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PH. D. THESIS ABSTRACT

Accurate Flexible Numerical Boundary Conditions for Multidimensional Transport and Diffusion

Precisas Flexibles Condiciones de Frontera Numéricas para el Transporte y Difusión Multidimensional

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Abstract

A method for numerical solution to the advection-diffusion-reaction equation in unbounded domains is developed. The method is based on the concept of artificial boundary conditions (ABCs), and employs the techniques of time and dimensional splitting of the partial differential equation coupled with domain decomposition of the original infinite space. The essentials of the method is that it is applicable for solving a wide class of mass transportation problems in domain of drastically complex geometries, realisable from the computation standpoint, and provides a highly accurate solution at minimal computational efforts.
Keywords: Artificial (numerical) boundary conditions, advection-diffusion-reaction equation, splitting, domain decomposition.

Resumen

Se desarrolla un método para la solución numérica de la ecuación de advección-difusión-reacción en dominios infinitos. El método se basa en el concepto de condiciones de frontera artificiales (CFAs), y utiliza las técnicas de escisión del operador por tiempo y por espacio junto con la de descomposición de dominio para el espacio original infinito. Los esenciales del método son lo que es aplicable para dar solución a una amplia clase de los problemas de transporte de masa en dominios de la geometría demasiado compleja, realizable desde el punto de vista numérico, y además proporciona una alta precisión de la solución con mínimos esfuerzos computacionales.
Palabras clave: Condiciones de frontera artificiales (numéricas), ecuación de advección-difusión-reacción, escisión del operador, descomposición de dominio.

1 Introduction

While numerically solving a differential problem originally formulated in an unbounded domain as a Cauchy problem, one has to reformulate it as a boundary value problem (BVP) for a finite computational domain. Therefore, the question of imposing adequate boundary conditions on the artificial boundary arises.

The simplest approach is to place the boundary rather far from the region of interest and impose the known boundary condition at infinity there. Obviously, the main disadvantage of this approach is wasteful use of computer resources; in particular, the calculation time increases dramatically, especially when solving multidimensional problems. To minimise the computational efforts, one can employ the nested grids method when the solution is recalculated sequentially from a coarser grid onto a finer one. However, this introduces an essential error into the final solution.

Approximately from the 1970’s there has been developed the approach of *artificial boundary conditions* (ABCs) (Givoli, 1992; Tsynkov, 1998). Within the framework of this approach it is supposed that outside the region of interest the problem admits the exact or approximate analytical solution. This simplification permits reducing the construction of boundary conditions to seeking for a solution in the exterior domain, which is further used as an ABC.

All the existing methods of constructing ABCs can be classified in two groups.

Methods of the first group, so-called *global*, lead to exact artificial boundary conditions, which are, however, unrealisable from the computational point of view. The latter is because the standard apparatus for constructing exact ABCs is integral (Fourier and/or Laplace) transforms, and so, the boundary condition is represented as a non-local integral relation between the function to be sought and its derivative(s). Moreover, many of these methods are very exigent to the shape of artificial boundary.

Methods of the second group, so-called *local*, on the contrary, provide algorithmically simple boundary conditions not so exigent to the geometry of computational domain. Nevertheless, these ABCs are often of an unsatisfactory degree of precision.

It is important to emphasise that for solving complex differential equations that include several (two and more) different physical processes, advanced methods of constructing artificial boundary conditions are required. In particular, these should take into account the mathematical specifics of each of the processes to be modelled, which will allow more accurate treating the solution at the artificial boundary. A new method satisfying the aforesaid requirements is described further in this paper.

2 Construction of the ABCs

2.1 Problem Formulation

Consider the two-dimensional mass transportation problem

$$\frac{\partial \varphi}{\partial t} + \nabla \cdot (\mathbf{U}\varphi) - \nabla \cdot (\mu \nabla \varphi) + \sigma \varphi = f \,, \tag{1}$$

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0 \,, \tag{2}$$

$$\varphi\big|_{t=0} = g(x,y) \,, \tag{3}$$

$$\lim_{\sqrt{x^2+y^2} \to +\infty} \varphi = 0 \,. \tag{4}$$

Here $\varphi = \varphi(x,y,t)$ is the function to be sought, $\mathbf{U} = \left(u(x,y,t), v(x,y,t)\right)^{\mathrm{T}}$ is the vectorial field of velocities, $\mu = \mu(x,y,t) \geq 0$ is the diffusion coefficient, $\sigma = \sigma(x,y,t) \geq 0$ is the absorption coefficient, and $f = f(x,y,t)$ denotes the sources. We want to find the solution to problem (1)-(4) in a bounded convex domain Ω with a piecewise smooth artificial boundary Γ. Upon this we assume that outside $\overline{\Omega} = \Omega \bigcup \Gamma$ the parameters u, v and μ are constant, while the sources f are absent (cf., e.g., Gustafsson, 1982, 1988; Halpern, 1986, 1991; Tsynkov, 1995, 1998, 1999; Yudin, 1982, 1984).

2.2 Time Splitting

We split (1) into the three equations

$$\frac{\partial \varphi_1}{\partial t} + \frac{\partial (u\varphi_1)}{\partial x} + \frac{\partial (v\varphi_1)}{\partial y} = 0\,, \tag{5}$$

$$\frac{\partial \varphi_2}{\partial t} - \frac{\partial}{\partial x}\left(\mu \frac{\partial \varphi_2}{\partial x}\right) - \frac{\partial}{\partial y}\left(\mu \frac{\partial \varphi_2}{\partial y}\right) = 0\,, \tag{6}$$

$$\frac{\partial \varphi_3}{\partial t} + \sigma\varphi_3 = f\,, \tag{7}$$

corresponding to the advective, diffusive and absorptive processes. (Without loss of generality the function f can be written on the right-hand side of (7) only.) Then the solution to the i th problem is the initial condition for the $(i+1)$ th one, i.e.,

$$\varphi_1\big|_{t=0} = g(x,y)\,, \tag{8}$$

$$\varphi_2\big|_{t=0} = \varphi_1(x,y,t)\big|_{t=\tau}\,, \tag{9}$$

$$\varphi_3\big|_{t=0} = \varphi_2(x,y,t)\big|_{t=\tau}\,. \tag{10}$$

Here τ is the timestep used in the numerical calculations. It can be shown that the sequential solution to problems (5), (8), (6), (9), and (7), (10) is equivalent (in the small) to the solution to original problem (1)-(4).

