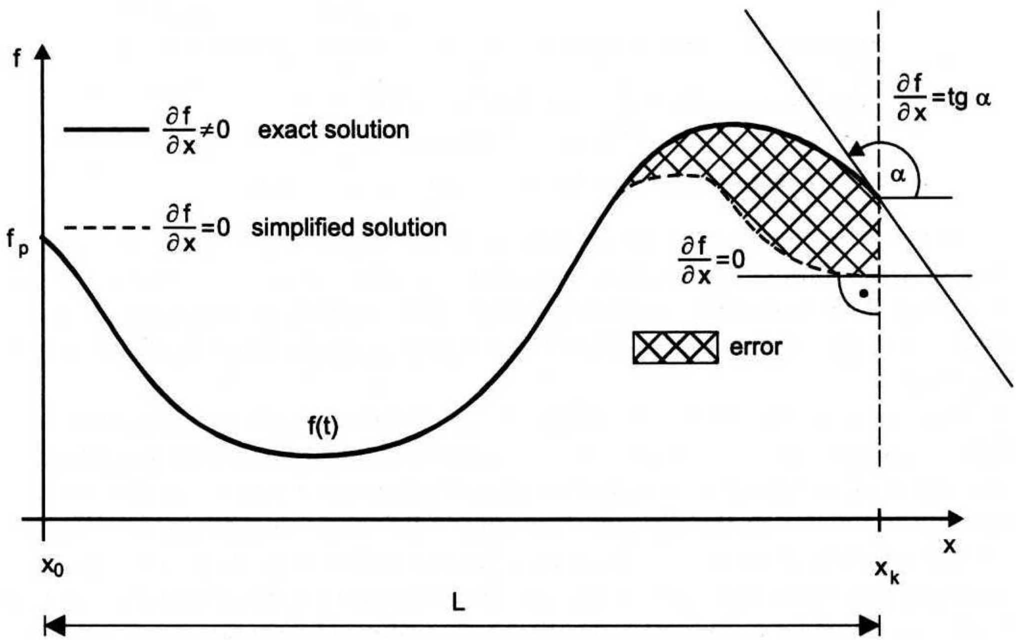

Fig. 8. Interpretation of approximated boundary condition as $\partial f/\partial x = 0$

4.3. Constant Value of Function on Boundary

Pollutants transport problems in case of rivers or channels that discharge to large reservoirs (sea, lake) are very important in practice. In these cases it is frequently assumed that a constant value of the unknown function is accepted (constant concentration or temperature – dashed line). It is an important simplification, as in reality we deal with so-called "close zone" which follows a gentle change of the f function value to the value of "background". Omission of the mixing zone causes non-physical deformation of solution on the boundary and inside computational demand (Fig. 9). In such case we will receive a more accurate solution using "zero flux" condition (dash-dot line).

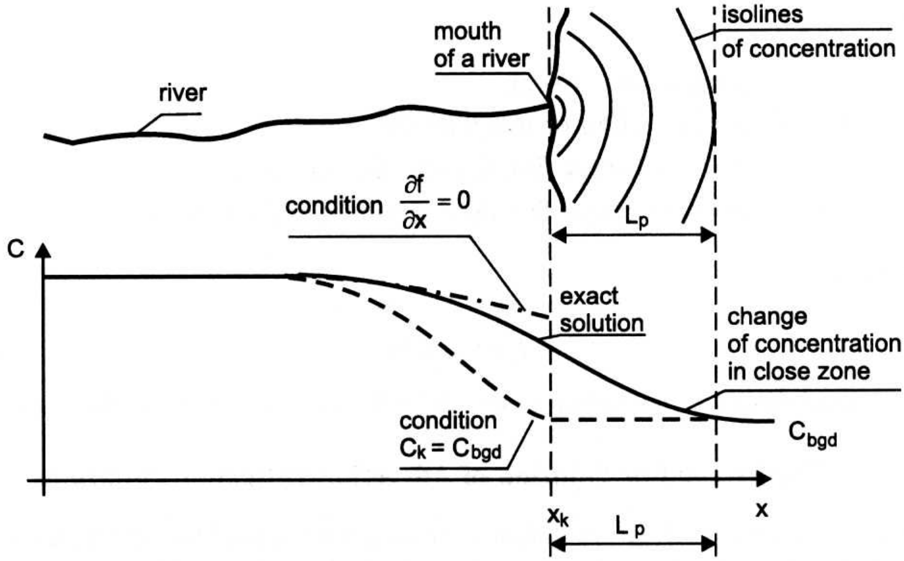

Fig. 9. Deformation of solutions caused by omission of close zone of mixing

4.4. Mass or Energy Balance Equation as Boundary Condition

In cases of calculations of pollutants transport in sewage-plants, when at the end of domain we have a receiver of small capacity (Fig. 10), the following condition is used:

$$f(x = x_k, t) = f_k(t). \tag{18}$$

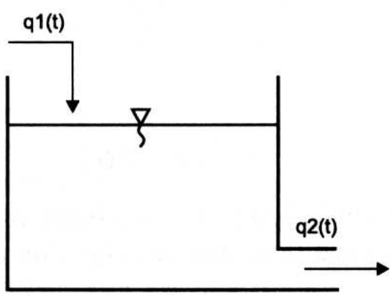

Fig. 10. Model of flow for mass or energy balance equation

Expression (18) is the solution of differential equation, which gives the balance of mass or energy (Sawicki 1993):

$$\frac{d(V \cdot \varphi)}{dt} = q_1(t) - q_2(t), \tag{19}$$

where:

