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MATHEMATICS METHODS AND INFORMATION SYSTEMS IN CHEMICAL TECHNOLOGY

ABOUT SOME SUPPLEMENTARY POSSIBILITY FOR NUMERICAL SOLUTION OF PARTIAL DIFFERENTIAL EQUATIONS

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A substitution of an non-homogeneous term and of a differential operator by the difference of Laplace operators in the direct co-ordinate system and in the turned one in the partial differential equations of first, second and third order is proposed. The numerical solution obtained by solving the substituting equation corresponds to the exact solution of the initial equations.

Keywords: *Poisson equation, partial differential equation, boundary value problem, difference of Laplace operators, turned co-ordinate system, method of transition to a steady state, substituting equation, Milne operator, structure of function, computer simulation.*

The computer modeling of chemical processes based on solving differential equation systems of various orders requires improving the solution methods and checking the obtained results. The development of numerical methods inevitably requires searching and checking new principles of numerical representation of individual chemical objects. Formulating the research objective as boundary value problems is most convenient for chemical technology. Such approach becomes necessary when specifying NMR data of unstable samples, designing and controlling processes of rare elements liquid extraction and forecasting the behavior of materials in case of long influence of media inaccessible to experiment.

When solving a boundary value problem by the grid method, it is required to determine the values of $\Phi(x, y)$ function satisfying a given differential equation in a range with specified boundary conditions. The search range is covered by a set of equidistant points (grid). The distance to any adjacent point is equal to the grid size $\Delta_{grid}=\Delta x=\Delta y$. Let us replace members containing differentiation in the differential equation with members containing algebraic operations. (This is referred to as creating approximation equations.) Let us solve the obtained system of equations. The requirement of obtaining a high precision of the numerical solution can be satisfied by applying more precise forms of approximation equations. In order to do this, the function values in the grid nodes (x+Δx, y+Δy), (x+Δx, y-Δy), (x-Δx, y+Δy) and (x-Δx, y-Δy) are usually introduced in the derivatives of the finite-difference operator along with the function values in the grid nodes (x, y), (x +Δx, y), (x, y +Δy), (x-Δx, y) and (x, y-Δy) [1]. This introduction in the process of the Laplace operator creation can be defined as the simultaneous use of the direct and rotated operators.

The possibility of using the Laplace operator in a rotated coordinate system was used in [1] and [2] for solving the Poisson equation at boundary conditions corresponding to the precise solution.

When solving the equation with the use of the finite difference method, the initial second-order differential equation $\frac{\partial^2\Phi}{\partial x^2}+\frac{\partial^2\Phi}{\partial y^2}+f(x, y)=0$ was replaced with the equation

$$\frac{\partial^2\Phi}{\partial x^2}+\frac{\partial^2\Phi}{\partial y^2}-\left(\frac{\partial^2\Phi}{\partial x'^2}+\frac{\partial^2\Phi}{\partial y'^2}\right)=0,$$

where $\frac{\partial^2\Phi}{\partial x^2}+\frac{\partial^2\Phi}{\partial y^2}$ is the Laplace operator in the Cartesian coordinate system *(x,y)*, and $\frac{\partial^2\Phi}{\partial x'^2}+\frac{\partial^2\Phi}{\partial y'^2}$ is the Laplace operator in the coordinate system (x', y') rotated by 45° with respect to the ordinary coordinate system. Such difference in the Laplace operators corresponds to the Miln operator presented in [4]. The possibility of such replacement was explained in [2] by the equality of the direct and rotated Laplace operators in coordinate systems (x, y) and (x', y') in the whole range including the boundaries. In the process of the study researchers were forced to discard this explanation.