2.3 Advection

Consider the transport equation

$$\frac{\partial \varphi}{\partial t} + \frac{\partial (u\varphi)}{\partial x} + \frac{\partial (v\varphi)}{\partial y} = f \tag{11}$$

subject to conditions (2)-(4). (For the sake of generality, hereafter the numerical subscripts at the function φ are omitted, while the sources f are distinct from zero on the right-hand side.) In accordance with the technique of domain decomposition, we represent the plane $\mathbb{R}^2$ as a union of a convex interior (denoted as D_I) and exterior (denoted as D_E) domains such that $D_I \supset \overline{\Omega}$, $D_E \overset{def}{=} \mathbb{R}^2 \setminus \overline{\Omega}$ (Fig. 1).

Then we consider the exterior problem. On the set $\partial D_I^- \overset{def}{=} \{(x,y) \in \partial D_I \;:\; \mathbf{U} \cdot \boldsymbol{n} \le 0\} \subset D_E$ its solution is determined by the formula

$$\varphi_E(x,y,t)\big|_{(x,y)\in\partial D_I^-} = g(x-ut, y-vt)\big|_{(x,y)\in\partial D_I^-}\,, \tag{12}$$

which due to the requirement of continuity of the function φ on ∂D_I^- leads to the exact local ABC for the interior problem

$$\varphi_I(x,y,t)\big|_{(x,y)\in\partial D_I^-} = g(x-ut, y-vt)\big|_{(x,y)\in\partial D_I^-}\,. \tag{13}$$

Here the subscripts I and E correspond to the interior and exterior problems, respectively, ∂D_I^- is the inflow part of the boundary ∂D_I, and $\boldsymbol{n}$ is the outward unit normal to ∂D_I.

Constructing an energetic Hilbert space with an adequate norm, it can be proved that the interior problem with boundary condition (13) is well-posed in the sense of existence, uniqueness and stability of solution (Filatov).

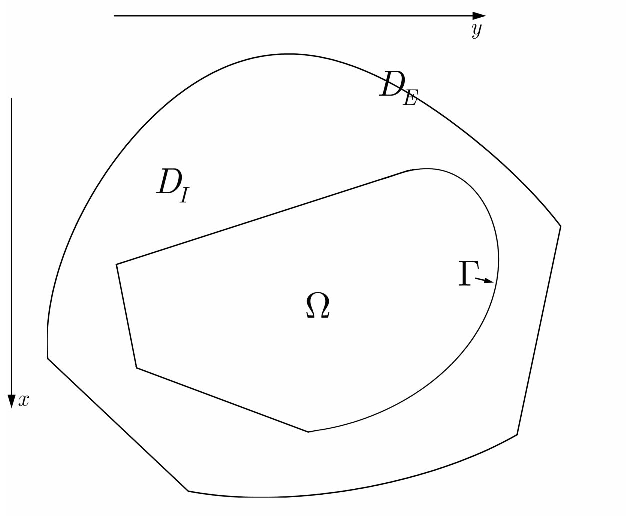

Fig. 1. Decomposition of the plane $\mathbb{R}^2$

2.4 Diffusion

Consider the diffusion equation

$$\frac{\partial \varphi}{\partial t} - \frac{\partial}{\partial x}\left(\mu \frac{\partial \varphi}{\partial x}\right) - \frac{\partial}{\partial y}\left(\mu \frac{\partial \varphi}{\partial y}\right) = f \tag{14}$$

with conditions (3), (4). Similarly to the advective problem, we decompose the infinite plane and solve the exterior diffusive problem: applying the Laplace transform in time, coordinate splitting and spline interpolation, we construct an infinite family of approximate solutions of the form

$$\varphi_{E,\,d}\left(x,y,t\right)\Big|_{(x,y)\in D_E} = \left[g\left(x,y\right) + \sum_{m=1}^{(d-1)/2} \frac{\mu^m t^m}{m!} \nabla^{2m} g\left(x,y\right) \right]\Bigg|_{(x,y)\in D_E} \tag{15}$$

Here $d \geq 3$ is the spline order (odd). This leads to the infinite family of local approximate ABCs for the interior problem

$$\varphi_I\left(x,y,t\right)\Big|_{(x,y)\in \partial D_I} \approx \left[g\left(x,y\right) + \sum_{m=1}^{(d-1)/2} \frac{\mu^m t^m}{m!} \nabla^{2m} g\left(x,y\right) \right]\Bigg|_{(x,y)\in \partial D_I} \tag{16}$$

One can make sure that boundary conditions (16) are asymptotically correct (or admissible) in time with any *finite* timestep τ (Filatov). For each odd $d \geq 3$ for the corresponding error we derive the estimate

$$\left|\varepsilon_d\right| \leq 2\mu \left[c_1 \frac{\left(\mu t\right)^{(d-1)/2}}{\left(\frac{d-1}{2}\right)!} + c_2 \sum_{m=1}^{(d-1)/2} \frac{\left(\mu t\right)^m}{m!} \right], \tag{17}$$

where $c_1 = \max\limits_{(x,y)\in\partial D_I}\left\{\left|\frac{\partial^{d+1}g(x,y)}{\partial x^{d+1}}\right|,\left|\frac{\partial^{d+1}g(x,y)}{\partial y^{d+1}}\right|\right\}$ and $c_2 = \max\limits_{(x,y)\in\partial D_I,\,1\le m\le (d-1)/2}\left\{\left|\frac{\partial^{2(m+1)}g(x,y)}{\partial x^2\partial y^{2m}}\right|,\left|\frac{\partial^{2(m+1)}g(x,y)}{\partial y^2\partial x^{2m}}\right|\right\}$.