V	–	capacity of receiver,
$\varphi(t)$	–	concentration or temperature,
$q_1(t)$	–	mass or energy flux flowing into receiver,
$q_2(t)$	–	mass or energy flux flowing out from the receiver;

and finally:

$$f_k(t) = \varphi(t). \tag{20}$$

This method describes individual cases and will not be analysed in this paper.

5. The Method of Solution of Advection-Diffusion Equation

In order to solve the advection-diffusion equation we should use the method that will reduce or eliminate problems with numerical solutions. This approach enables examining the influence of solution of accepted reductions on the "outflow" boundary. It is very important to isolate error that is only the result of accepted reductions on the boundary. Problems connected with numerical solutions of advection-diffusion equations are well known (Szymkiewicz 2000). There is no general method that would permit solution of the equation (5) with satisfactory accuracy. Taking into consideration the nature of advection-diffusion equation the splitting technique was used (Szymkiewicz 1993). This technique enables decomposition the equation (5) according to the processes. We solve the advection equation in each time step (in accordance with rules of splitting technique):

$$\frac{\partial f^{(1)}}{\partial t} + u\frac{\partial f^{(1)}}{\partial x} = 0 \tag{21}$$

with initial condition

$$f_t^{(1)}(x) = f_t(x). \tag{22}$$

As a result we can obtain $f_{t+\Delta t}^{(1)}(x)$. It is the value of function $f(x)$ on the next time level. Next, in the same time step, the diffusion equation is solved:

$$\frac{\partial f^{(2)}}{\partial t} - D_e\frac{\partial^2 f^{(2)}}{\partial x^2} = 0 \tag{23}$$

with initial condition

$$f_t^{(2)}(x) = f_{t+\Delta t}^{(1)}(x). \tag{24}$$

We obtain on the next time level $t + \Delta t$:

$$f_{t+\Delta t}(x) = f^{(2)}_{t+\Delta t}(x). \tag{25}$$

The solution of the advection equation (21) has the following form (Fletcher 1991):

$$f(x,t) = f\left(x_0 = x - ut,\ t_0 = t - \frac{x - x_0}{u}\right). \tag{26}$$

If we introduce the net of nodes such that

$$u\frac{\Delta t}{\Delta x} = 1, \tag{27}$$

the solution describes the characteristic lines which correspond with the points of the accepted nets of nodes (Fig. 11). In the opposite cases different ways of interpolation are used to calculate the value of points located among nodes (e.g. Cunge, Holly, Verwey 1980, Szymkiewicz 1993, Holly, Preissmann 1977).

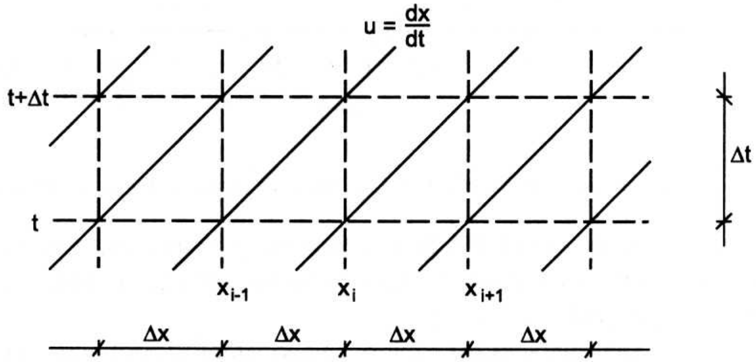

Fig. 11. Run of characteristics, when $u\frac{\Delta t}{\Delta x} = 1$

The solution of the diffusion equation (because of its character) does not cause difficulties of a numerical nature (Szymkiewicz 2000). To solve this equation the finite elements method (Galerkin scheme) was used (Zienkiewicz 1972, Anderson, Tannenhil, Pletcher 1984). Tests of the accepted methods of solution of advection-diffusion equation were checked before each series of calculations. The error was small and did not exceed 0.1%. The example of a test result is presented on Fig. 12.

6. Examining the Influence of Diffusion Term Omission on the Boundary of Domain

Each solution of the advection-diffusion equation has a very clear geometrical interpretation.

