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FINITE VOLUME METHOD DEVELOPMENT FOR AN AXISYMMETRIC POLLUTANT DIFFUSION PROBLEM

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ABSTRACT
The propagation of a pollutant and reactions that a toxic particle undergoes, are important aspect of a pollutant's fate in the environment. In this paper, we research the process of natural non-stationary mass transport in atmosphere. We deal with the system consisted of fluid (air – continuum) in which a toxic pollutant is added. The distribution of pollutants in atmosphere is described by the concentration field ***c(r,*** *t). Diffusion, as the mixing process caused by random walk of molecules (or particles) which, from macroscopic point of view, hardly occupy the configuration with maximum entropy (in absence of outer forces - homogeneous mixture), can be appeared on molecular level or with velocity gradients caused by shear forces (like wind shear). The second case show greater degree of mixing, known as dispersion. In our case, the pollutants diffuse through the medium and the propagation of them is expressed by mass flux rate vector field* ***q(r****,t). We consider also the possibility of the contaminant's creation (or vanish), which is given by scalar source field* ***s(r****,t). For calculation of pollutant transport upon given conditions, we developed a diffusive model in integral form and finite volume method for a specific case of axisymmetrical diffusion. The finite volume discretisation method gives very clear physical interpretation and possibility of reaching very valuable reliable results. For different combination of location of pollutant source, wind direction and other related parameters, it is possible to obtain an optimum solution in terms of achieving satisfactory level of chemical pollution.*
Keywords: axisymmetrical diffusion, finite volume method, discretisation

1. THEORETICAL BASE
The subject of interest is a fluid system (medium) in which a pollutant is added. The pollutant distribution is represented by *scalar field of concentration* $c(\vec{r},t)$ [1]. *The diffusion* is the process of mixing fluid components, caused by random moving of molecules, which, by microscopic point of view, hardly occupy a configuration of maximal entropy (in absence of outer forces this is the state of homogenous mixture). In our case the molecules diffuse throughout the medium, and this spreading can be described by *vector field of mass flux rate* $\vec{q}(\vec{r},t)$ [2]. We took into account possibility of pollutant production (or disappearing) which can be described by *scalar field of source* $s(\vec{r},t)$ [3].

The basic equations are equations of conservation of some property and constitutive equations. In the simplest case the diffusion problem is based on a conservation equation – equation of continuity and a constitutive equation – Fick's law of diffusion [1].

Continuity equation: $$\frac{\partial c}{\partial t}+\nabla\cdot\vec{q}=s \qquad (1.1)$$

[1] Concentration (amount of substance per volume) ML^{-3}
[2] Amount of substance which passing through unit cross section in unit of time or areal mass flux rate ($ML^{-2}T^{-1}$)
[3] Amount of substance which has been created in a volume around a space point **r** in unit of time ($ML^{-3}T^{-1}$)

Fick's law determined that mass transfer by diffusion is proportional to the cross-sectional area and steepness of the concentration gradient, with respect to time: $\vec{q} = -D\nabla c$ (1.2)
where ***D*** is diffusivity or diffusion coefficient [L^2T^{-1}].

Putting (1.2) in (1.1) we obtain $\frac{\partial c}{\partial t} - \nabla\cdot(D\nabla c) = s$. Using Gauss theorem this equation takes an integral form: $\frac{\partial}{\partial t}\int_V c\,dV - \int_S D\nabla c\cdot\vec{n}\,dS = \int_V s\,dV$ (1.3)

The finite volume method (FVM) is powerful discretisation method with very clear physical interpretation [2]. The continuous space and time coordinates will be transformed to a discrete form. **The time** is turning discrete by arbitrary number of time steps $\{t_0, t_1, t_2, \ldots\}$, separated by elementary time interval δt. **The space** is divided into finite number of control volumes (cells), which generally, can have different forms and volumes. In the simplest case these are cubes of same cubic volume. The grid nodes are taken in the center of each control volume. The boundary nodes are located in the centers of volume surfaces.

We have chosen an axisymmetric system (like the point source of pollutant propagation in atmosphere) in order to reduce the dimension of the system. For this reason we transform the Cartesian coordinates (x,y,z) to the cylindrical (r,ϕ,z), where z-axis is oriented to the axis of symmetry. Because of that, scalar fields $c(\vec{r},t)$ and $s(\vec{r},t)$ will not depend of angular coordinate ϕ. The discretisation of the space is made by splitting it to the families of coordinate planes as follow:

$\{ r = r_j = j\cdot\delta l, \quad j\in N \}$ (*cylinders around the axis*)

$\{ z = z_k = k\cdot\delta l \quad k\in N \}$ (*planes orthogonal to the axis*)

$\{ \phi = \phi_m = m\cdot\delta\phi, \ m = 0,1,2,\ldots n-1) \}$ (*planes through the axis*)

The cells are indexed as $V_{jk}^m = \{(r,\phi,z)\in(r_j, r_{j+1})\times(\phi_m,\phi_{m+1})\times(z_k, z_{k+1}) \}$.