Analogically, in an energetic Hilbert space and a specially chosen norm, it can be demonstrated that for each odd $d \ge 3$ the interior problem with the corresponding boundary condition (16) is well-posed in the sense of existence, uniqueness and stability of solution.

2.5 Reaction

The absence of spatial derivatives in (7) does not require imposing boundary conditions when solving the absorptive subproblem.

3 Numerical Results

3.1 Preliminaries

In the numerical experiments as the sets $\overline{\Omega}$ and $\overline{D_I}$ we considered the domains $\overline{\Omega} = [0,1]\times[0,1]$ and $\overline{D_I} = [-0.5,1.5]\times[-0.5,1.5]$. The experiments were performed for the following three problems: the purely advective problem, the purely diffusive problem, and the general advection-diffusion-reaction problem. For each of the problems the experiments can be classified in the three groups: in the first two groups the problems were solved in the domain $\overline{D_I}$; upon this, the parameters of the model were varied in some ranges being constant and non-constant, respectively; in the third group the problems were solved without ABCs for a fixed set of the parameters in domains with increasing sizes from $[-2,3]\times[-2,3]$ to $[-14,15]\times[-14,15]$. The aim of the experiments of the first two groups was to confirm the functionality of the ABCs constructed in the previous chapter; the experiments of the third group were performed in order to substantiate the approach of ABCs from the point of view of saving of computer resources.

The spatial grid steps were $\Delta x = \Delta y = 0.05$, the time of modelling was $T = 12$. The numerical solutions were compared with the appropriate "exact" ones computed in the square $\overline{S} = [-2,3]\times[-2,3]$. When solving the purely advective and diffusive problems, the timestep for the "exact" solution was equal to $\tau^{(exact)} = 0.001$, while for the general advection-diffusion-reaction equation it coincided with $\tau^{(num)} = 0.005, 0.004, 0.003$. Such a practice of comparison of results is typical in the literature (Gustafsson, 1988; Halpern, 1986). The initial condition was chosen to be zero, the sources were computed by the formula $f(x,y,t) = f(t)f(x,y)$, where $f(t) = 0.6t^2e^{-0.273\sqrt{t^3}}(\cos t + 1)$, $f(x,y) = 0.25[1-\cos 4\pi(x-0.35)][1-\cos 4\pi(y-0.1)]$, $(x,y)\in[0.35,0.85]\times[0.1,0.6]$. Such a function reflects the behaviour of real sources used in practical modelling.

3.2 Advection

To discretise the differential operator of equation (11), we employed the explicit conditionally stable first order upwind finite differencing scheme (Press *et al.*, 1992). On the artificial boundary the solution was computed by formula (13). For each of the experiments we computed the absolute errors in the norms of the spaces $L_2\left(\overline{\Omega}\right)$ and $L_2\left(\overline{\Omega}\times(0,T]\right)$: $\varepsilon_{\overline{\Omega}} \equiv \left\|\varphi^{(num)} - \varphi^{(exact)}\right\|_{L_2(\overline{\Omega})}$, $\varepsilon_{\overline{\Omega}\times(0,T]} \equiv \left\|\varphi^{(num)} - \varphi^{(exact)}\right\|_{L_2(\overline{\Omega}\times(0,T])}$.

Figures 2–4 correspond to the first group of experiments (the field of velocities $\mathbf{U} = \mathbf{U}^{const}$ is constant). In Fig. 2 we plot the variation of the $\varepsilon_{\overline{\Omega}}$-error in time at $\mathbf{U} = (0.3, 0.24)$ and $\tau^{(num)} = 0.005$. It can be easily verified that the behaviour of the function $\varepsilon_{\overline{\Omega}} = \varepsilon_{\overline{\Omega}}(t)$ qualitatively repeats the behaviour of the function $f(t)$. Figure 3 shows the dependence of the mean error $\varepsilon_{\overline{\Omega}\times(0,T]}$ on modulus of the field $\mathbf{U}$. One can see that for $\mathbf{U}$ less than some critical $\mathbf{U}^*$ the quantity $\varepsilon_{\overline{\Omega}\times(0,T]}$ increases, while it decreases when $\mathbf{U} > \mathbf{U}^*$. In other words, in case of $\mathbf{U} < \mathbf{U}^*$ the error between the numerical and "exact" solutions is simply growing with the growth of $\mathbf{U}$ due to the temporal discretisation of the problem, while for $\mathbf{U} > \mathbf{U}^*$ it is additionally transported (or "pushed") rapidly out of the region $\overline{\Omega}$ under the essential influence of the advective process itself.