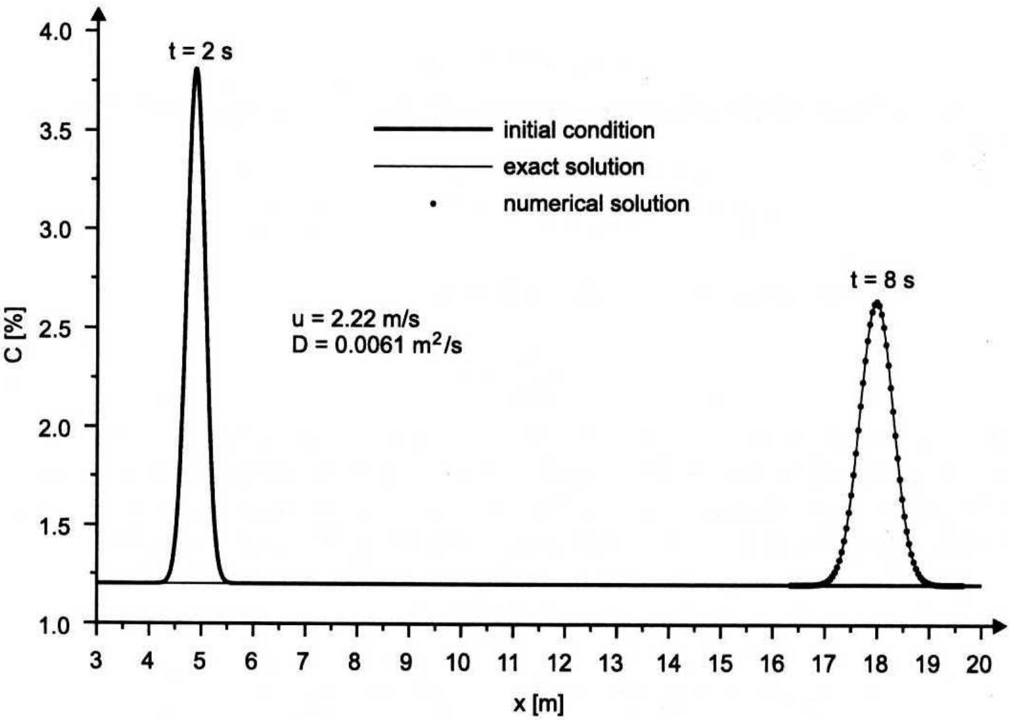

Fig. 12. The results of test solution of advection-diffusion equation using splitting technique

This solution can be visualised by the surface $f = f(x, t)$, which is chart of the function describing the concentration of dissolved matter (when $f = c$) or the temperature of liquid (when $f = T$).

We may receive two surfaces for each of the considered problems. The first one ($f_e = f_e(x, t)$) describes the solution for real boundary conditions (in this paper it was obtained on the basis of analytical solution). The second one ($f_a = f_a(x, t)$) is the solution for boundary condition (17) (Fig. 13).

The following analytical solutions of the considered equation was used in this paper (5) (Crank 1975):

1) for the initial condition in rectangular form (height C_0 and width $2d = e$):

$$c^A(t, x - v \cdot t) = c(t, x), \tag{28}$$

2) for the signal of impulse M type:

$$C^A(x, t) = \frac{M}{2\sqrt{D_e \pi t}} \exp\left(-\frac{(x - ut)^2}{4D_e t}\right), \tag{29}$$

where:

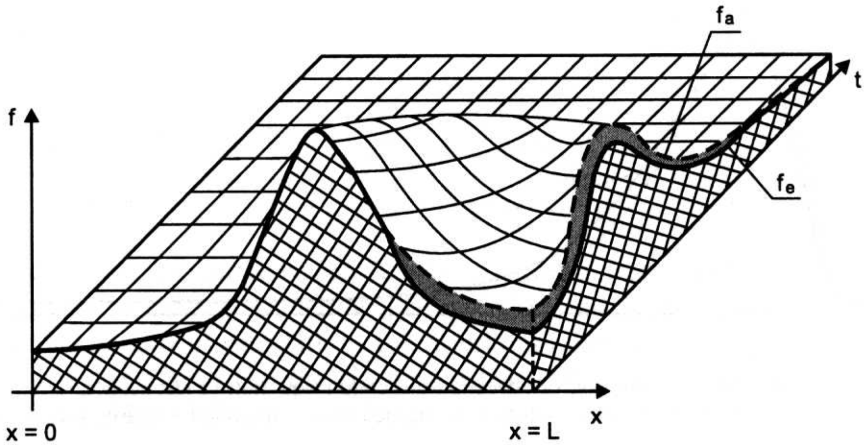

Fig. 13. Solution of advection-diffusion equation in $x - t$ space

M – mass rate of inflow of pollutants (Mitosek 2001) $M = Q_z \cdot C_0$ [kg/s],

Q_z – rate of inflow of pollutants [m^3/s],

C_0 – concentration of pollutants at injection point [kg/m^3];

3) for the "front" of pollutants:

$$C^A(x,t) = \frac{1}{2} C_0 erfc\left(\frac{(x - ut)}{2\sqrt{D_e t}}\right). \tag{30}$$

Because of the practical possibilities of the description of physical effects, the influence of reductions of boundary condition in the end section of the considered domain ($x = L$; "outflow" boundary) was tested in the paper. In geometrical interpretation which means that surfaces $f_e(x,t)$ and $f_a(x,t)$ have identical courses in first section ($x = 0$; "outflow" boundary).

$$f_e(0,t) = f_a(0,t) \tag{31}$$

Both surfaces split for increasing values of x and t (Fig. 13). For practical reasons the author focused on the estimation of difference of both solutions in the end section ($x = L$), where error has the greatest value (Fig. 14).