Particularly, it was found that finite-difference equation $\frac{\Delta^2\Phi}{\Delta x^2}+\frac{\Delta^2\Phi}{\Delta y^2}=\frac{\Delta^2\Phi}{\Delta x'^2}+\frac{\Delta^2\Phi}{\Delta y'^2}$ is true only for some functions and under conditions $\Delta x=\Delta y;\ \Delta x'=\Delta y'=\sqrt{\Delta x^2+\Delta y^2}$. But Δx and Δy values can be both tending to zero and finite. It is obvious that the case in point is the existence of a structure expressed by the above equation in such functions. Using this equation allowed obtaining precise solutions only by means of the values of the corresponding function at the boundary without using source functions *f (x,y)* (which are present in the Poisson equation) in the finite-difference equations. In a more general case the structure of the functions is expressed by equation $\frac{\Delta^2\Phi}{\Delta x^2}+\frac{\Delta^2\Phi}{\Delta y^2}=\frac{\Delta^2\Phi}{\Delta x'^2}+\frac{\Delta^2\Phi}{\Delta y'^2}+F(x,y,\Delta x,\Delta y)$, where $F(x,y,\Delta x,\Delta y)$ is a function depending on x, y, Δx and Δy. For example, in case of function $f(x,y)=x^2y^2$ (under condition $\Delta x=\Delta y$; $\Delta x'=\Delta y'=\sqrt{\Delta x^2+\Delta y^2}$) the structural equation takes the form $\frac{\Delta^2\Phi}{\Delta x^2}+\frac{\Delta^2\Phi}{\Delta y^2}=\frac{\Delta^2\Phi}{\Delta x'^2}+\frac{\Delta^2\Phi}{\Delta y'^2}+\Delta x^2+\Delta y^2$, Δx and Δy either tending to zero or tending to large numbers.

In this study we suggest developing the method for solving boundary value problems presented in [1] and [2].

We have differential equation

$$\frac{\partial^2\Phi}{\partial x^2}+\frac{\partial^2\Phi}{\partial y^2}+f_1(x,y)=0, \tag{1}$$

having precise solution $\Phi(x,y)$. This solution can be the solution of a number of other differential equations. Such equations are, for example:

$$\frac{\partial\Phi}{\partial x}+\frac{\partial\Phi}{\partial y}+f_2(x,y)=0, \tag{2}$$

$$\frac{\partial^3\Phi}{\partial x^3}+\frac{\partial^3\Phi}{\partial y^3}+f_3(x,y)=0, \tag{3}$$

$$\frac{\partial^2\Phi}{\partial x^2}+\frac{\partial^2\Phi}{\partial y^2}-\left(\frac{\partial^2\Phi}{\partial x'^2}+\frac{\partial^2\Phi}{\partial y'^2}\right)=0,$$

where $\partial x'=\partial y'=\sqrt{\partial x^2+\partial y^2}$. (4)

The solution of each of the equations is an independent boundary value problem with the choice of the corresponding difference scheme. However, the boundary conditions for these tasks are identical. So, the same solution should be obtained. This enables choosing the most appropriate equation. It may be assumed that equation (4) applied in [1] and [2] is such an equation.

The following example illustrates the use of this method.

Function

$$\Phi(x,y)=x^4+y^4-4x^3y-4xy^3-\sin^5(x^3-2)-\exp(\alpha y^2+1) \tag{5}$$

is a precise solution of the following partial differential equations:

$$\frac{\partial\Phi}{\partial x}+\frac{\partial\Phi}{\partial y}+12x^2y+12y^2x+15x^2\sin^4(x^3-2)\cos(x^3-2)+2\alpha y\exp(\alpha y^2+1)=0; \tag{6}$$

$$\begin{aligned}&\frac{\partial^2\Phi}{\partial x^2}+\frac{\partial^2\Phi}{\partial y^2}+48xy+12x^2+12y^2+30x\sin^4(x^3-2)\cos(x^3-2)+\\&180x^4\sin^3(x^3-2)\cos(x^3-2)+45x^4\sin^5(x^3-2)+(2\alpha+4\alpha^2y^2)\exp(\alpha y^2+1)=0\end{aligned}; \tag{7}$$

$$\begin{aligned}&\frac{\partial^3\Phi}{\partial x^3}+\frac{\partial^3\Phi}{\partial y^3}+1620x^6\sin^2(x^3-2)\cos^3(x^3-2)-1755x^6\sin^4(x^3-2)\cos(x^3-2)+\\&1080x^3\sin^3(x^3-2)\cos^2(x^3-2)-270x^3\sin^5(x^3-2)+30\sin^4(x^3-2)\cos(x^3-2)+\cdot\\&(8\alpha^3y^3+12\alpha^2y)\exp(\alpha y^2+1)=0\end{aligned} \tag{8}$$

Solving these equations numerically is difficult. The first- and third-order equations cannot be solved due to the instability of the difference schemes. The solution of the second-order differential equation is prevented by the cumbersome source function. In this case we foreknow that a solution of any of the suggested equations is a solution of equation (4). Let us use the possibility of substitution. The procedure of solving this substituting equation presents no problems. Such features as the absence of the source function, the possibility of coincidence of the numerical solution with the precise solution and the independence of the obtained solution on the stride parameter along the space facilitate the solution check.