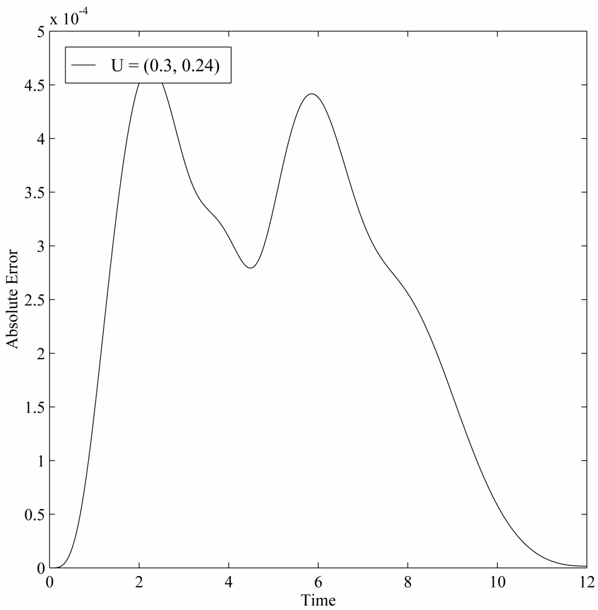

Fig. 2. Behaviour of the $\varepsilon_{\overline{\Omega}}$-error in time

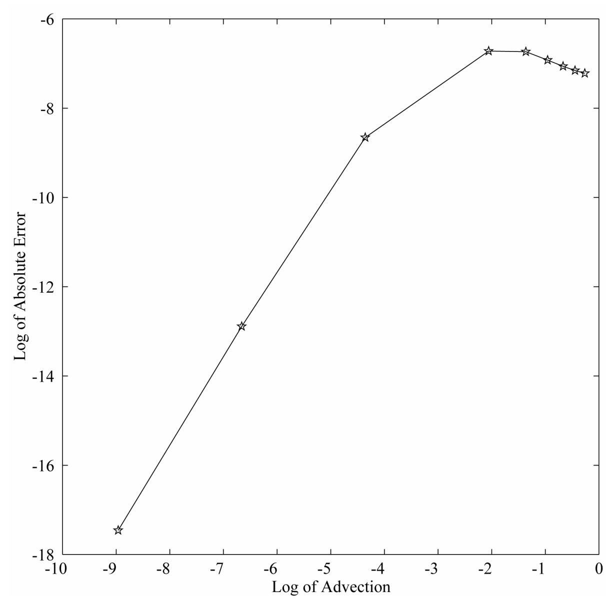

Fig. 3. Dependence of the mean $\varepsilon_{\overline{\Omega}\times(0,T]}$-error on modulus of the field $\mathbf{U}$

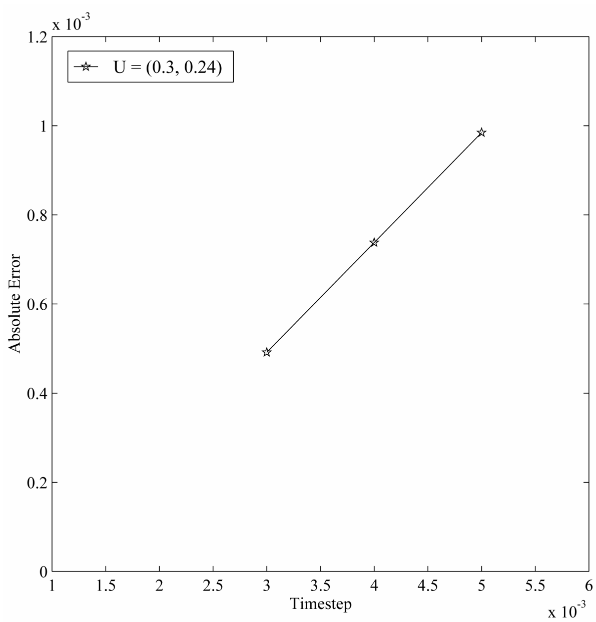

Fig. 4. Dependence of the mean $\varepsilon_{\overline{\Omega}\times(0,T]}$-error on the timestep $\tau^{(num)}$

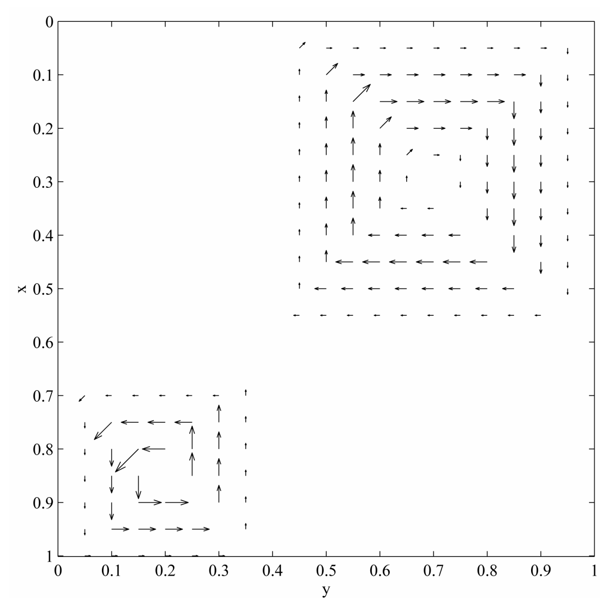

Fig. 5. Portrait of the field $\mathbf{U}^{var}$ in the domain $\overline{\Omega}$

In Fig. 4 we plot the dependence of the mean $\varepsilon_{\overline{\Omega}\times(0,T]}$-error on the timestep $\tau^{(num)}$. Extrapolation of the curve to the point $\tau^{(num)} = \tau^{(exact)} = 0.001$ yields zero value of the error, which confirms that expression (13) is the *exact* artificial boundary condition.

Figure 5 represents the portrait of the field $\mathbf{U}^{var} = \mathbf{U}^{var}(x,y)$ for the second group of experiments (the general field of velocities $\mathbf{U} = \mathbf{U}^{const} + \mathbf{U}^{var}$ is variable; upon this, the vector-function $\mathbf{U}^{var}$ satisfies the finite differencing analogue of condition (2)). The results are almost identical (the difference is about 4%) to those presented above. Consequently, boundary condition (13) "catches" well variations of the parameter $\mathbf{U}$ in the region of interest $\overline{\Omega}$.

