Study of the simplest solutions of the semiempirical turbulent diffusion equation closed using the second order closure methods

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A number of exact solutions of the one-dimensional turbulent diffusion equation have been obtained using a second order closure method. Obtained results have been compared with solutions of the semiempirical equation closed with the help of the simplest gradient hypothesis. Analysis of obtained results has been performed.

The semiempirical turbulent diffusion equation is widely used for description of the process of atmospheric impurities propagation[1]:

$$\frac{\partial \overline{C}}{\partial t} + \overline{U}_i \frac{\partial \overline{C}}{\partial x_i} + \frac{\partial q_i}{\partial x_i} = \overline{Q}, \qquad (1)$$

where $\overline{C}$ is the average impurity concentration; $\overline{U}_i$ is the average ith component of wind speed; q_i is the ith component of turbulent impurity flow; $\overline{Q}$ describes the impurity sources. An over-bar denotes averaging over statistical ensemble and repeating indices – summing.

Equation (1) illustrates the common property of all averaged equations of turbulent medium mechanics: it is nonclosed as it involves unknown variables q_i. By analogy with the Brownian diffusion process, Eq. (1) is usually closed using the semiempirical gradient hypothesis

$$q_i = -K_{ij} \frac{\partial \overline{C}}{\partial x_j}. \qquad (2)$$

Thus, instead of three unknown components of turbulent flow in the general case, six unknown variables K_{ij}, commonly called turbulent diffusion coefficients, are to be known. Definition of these variables is a complicated problem. The spectrum of such problems is considered in Refs. 1 and 2. Attempts of rigorous proof of the gradient hypothesis (2) have been made in Ref. 3. In Ref. 4, an approach allowing estimation of the turbulent diffusion coefficients is experimentally justified using a recursive technique.[3] Justification of the coefficients proportionality to respective components of the Reynolds viscous stress tensor is given as well. However, when using the semiempirical equation in practice, objective definition of the turbulent diffusion coefficients seems to be the main weakness of the semiempirical approach.

The second order closure methods relates to solution of equations for impurity flows.[5,6] These equations are also nonclosed and involve some unknown variables, which are excluded from the obtained equations with the use of the simplest hypothesis based on dimensionality analysis, tensor structure of equations, and some other physical reasons. So closed equations involve constants, which values can be estimated experimentally.

A number of exact solutions of the one-dimensional turbulent diffusion equation have been obtained in the work using a second order closure method.

Equations for turbulent flows q_i are derived from the medium continuity equation by multiplying its terms by unaveraged components of wind speed U_i (Ref. 6) and following averaging over statistical ensemble. After calculations with the use of the Navier–Stokes equation, we obtain:

$$\frac{\partial q_i}{\partial t} + \overline{U}_j \frac{\partial q_i}{\partial x_j} + \frac{\partial}{\partial x_j}(\overline{\hat{U}_i \hat{U}_j \hat{C}} + \frac{\delta_{ij}}{\rho}\overline{\hat{p}\hat{C}}) + \overline{\hat{U}_i \hat{U}_j} \frac{\partial \overline{C}}{\partial x_j} + q_j \frac{\partial \overline{U}_i}{\partial x_j} - \frac{1}{\rho}\overline{\hat{p}\frac{\partial \hat{C}}{\partial x_i}} - \nu \overline{\hat{C}\Delta \hat{U}_i} = 0, \qquad (3)$$

where $\hat{U}_i$, $\hat{C}$, and $\hat{p}$ are the pulsations of components of wind speed, concentration, and pressure, respectively; ρ is the air density; ν is the air kinematic viscosity; δ_{ij} is the Kronecker symbol; and Δ is the Laplace operator.

The first term in Eq. (3) describes time variations of turbulent flow; the second one is advective, and the third one is diffused. Next two terms are elements of the flow generation by averaged characteristics. The next to last term describes the flow generation by correlations of pressure pulsations with gradients of concentration pulsations. And the last one reflects the presence of viscous dissipation. The third, next to last, and the last terms are to be closed in Eq. (3).

As a rule, the closure procedure of Eq. (3) is the following. The tensor variable $\nu\overline{\hat{C}\Delta \hat{U}_i}$ has an odd number of indices so it should reverse its sign when

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reflecting. An assumption of local isotropy of turbulence should lead to tensor invariability by reflecting. Hence, the term responsible for viscous dissipation is equal to zero under such assumption.

Usually the diffused term is approximated by the gradient equation[6]

$$-C_1\frac{\partial}{\partial x_j}\frac{b^2}{\varepsilon}\left(\overline{\hat{U}_k\hat{U}_j}\frac{\partial q_i}{\partial x_k}+\overline{\hat{U}_k\hat{U}_i}\frac{\partial q_j}{\partial x_k}\right),$$

where b^2 and ε are the kinetic energy of turbulence and the rate of its dissipation, respectively. Their ratio is some kind of speed scale. The constant C_1 is estimated to be equal to 0.11.[6]

Finally, the following approximation is used for the term remaining nonclosed[6]:

$$C_2 q_j\frac{\partial\overline{U}_i}{\partial x_j}-C_3\frac{\varepsilon}{b^2}q_i.$$

According to different authors,[5,6] empirical constants $C_2 = 0.33–0.5$ and $C_3 = 3.0–3.2$.