6.1. Accepted Tests of Convergences

The basic question considered in this paper is the problem of the quantitative description of difference between the exact solution (f_e) and the approximate solution (f_a). From the formal point of view it is the question of choosing the agreement criteria of the courses of two lines:

$$f_e(x = x_u, t) \quad \text{and} \quad f_a(x = x_u, t) \tag{32}$$

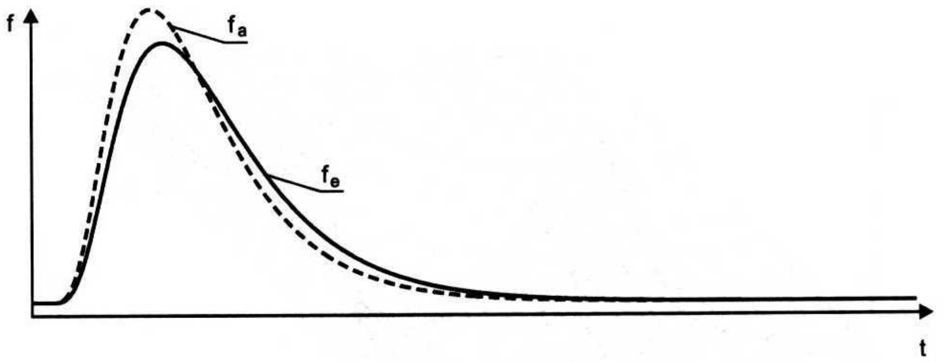

Fig. 14. The solution of advection-dispersion equation in last section (continuous line – exact solution f_e, dashed line – simplified solution f_a)

where x_u is a fixed value of space variable x. In last section $x_u = L$.

We meet the problem of choice of agreement criterion during the analysis of divergence of exact and simplified solution. There are numerous measure criteria that permit estimation of the divergences between two functions. In this paper the following criteria were used:

– ratio of average value of absolute error to average value of f_e

$$SBW = \frac{\left[\sum_{i=1}^{M} |f_{ei} - f_{ai}|\right]}{\sum_{i=1}^{M} f_{ei}} \cdot 100[\%], \tag{33}$$

– correlation coefficient

$$WK = \frac{\sum_{i=1}^{M} (f_{ei} \cdot f_{ai})^2}{\sum_{i=1}^{M} (f_{ei}^2) \cdot \sum_{i=1}^{M} (f_{ai}^2)} [\%]. \tag{34}$$

6.2. Formulating of Research Problems

Formally the difference between the exact and approximate solution may attain an infinitely great value. Real advection velocity in the range of from 0.1 m/s to 2.0 m/s was examined. The transport coefficient was obtained from different formulas for real conditions. During computer simulation, velocity and dispersion coefficient changed in range as follows:

$$D_l \in < 0,0005; 0,1; 0,5; 1,0; 1,3 > \ [\mathrm{m}^2/\mathrm{s}]$$
$$u \in < 0,1; 0,5; 1,0; 1,5; 2,0 > \ [\mathrm{m/s}]$$

The calculations were performed in the L length domain:

$$L \in < 10; 20; 80; 1000; 10000; 100000 > \text{ [m]}$$

The L domain was divided into a different quantity of nodes:

$$n \in < 225; 450; 900 >$$

In the first step, single wave propagation was considered. An analytical solution of the advection-diffusion equation in form (28) and (29) was used. As initial condition to numerical calculations the solution of equation (28) or (29) in form $f(t, x = x_p)$ was taken. For the right boundary condition ($x = x_k$) in form (17) was accepted (Fig. 15).

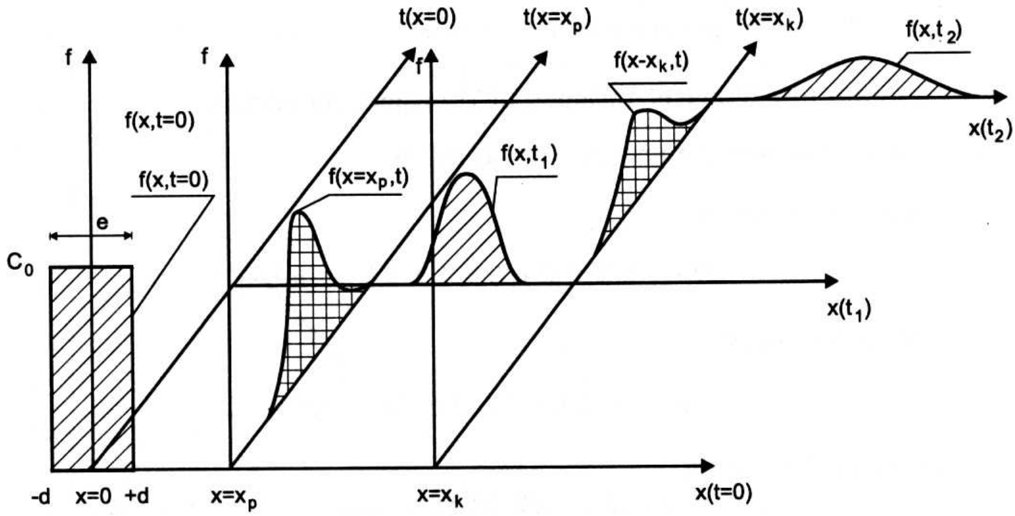

Fig. 15. An example of formulating of research problem

6.3. Definition of Dimensionless Parameters

The most essential element in the presented problem is the connection of investigated error with the characteristic parameters of the analysed phenomenon. In this paper (taking into consideration the physical aspects of processes of mass and energy transfer and aspects of numerical solutions), the following parameters were used (Puzyrewski, Sawicki 2000):