Figure 6 corresponds to the third group of experiments (we compared the calculation time required for solving the problem without ABCs in a series of domains with increasing sizes and when solving it with the ABC in the domain $\overline{D_I}$). As it follows from the graph, the behaviour of the curve is of a quadratic character with respect to linear size of the computational domain. This determines the importance of using ABCs from the point of view of saving of computer resources when solving the purely advective problem.

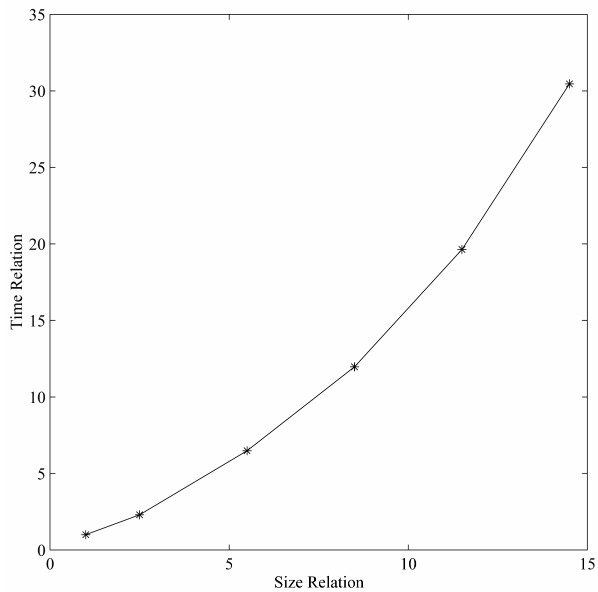

Fig. 6. Dependence of the calculation time on linear size of the computational domain

3.3 Diffusion

To discretise the differential operator of equation (14), we employed the explicit conditionally stable "Forward Time, Centred Space" finite differencing scheme of the first order in time and the second order in space (Press *et al*., 1992). We investigated the first three boundary conditions $d = 3, 5, 7$. To compute the spatial derivatives of orders 2, 4 and 6 in expression (16), we used the discrete exponential extrapolation of the function φ beyond the artificial boundary:

$$\varphi_{-p} = \frac{\varphi_0^{p+1}}{\varphi_1^{p}}, \quad p \in \mathbb{N}, \tag{18}$$

and employed the central finite differences of second order (Korn, 1968). We compared the solutions in the norms: $\varepsilon_{\partial D_I,\, d} \equiv \left\|\varphi_d^{(num)} - \varphi^{(exact)}\right\|_{L_2(\partial D_I)}$, $\varepsilon_{\partial D_I\times(0,T],\, d} \equiv \left\|\varphi_d^{(num)} - \varphi^{(exact)}\right\|_{L_2(\partial D_I\times(0,T])}$.

Figures 7–9 correspond to the first group of experiments (the diffusion coefficient $\mu = \mu^{const}$ is constant). Figure 7 shows the variation of the $\varepsilon_{\partial D_I, d}$-error in time at $\mu = 0.05$, $\tau^{(num)} = 0.005$ and $d = 3$. One can see that there is a growth of the error in time caused by an inaccuracy of extrapolation (18). Therefore, that extrapolation should be used for short time modelling only, when the error is within acceptable limits. In Fig. 8 we plot the dependence of the mean $\varepsilon_{\partial D_I \times (0,T], d}$-errors on the diffusion coefficient.

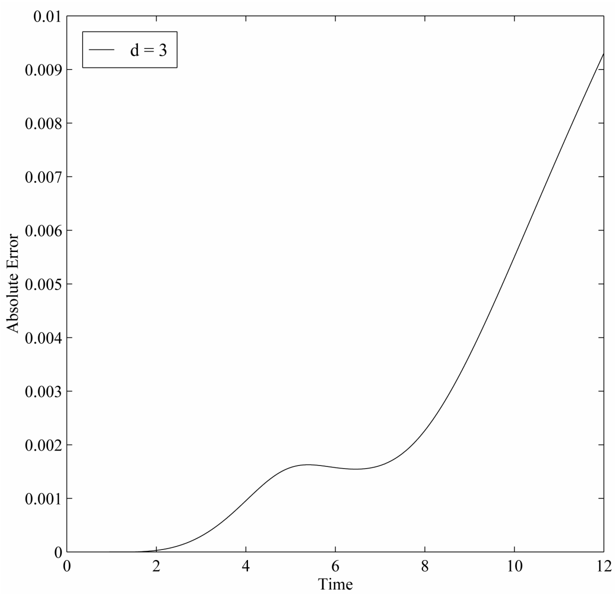

Fig. 7. Behaviour of the $\varepsilon_{\partial D_I, d}$-error in time

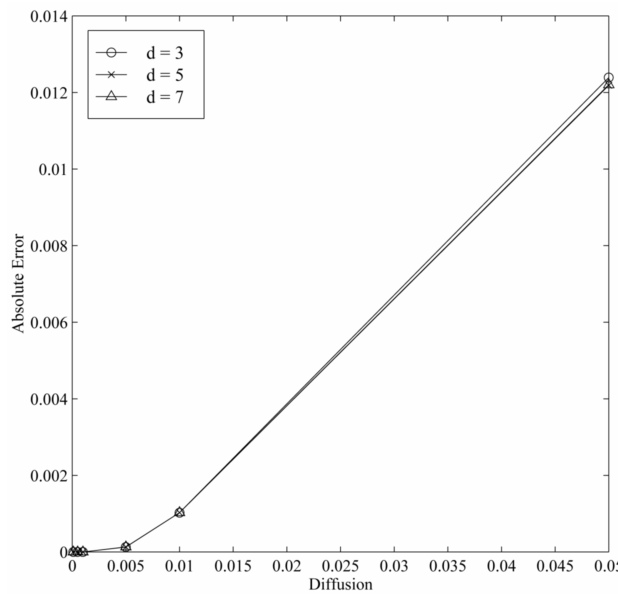

Fig. 8. Dependence of the mean $\varepsilon_{\partial D_I \times (0,T], d}$-errors on the diffusion coefficient μ