We reduced the dimension by integrating cyclic polar variable ϕ and excluding it out of consideration.

Turn on the equation (1.3) and take a cell V_{jk}^m for the observed volume. **The volume integral** of a scalar function $s(r,z)$ over a control volume can be expressed as:

$$\int_{V_{jk}^m} s(r,z)\,dV = \int_{V_{jk}^m} s(r,z)\,r\,d\phi\,dr\,dz = \delta\phi\int_{v_{jk}} s(r,z)\,r\,dr\,dz \qquad (1.4)$$

where v_{jk} represents corresponding surface in *r*-*z* plane.

In the consideration of surface integrals we calculate the term which represents the flux through the boundary control volume (the second term in (1.3)) by dividing the integral over the surfaces into the integrals over different coordinate planes. The differential *dS* has different shapes as:

$$dS = \begin{cases} r\,d\phi\,dz, & r = const \\ dr\,dz, & \phi = const \\ r\,d\phi\,dr, & z = const \end{cases} \qquad (1.5)$$

When we sum up the integrals over the planes $\phi = const$, the result is zero, as their contributions can be canceled. In final equation we write 2π instead $\delta\phi$. So we get the ring (actually it is square 2-dimensional cell in *r*-*z* plane) which we note as $V_{jk} = \bigcup_{m=0}^{m=n-1} V_{jk}^m$. With this, we can write:

$$\int_{V_{jk}} s(r,z)\,dV = 2\pi\int_{v_{jk}} s(r,z)\,r\,dr\,dz \qquad (1.6)$$

$$\int_{S_{jk}} q\cdot n\,dS = 2\pi\left[r_{j+1}\int_{z_k}^{z_{k+1}} q_r(r_{j+1},z)\,dz - r_j\int_{z_k}^{z_{k+1}} q_r(r_j,z)\,dz \right] + 2\pi\left[\int_{r_j}^{r_{j+1}} q_z(r,z_{k+1})\,rdr - \int_{r_j}^{r_{j+1}} q_z(r,z_k)\,rdr \right] \tag{1.7}$$

It should be mentioned that the (*r*,*z*) metrics in 2D is not Euclidian. The points with greater ***r*** have "greater weight", since in 3D actually, they represent the circles about axis, and greater ***r*** means greater radius of circle. The (*r*,*z*) metrics is given by expression: $ds^2 = (2\pi r)^2\,dr^2 + dz^2 \;\; i.e.\, \mu = \begin{bmatrix} (2\pi r)^2 & 0 \\ 0 & 1 \end{bmatrix}$.

The differential of 2-D volume (surface) in this metrics is equal $dv = 2\pi r\,dr\,dz$. In 3D this is the volume of the ring which radius is equal ***r*** and linear transversal dimensions ***dr*** and ***dz***.

In order to complete transfer to the 2D form, we note 2-D cells with v_{jk}. The volume of v_{jk} cell is:

$$|v_{jk}| = \int_{v_{jk}} dv = \int_{v_{jk}} 2\pi r\,dr\,dz = 2\pi\frac{r_{j+1}^2 - r_j^2}{2}(z_{k+1} - z_k) = (2j+1)^2\,\pi\,\delta l^3 \tag{1.8}$$

If we note with X_{jk} the centers of cells v_{jk}, we will have the coordinates of these centers as:

$$X_{j,k}^{(r)} = \frac{1}{|v_{jk}|}\int_{v_{jk}} r\,dv = \frac{3j^2+3j+1}{2j+1}\delta l, \qquad X_{j,k}^{(z)} = \frac{1}{|v_{jk}|}\int_{v_{jk}} z\,dv = (k+\frac{1}{2})\,\delta l \tag{1.9}$$

Thus, *z*-coordinate is located in the middle to z-direction, but *r*-coordinate is moved in relation to the Euclidian's center in the opposite direction of axis.

2. DISCRETISATION OF EQUATION

a) A scalar field $u(\vec{r},t)$ can be transform into a discrete quantity by $u_i(t) = \frac{1}{|V_i|}\int_{V_i} u(\vec{r},t)\,dV$, where $|V_i|$ is the volume of cell V_i. These discrete quantities are join to the points in the centers of the control volumes. In our case, scalar fields $c(r,z,t)$ and $s(r,z,t)$ are transformed into discrete mean values $c_{jk}(t)$ and $s_{jk}(t)$ averaged over control volumes, and correspond to the centers of control volumes X_{jk}.

b) We also should express surface integrals by dicrete quantities. The expression (1.7) in cylindrical coordinates will have the forms: $q_r = -D(\frac{\partial c}{\partial r} + \frac{c}{r})$; $q_z = -D\frac{\partial c}{\partial z}$. (2.1)

q_r and q_z appear in the linear integrals on the edges of cells, so we can approximate them with mean values on corresponded lines. The partial derivation over ***z*** is equal the difference of mean values of ***c*** on two adjacent cells divided by the distance between these cells, that is: $\left.\frac{\partial c}{\partial z}\right|_{\partial v_{jk}\cap\partial v_{jk+1}} = \frac{c_{jk+1} - c_{jk}}{d(X_{jk+1,}X_{jk})}$.