– Peclet number (Pe)

$$Pe = \frac{ul}{D_e}, \tag{35}$$

where:

u – average advection velocity,
l – characteristic linear dimension,
D_e – dispersion coefficient;

– Strouhal number (Sth)

$$Sth = \frac{t_e}{t_L} = \frac{t_e u}{t_z u} = \frac{e}{L}, \tag{36}$$

where:

t_e – time of disturbance,
t_L – time of signal along L domain,
e – length of pollutants wave,
L – length of domain.

6.4. Range of Variation of Transport Parameters

The values of transport parameters were as follow:

1) dispersion coefficient

$$D \in < 0.005; 0.1; 0.5; 1.0; 1.3 > \ [\mathrm{m^2/s}]$$

2) advection velocity

$$u \in < 0.1; 0.5; 1.0; 1.5; 2.0 > \ [\mathrm{m/s}]$$

3) length of the domain

$$L \in < 10; 20; 80 > \ [\mathrm{m}]$$

4) length of injected pollutants wave

$$e \in < 0.2; 2.0; 5.0 > \ [\mathrm{m}]$$

5) number of nodes in domain

$$n \in < 225; 450; 900 > [/]$$

Single "wave" was considered as the input function.

For each consideration of the data, an average relative error SBW was determined according to equation (33). New formula was proposed for received set of SBW values. In this formula the average relative error depends on the dimensionless parameters (35) and (36). Initial analysis of results of numerical calculations shows that error connected with accepted boundary condition $\partial f/\partial x = 0$ on "outflow" boundary depends on:

1) the influence of advection and diffusion processes in the effective transport of dissolved matter or thermal energy,
2) relation between width of pollutants wave e and length of domain L,
3) quantity of error does not depend on accepted numbers of computational nodes, on condition that selection of step Δx was proper. In this regard the constant number of nodes was used in numerical calculation, and $n = 900$.

7. Definition of Formula that Describes the Dependence SBW on Dimensionless Parameters

The solution of equation (5) (for the combination of all parameters presented above) was used as research material for qualifying the influence of reductions on boundary. The examples of calculation results are presented in Fig. 16. Accurate courses (analytical solution) on boundary were drawn as continuous lines corresponding to length of wave e (the highest one $e = 5$ m, the middle $e = 2$ m, the lowest one $e = 1$ m). Approximated solution (dashed line) was drawn for each case.

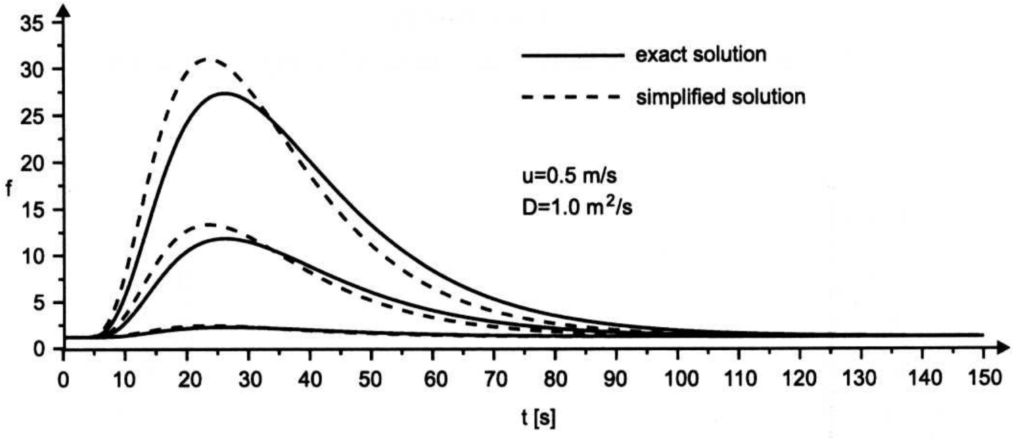

Fig. 16. Example of research results

The next step was the comparison of accurate solutions with adequate approximated solutions. The dependence of average relative error (SBW) on Peclet number (35) was found. The length of computational area L and length of wave e were taken as characteristic dimensions. In this way two Peclet numbers were received: $Pe(e)$ and $Pe(L)$. The value of SBW does not only depend on ratio of advection to diffusion process (defined by Peclet number), but on other parameters also. The detailed analysis has enabled finding of a certain relation to the Strouhal number. The results $SBW(Pe(e))$ and $SBW(Pe(L))$ for example Strouhal numbers (36)) are shown on Fig. 17–18 and 19–20. The points on $SBW(Pe)$ chart (for definite Sth numbers) may be approximate as follows:

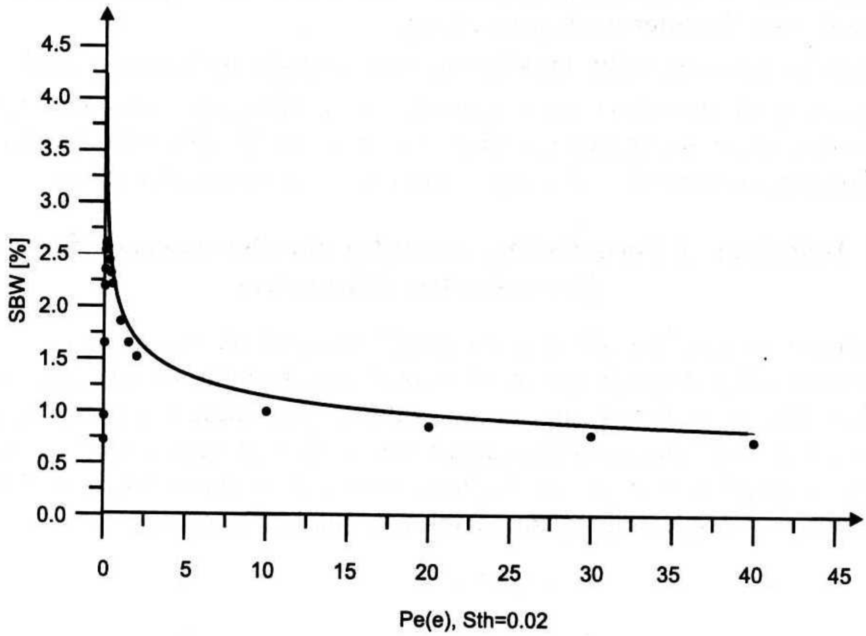

Fig. 17. Dependence of SBW on $Pe(e)$ for number $Sth = 0.02$ (equation (41))

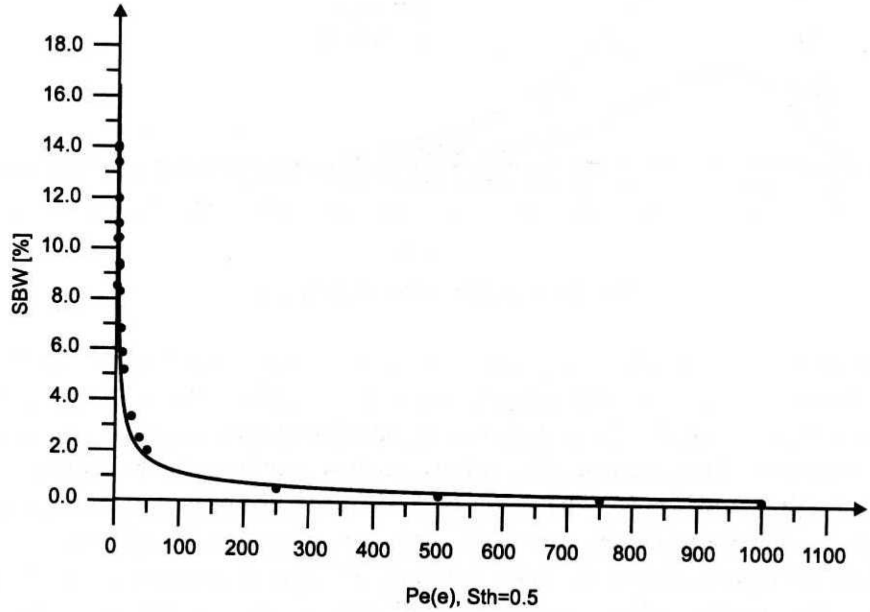

Fig. 18. Dependence of SBW on $Pe(e)$ for number $Sth = 0.5$ (equation (41))

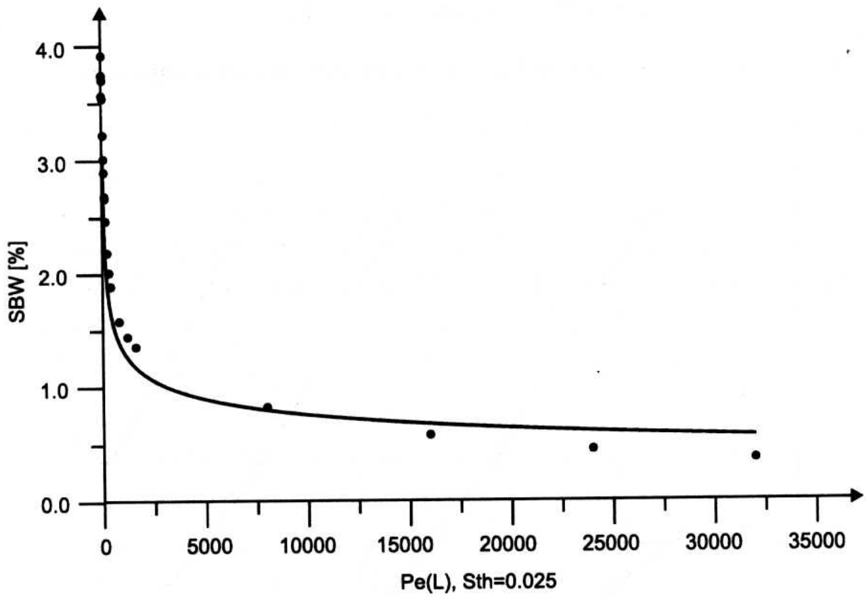

Fig. 19. Dependence of SBW on $Pe(L)$ for number $Sth = 0.025$ (equation (42))