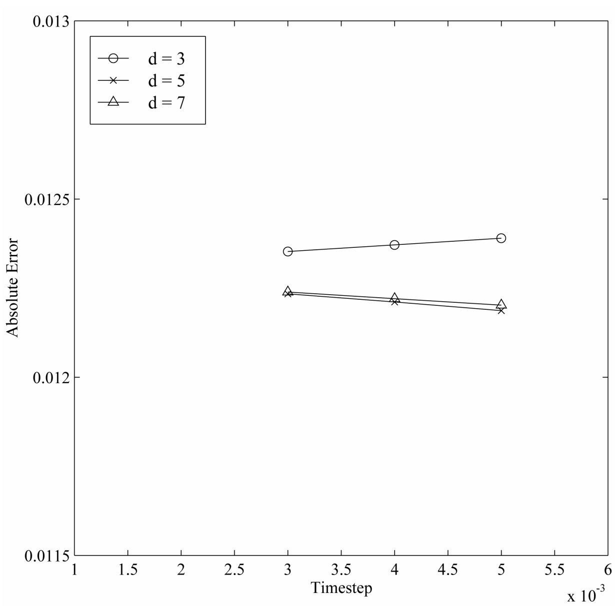

Fig. 9. Dependence of the mean $\varepsilon_{\partial D_I \times (0,T], d}$-errors on the timestep $\tau^{(num)}$

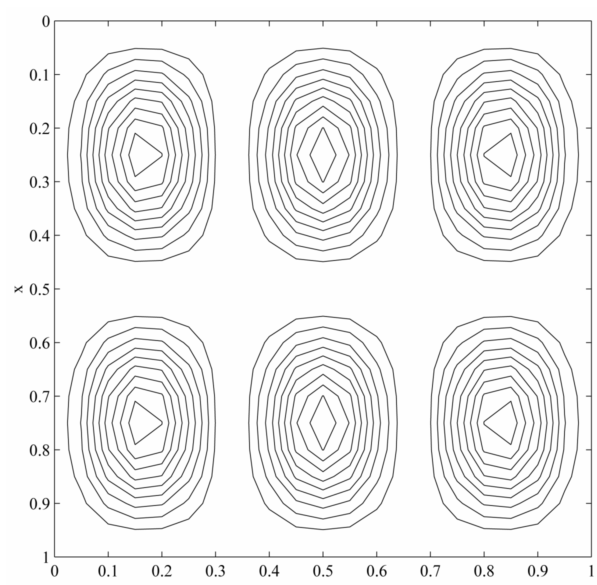

Fig. 10. Portrait of the function μ^{var} in the domain $\overline{\Omega}$

Although $\varepsilon_{\partial D_I \times (0,T],\, d}$ decrease when increasing d, the benefits in precision are rather small and observable only for $\mu = 0.05$. Also, it can be seen that when $\mu \geq 0.01$ the character of the dependence is not polynomial, which contradicts estimate (17). This means that for large values of μ a more accurate extrapolation than (18) is required for calculating the spatial derivatives in expression (16). Figure 9 shows the dependence of the errors on the timestep. Again, quasi-constancy of the errors contradicts estimate (17), which confirms that the influence of the inaccuracy of extrapolation (18) is essential.

In Fig. 10 there is represented the portrait of the function $\mu^{var} = \mu^{var}(x,y)$ from the second group of experiments (the diffusion coefficient $\mu = \mu^{const}(1+\mu^{var})$ is variable). The corresponding results differ very little (the difference does not exceed 4%) from those shown above, which indicates the sensitivity of boundary conditions (16) to variations of the parameter μ in the domain $\overline{\Omega}$.

The results of the third group on solving the diffusive problem are analogous to the corresponding advective ones. This determines the importance of the approach of ABCs for the diffusive problem.

3.4 Advection-Diffusion-Reaction

For discretisation of the advective and diffusive terms of the mass transportation equation we used the explicit upwind and "Forward Time, Centred Space" finite differencing schemes, respectively. The numerical solution was computed by the split scheme, while for the "exact" solution we employed the unsplit differencing scheme. We considered the case when the influence of diffusion is negligible out of the domain $\overline{D_I}$ in comparison with the advective component, which is valid for many practical problems (Bayliss and Turkel, 1982; Incropera and De Witt, 1996; Marchuk, 1986; also Herrera, 1988, 1989).

There were tested the diffusive ABCs corresponding to $d = 3, 5, 7$; for the "exact" solution on the boundary ∂D_I we imposed the ABC corresponding to $d = 9$. For the advective process there was imposed ABC (13) with absorption. The solutions were compared in the norms of the spaces $L_2\left(\overline{\Omega}\right)$ and $L_2\left(\overline{\Omega}\times(0,T]\right)$.

Figures 11–14 correspond to the first group of experiments (the field $\mathbf{U} = \mathbf{U}^{const}$ and the coefficient $\mu = \mu^{const}$ are constant). In Fig. 11 we show the variation of the $\varepsilon_{\overline{\Omega},\, d}$-error in time at $\mathbf{U} = (0.3, 0.24)$, $\mu = 0.05$, $\tau^{(num)} = 0.005$ and $d = 3$. It can be seen that the behaviour of the function $\varepsilon_{\overline{\Omega},\, d} = \varepsilon_{\overline{\Omega},\, d}(t)$ is similar to the behaviour of the temporal component of the source function. In Figs. 12 and 14 there are shown the dependences of the mean $\varepsilon_{\overline{\Omega}\times(0,T],\, d}$-errors on modulus of the field of velocities and on the diffusion coefficient, respectively. As it follows from the figures, when $\mathbf{U} \gg \mu$ the order d of the diffusive ABCs does not affect the precision of the solution; however, it does affect it when the influences of the processes are comparable. This fact indicates the importance of using diffusive ABCs of high orders in case of small velocities. In Fig. 13 we plot the dependence of the mean $\varepsilon_{\overline{\Omega}\times(0,T],\, d}$-errors on the timestep $\tau^{(num)}$. One can easily see that decreasing the step yields decreasing the error, which together with the data of Fig. 11 (the absence of divergence of the numerical solution from the "exact" one) indicates the convergence of the solution to the split BVPs to the solution to the original, unsplit boundary value problem.