Boundary conditions for equation (4) remain the same. The calculations were carried out according to the finite-difference scheme

$$\frac{1}{\Delta t}\left(\Phi_{x,y}^{j+1}-\Phi_{x,y}^{j}\right)=\frac{1}{(\Delta x)^2}\left(\Phi_{x+1,y}^{j}-2\Phi_{x,y}^{j}+\Phi_{x-1,y}^{j}\right)+\frac{1}{(\Delta y)^2}\left(\Phi_{x,y+1}^{j}-2\Phi_{x,y}^{j}+\Phi_{x,y-1}^{j}\right)-$$
$$-\frac{1}{(\Delta x)^2+(\Delta y)^2}\left(\Phi_{x+1,y-1}^{j}-2\Phi_{x,y}^{j}+\Phi_{x-1,y+1}^{j}\right)-\frac{1}{(\Delta x)^2+(\Delta y)^2}\left(\Phi_{x+1,y+1}^{j}-2\Phi_{x,y}^{j}+\Phi_{x-1,y-1}^{j}\right) \quad (9)$$

for orthogonal region $0 \le x \le 6$, $0 \le y \le 6$ by the relaxation method. The stride parameter along the space $\Delta x = \Delta y = 1$.

The difference between the approximate solution and the precise one (the residual) was calculated by the formula

$$\sigma = \sum \left\| \Phi precise \right| - \left| \Phi calculated \right\|, \quad (10)$$

where the sum was calculated for all the reference points of the range. For checking purposes a numerical solution was carried out at a step along the space $\Delta x = \Delta y = 0.5$.

The calculation results are presented in Table.

Results of the numerical solution of equations (6), (7), (8) and (4)

Differential equation	Precise solution	Residual
$\frac{\partial \Phi}{\partial x}+\frac{\partial \Phi}{\partial y}+12x^2y+12y^2x+$ $15x^2\sin^4(x^3-2)\cos(x^3-2)+$ $2\alpha y\exp(\alpha y^2+1)=0$		no numerical solution was obtained
$\frac{\partial^2 \Phi}{\partial x^2}+\frac{\partial^2 \Phi}{\partial y^2}+48xy+12x^2+12y^2+$ $30x\sin^4(x^3-2)\cos(x^3-2)+$ $180x^4\sin^3(x^3-2)\cos(x^3-2)+$ $45x^4\sin^5(x^3-2)+(2\alpha+4\alpha^2y^2)\exp(\alpha y^2+1)=0$	$\Phi(x,y)=$ $x^4+y^4-4x^3y-$ $4xy^3-\sin^5(x^3-2)-$ $\exp(\alpha y^2+1)$	no numerical solution was obtained.
$\frac{\partial^3 \Phi}{\partial x^3}+\frac{\partial^3 \Phi}{\partial y^3}+1620x^6\sin^2(x^3-2)\cos^3(x^3-2)-$ $1755x^6\sin^4(x^3-2)\cos(x^3-2)+$ $1080x^3\sin^3(x^3-2)\cos^2(x^3-2)-$ $270x^3\sin^5(x^3-2)+30\sin^4(x^3-2)\cos(x^3-2)+$ $(8\alpha^3y^3+12\alpha^2y)\exp(\alpha y^2+1)=0$		no numerical solution was obtained.
$\frac{\partial^2 \Phi}{\partial x^2}+\frac{\partial^2 \Phi}{\partial y^2}-\left(\frac{\partial^2 \Phi}{\partial x'^2}+\frac{\partial^2 \Phi}{\partial y'^2}\right)=0$		$< 1.0\cdot10^{-14}$ $\Delta x = \Delta y = 1.0$ $\Delta t = 0.257$ $< 3.0\cdot10^{-12}$ $\Delta x = \Delta y = 0.5$ $\Delta t = 0.06$

The conducted substitution of the initial equation by the simpler one can be useful when creating algorithms for the numerical solution of partial equations.

The author is grateful to associate professor A.S. Litvinovich for the necessary criticism of the studied method and for the help in the results discussion, as well as to all the staff of the physics department for the support during the whole work period.

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