By analogy we get the result for the first term in (1.7) as $\left.\frac{\partial c}{\partial r}\right|_{\partial v_{jk}\cap\partial v_{jk+1}} = \frac{c_{jk+1} - c_{jk}}{d(X_{jk+1,}X_{jk})}$ (2.2)

c) The distance in z-direction will be δl. But, in the r-direction it can be calculated by formula:

$$\delta r_j = \pi\left(X_{j+1k}^{(r)\,2} - X_{jk}^{(r)2} \right) = \pi\delta l \frac{72j^5 + 360j^4 + 684j^3 + 612j^2 + 256j + 40}{16j^4 + 64j^3 + 88j^2 + 48j + 9} \tag{2.3}$$

Now we have all expressions for partial derivations, so the equation (1.7) have final form as: $\int_{S_{jk}} \vec{q}\cdot\vec{n}dS = -2\pi D\delta l \left\{ \begin{array}{l} (j+1)\frac{\delta l}{\delta r_j}(c_{j+1k} - c_{jk}) - j\frac{\delta l}{\delta r_{j-1}}(c_{jk} - c_{j-1k}) + \\ \frac{1}{2}(c_{j+1k} + c_{jk+1} - c_{j-1k} - c_{jk-1}) + j(c_{jk+1} - 2c_{jk} + c_{jk-1}) \end{array} \right\}$ (2.4)

d) Discretisation of time. The time is discretised by using the Runge-Kutta method. For the sake of this discretisation, Equation (1.3) is devided by $1/|v_{jk}| = (2j+1)\pi\delta l^3$ which gives its term on the right hand side in the form:

$$\begin{aligned} \frac{\partial c_{jk}}{\partial t} = \frac{D}{(j+1/2)\delta t^2}\Big\{ & (j+1)\frac{\delta l}{\delta r_j}\left(c_{j+1k} - c_{j+1k}\right) - j\frac{\delta l}{\delta r_{j-1}}\left(c_{jk} - c_{j-1k}\right) + \\ & + \frac{1}{2}\left(c_{j+1k} + c_{jk+1} - c_{j-1k} - c_{jk-1}\right) + j\left(c_{jk+1} - 2c_{jk} + c_{jk-1}\right)\Big\} + s_{jk} \end{aligned} \tag{2.5}$$

This represents the system of equation by indexes *j* and *k*. If we use the matrix $[C(t)] = \{c_{jk}(t)\}$, we obtain the compact form of equation (2.5): $\frac{\partial[\mathbf{C}]}{dt}(t) = F([\mathbf{C}(t)])$ (2.6)

e) The Runge-Kutta algorithm. The calculation is done in discrete point in time: $t = t_n = n\delta t$

$$\mathbf{K}_1 = \delta t\, F(\mathbf{C}^n)\ ; \mathbf{K}_2 = \delta t\, F(\mathbf{C}^n + \frac{1}{2}\mathbf{K}_1)\ ;\ \mathbf{K}_3 = \delta t\, F(\mathbf{C}^n + \frac{1}{2}\mathbf{K}_2)\ ;\ \mathbf{K}_4 = \delta t\, F(\mathbf{C}^n + \mathbf{K}_3) \tag{2.7}$$

Based on this values, in the next time step one can obtain:

$$\mathbf{C}^{n+1} = \mathbf{C}^n + \frac{1}{6}(\mathbf{K}_1 + 2\mathbf{K}_2 + 2\mathbf{K}_3 + \mathbf{K}_4) \tag{2.8}$$

The equations (2.5) and (2.8) are enough for the numerical solution of problem.

3. AN EXAMPLE: THE POINT SOURCE OF POLLUTANT

As the illustration of FVM application a concrete problem of diffusion: A point source of in atmosphere at definite height H is given was considered. We wanted to find the spreading of pollutant concentration $c(\vec{r},t)$ for *t*>0. Initial condition for *t*=0, the pollutant concentration is equal zero in all points of space. The boundary conditions: the pollutants remain over the ground (*z*=0), actually the flux of pollutant through the plane *z*=0 is equal zero. Using the presented numerical procedure the standard results as could refereeing in [3] was obtained.

4. REFERENCES

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