The results of the second group (the field $\mathbf{U} = \mathbf{U}^{const} + \mathbf{U}^{var}$ and the coefficient $\mu = \mu^{const}(1+\mu^{var})$ are variable) are close (the difference is not greater than 5%) to the previously obtained ones. This means that boundary conditions (13), (16) "catch" well variations of the parameters $\mathbf{U}$ and μ in the domain $\overline{\Omega}$.

The results of the third group are analogous to the corresponding advective and diffusive ones, which substantiates the importance of the approach of ABCs when solving the general mass transportation problem.

3.5 Non-Square Computational Domain

Aside from the domain $\overline{\Omega} = [0,1]\times[0,1]$ we solved the advection-diffusion-reaction equation in the non-square domain $\overline{\Omega}$ shown in Fig. 15. The results of these experiments differ rather little from those analysed above, which confirms the functionality and accuracy of the constructed ABCs, as well as indicates their sensitivity to the shape of artificial boundary.

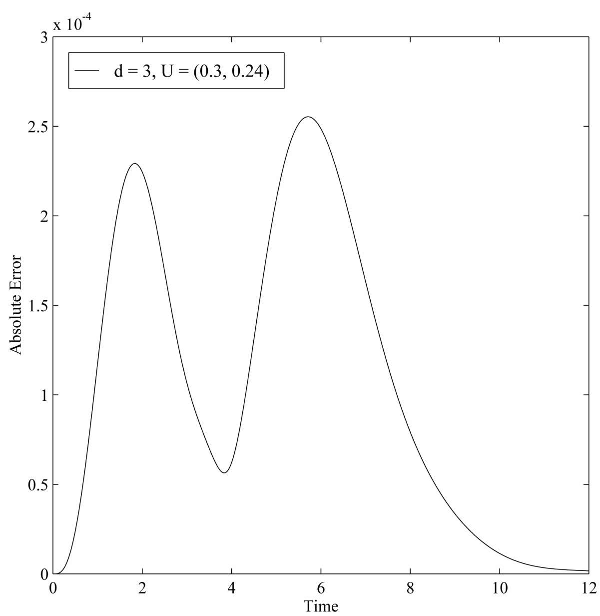

Fig. 11. Behaviour of the $\varepsilon_{\overline{\Omega},\,d}$-error in time

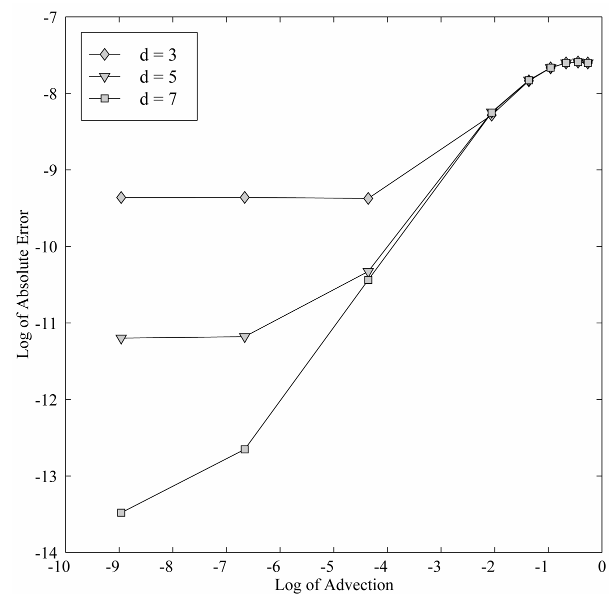

Fig. 12. Dependence of the mean $\varepsilon_{\overline{\Omega}\times(0,T],\,d}$-errors on modulus of the field $\mathbf{U}$

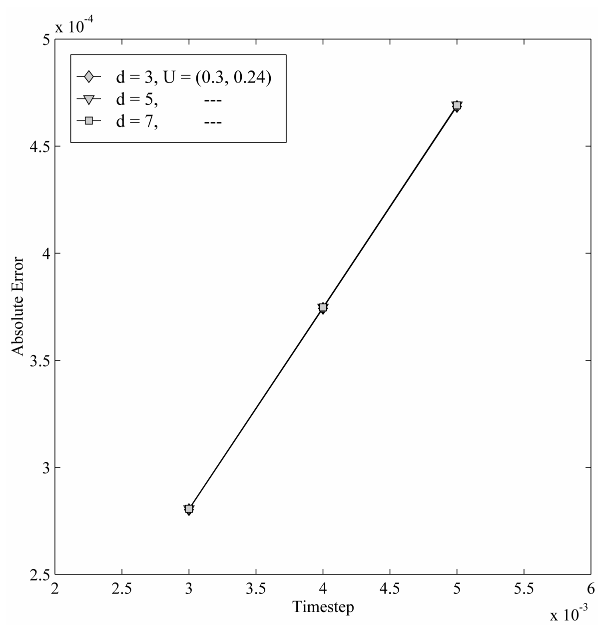

Fig. 13. Dependence of the mean $\varepsilon_{\overline{\Omega}\times(0,T],\,d}$-errors on the timestep $\tau^{(num)}$