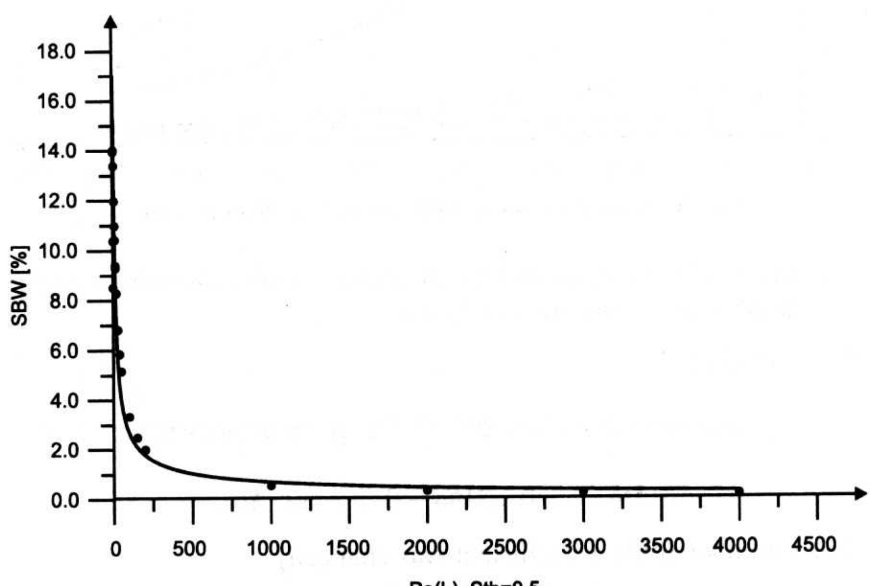

Fig. 20. Dependence of SBW on $Pe(L)$ for number $Sth = 0.5$ (equation (42))

$$SBW = a(Sth)Pe^{b(Sth)}\ [\%] \tag{37}$$

where: $a(Sth)$, $b(Sth)$ – coefficients depend on the Strouhal number.

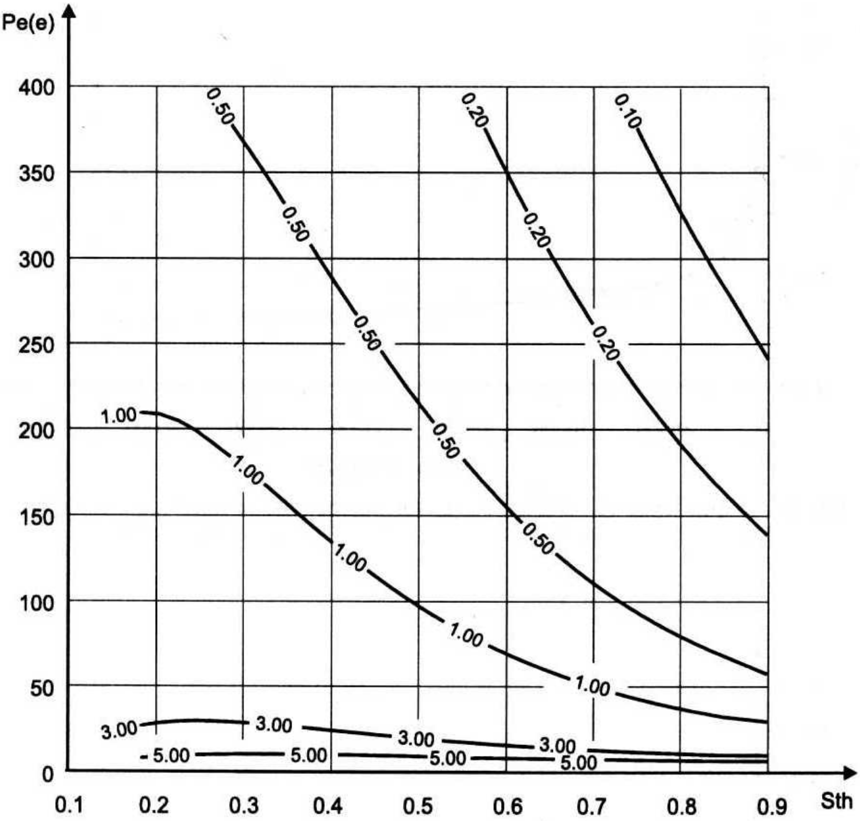

Fig. 21. Nomogram where SBW depend on $Pe(e)$ and Sth

The formulas of $a(Sth)$ and $b(Sth)$ coefficients were determined by the least squares method. Their forms are as follows:

– for $Pe(e)$ number

$$a(Sth) = 48.823497 Sth^{0.808480} \exp(-0.98545 Sth), \tag{38}$$

$$b(Sth) = -0,22148 - 0,713712 \cdot Sth, \tag{39}$$

– for $Pe(L)$ number (only a coefficient was changed)

$$a(Sth) = 117.598542 Sth^{0.759358} \exp(-1.27870 Sth). \tag{40}$$

Finally, the relation (37) can be expressed as follows:

– for $Pe(e)$ number

$$SBW = 48.823497 Sth^{0.80848} \exp(-0.98545 Sth) Pe(e)^{-0,22148-0,71371 \cdot Sth} \, [\%], \quad (41)$$

– for $Pe(L)$ number

$$SBW = 117.598542 Sth^{0.75936} \exp(-1.27870 Sth) Pe(L)^{-0,22148-0,71371 \cdot Sth} \, [\%]. \quad (42)$$

The formula (41) was determined for Strouhal numbers $Sth \in < 0.0025; 0.5 >$ and Peclet numbers $Pe(e) \in < 0; 1000 >$. This function may be represented as a nomogram for small numbers of $Pe(e) \in < 0; 400 >$ (Fig. 21) and for the high numbers of $Pe(L) \in < 0; 1000 >$ (Fig. 22). These nomograms represent the relation of average relative error (SBW) on Sth and Pe numbers. Very good conformity was received with numerical solution points in both cases of Sth number definitions.

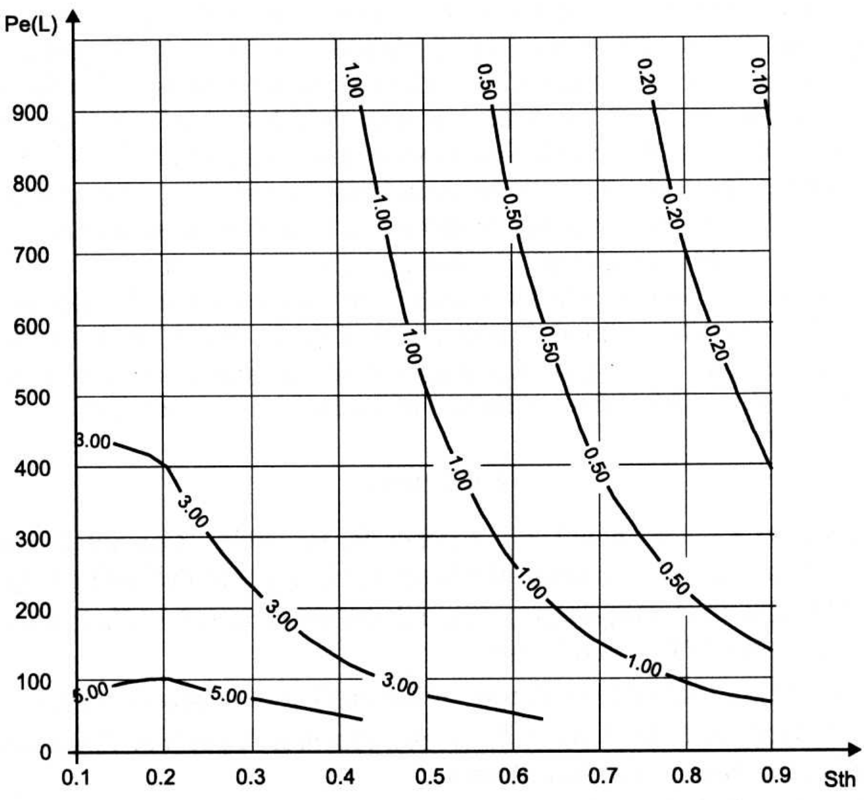

Fig. 22. Nomogram where SBW depend on $Pe(L)$ and Sth

8. Summary and Conclusions

The problem of "outflow" boundary condition appears very often in numerical solutions of advection-dispersion equations. It is impossible to pose them precisely, so some simplifying assumptions are necessary. Especially the following methods are often used:

- "distant boundary" method,
- omission of diffusive term in the "outflow" section of the stream ($\partial f/\partial x = 0$),
- constant value of function f on boundary (constant value of concentration or temperature).

The "distant boundary" method is very precise but has some limitations. First of all it is connected with an artificial extension of the solution area. It results in longer time of calculations of problem solution. The length of domain is limited, hence this method can be used for solving problems connected with propagation of a single wave of pollutants. This method is useless when dealing with continuous changes of concentration or temperatures (continuous "waves").

The most often used simplification in relation to the required boundary condition is acceptance on the "outflow" boundary of the zero diffusive flux (condition $\partial f/\partial x = 0$). This approach generates an error, which depends on shares of advection and diffusion. When diffusion prevails (low Peclet number) this error may be meaningful (average relative error even between ten and twenty percent was obtained during the investigation). When the advection process dominates (high Peclet numbers) this error drops to a few percent.

The results of the performed research show that the error that occurs while applying the generally accepted simplifications of the boundary condition on "outflow" boundary may have significant influence on the final solution of pollutants transport problem. This influence should be taken into consideration.

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