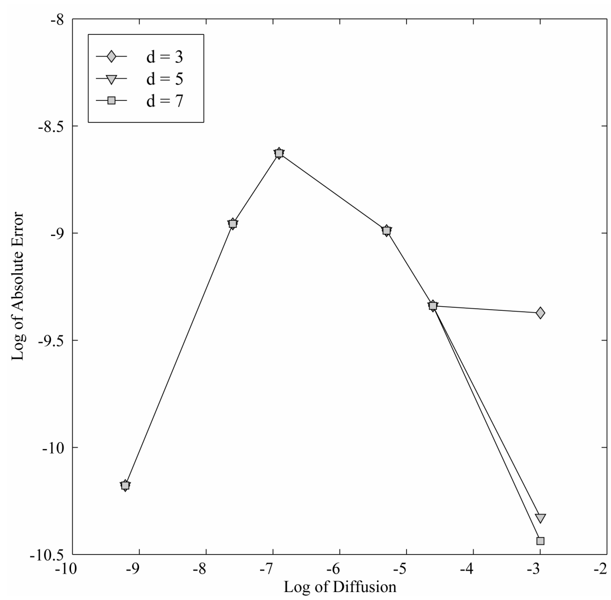

Fig. 14. Dependence of the mean $\varepsilon_{\overline{\Omega}\times(0,T],\,d}$-errors on the diffusion coefficient μ

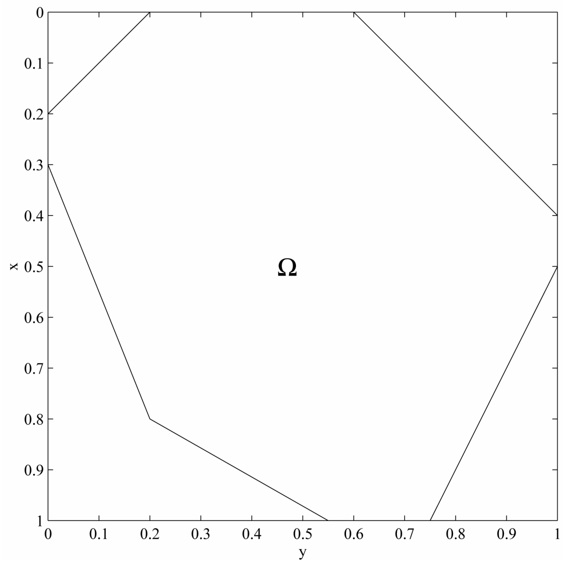

Fig. 15. Non-square computational domain $\overline{\Omega}$

3.6 Experiments with Real Data

A few series of experiments with real data were also performed to test the developed method. Specifically, we modelled the propagation of a polluting substance in the atmosphere of Mexico City. As the pollution sources, we considered the contribution of the city traffic in five principal streets. The data were obtained from the archives of RAMA (Automatic Net for Atmospheric Monitoring) of the Mexico City Government.

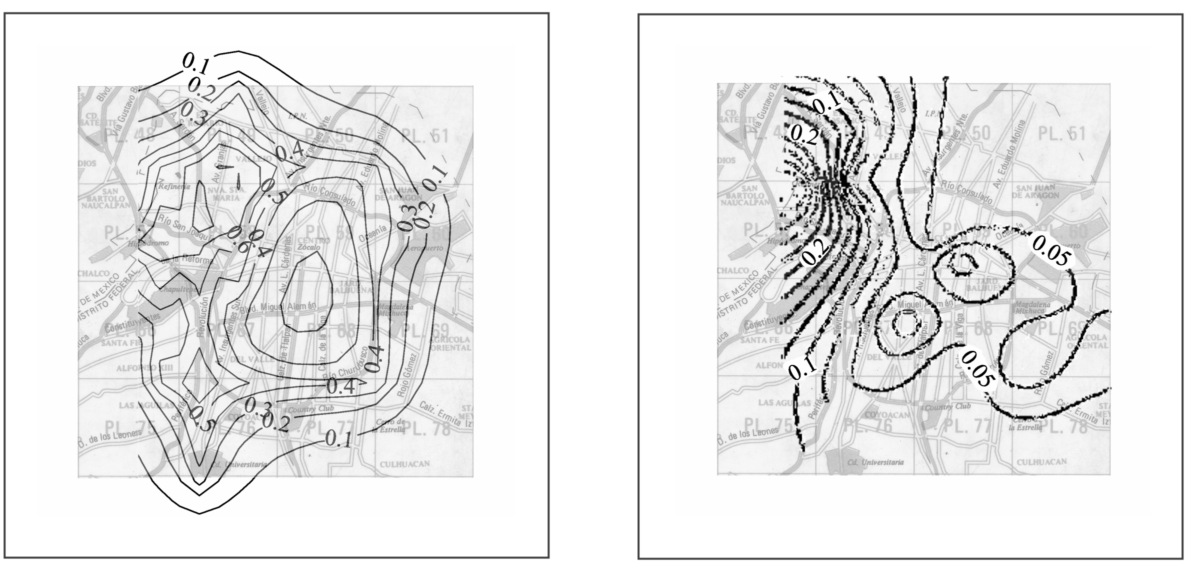

Fig. 16. Experiments with real data: numerical solution (left) and real situation (right)

Figure 16 shows an example of numerical modelling and the real situation (the results are averaged). It can be seen that the numerical solution *qualitatively* repeats the data of observation. In particular, one can see a maximum in the city centre (Fig. 16, left) that corresponds to the two maximums in Fig. 16, right. Yet, there is a family of isolines in the west observed in both figures (with some local maximums in Fig. 16, left, as well). Thus, the method can be used for accurate simulation while numerically solving a wide range of practically important problems described by the mass transportation equation. We believe the method can further be investigated for a wider class of shapes of artificial boundaries.

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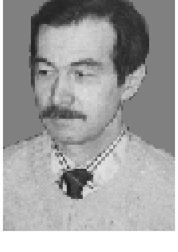

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