Thus, the equations for turbulent flow components take the form

$$\frac{\partial q_i}{\partial t}+\overline{U}_j\frac{\partial q_i}{\partial x_j}-C_1\frac{\partial}{\partial x_j}\frac{b^2}{\varepsilon}\left(\overline{\hat{U}_k\hat{U}_j}\frac{\partial q_i}{\partial x_k}+\overline{\hat{U}_k\hat{U}_i}\frac{\partial q_j}{\partial x_k}\right)+$$
$$+(1-C_2)q_j\frac{\partial\overline{U}_i}{\partial x_j}+C_3\frac{\varepsilon}{b^2}q_i-\overline{\hat{U}_i\hat{U}_j}\frac{\partial\overline{C}}{\partial x_j}=0. \qquad (4)$$

As is known, the time scale as the ratio of the dispersion of concentration pulsations σ_c^2 to the rate of its dissipation ε_c is more reasonable to use in closure equations instead of the b^2-to-ε ratio.[6] If to introduce the ratio of the two specified scales $R = \varepsilon\sigma_c^2(b^2\varepsilon_c)^{-1}$, then it is necessary to divide C_1 to R and multiply C_3 by the same value in Eq. (4).

When approximating the diffused term in the equation for dispersion of impurity concentration pulsations the following equation for the turbulent diffusion coefficients is obtained[6]:

$$K_{ij}=C_4\frac{b^2}{\varepsilon}\overline{\hat{U}_i\hat{U}_j}. \qquad (5)$$

Assuming the time scale to be small and neglecting the terms of 2-order infinitesimal in Eq. (4), Eq. (5) with the coefficient of proportionality $C_4 = R/C_3$ is to be obtained. According to some literature data, $C_4 = 0.13$.[6] This implies the estimation $R \approx 0.4$. Thus, closure of the semiempirical equation of turbulent diffusion with the help of Eq. (2) and the set of equations (4) gives virtually the same results at small values of the characteristic time scale of concentration (rate) pulsations. At the same time, the request for times of impurity propagation to be much greater than the considered time scales[4] is the condition of applicability of the semiempirical equation.

Consider other the simplest one-dimensional cases of diffusion. Using scales of time, length, concentration, and flow:

$$t_0=\frac{b^2}{\varepsilon};\quad x_0=\overline{U}t_0;\quad C_0;\quad q_0=\overline{U}C_0,$$

the set of equations

$$\frac{\partial\overline{C}}{\partial t}+\frac{\partial}{\partial x}(\overline{C}+q_x)=0;$$
$$\frac{\partial q_x}{\partial t}+\frac{\partial}{\partial x}(I^2\overline{C}+q_x)-2C_1I^2\frac{\partial^2 q_x}{\partial x^2}+C_3q_x=0 \qquad (6)$$

is obtained, where the previous designations are used for dimensionless variables and $I=\sigma_u/\overline{U}$ is the turbulence intensity (σ_u is the standard deviation of wind speed pulsations).

In case of a stationary point source of impurity, Eq. (6) has no terms with time derivatives. Locate the source in a point with the coordinate $x = 0$. Define the source term as $\overline{Q} = Q_0\delta(x)$, where $Q_0 = \text{const}$. Combining Eqs. (6), obtain

$$2C_1I^2\frac{\partial^2 q_x}{\partial x^2}-\left(1-I^2\right)\frac{\partial q_x}{\partial x}-C_3q_x=I^2Q_0\delta(x). \qquad (7)$$

The last term of Eq. (7) describes the impurity flow “decomposition.” Therefore, zero boundary conditions at infinity $\overline{C}(\pm\infty) = q_x(\pm\infty) = 0$ are admissible. A solution of Eq. (7) can be obtained employing continuity of the impurity flow at the point $x = 0$ (see Ref. 7):

$$q_x=-\frac{Q_0}{\left[(1-I^2)^2+8C_1C_3I^2\right]^{1/2}}\begin{cases}\exp(-\alpha_1 x), & x>0\\ \exp(+\alpha_2 x), & x<0\end{cases};$$
$$\alpha_{1,2}=\left[\left(\frac{1-I^2}{4C_1I^2}\right)^2+\frac{C_3}{2C_1I^2}\right]^{1/2}\mp\frac{1-I^2}{4C_1I^2}. \qquad (8)$$

It is also follows from Eq. (7) that $\overline{C}(x) = -q_x(x)$. The solution of semiempirical Eq. (1) closed with the gradient hypothesis (2) has the following form[7]:

$$\overline{C}(x)=Q_0\begin{cases}1, & x>0\\ \exp(C_3I^{-2}x), & x<0\end{cases}. \qquad (9)$$

Note, that there is no impurity decomposition in Eq. (1), therefore the impurity concentration is constant at $x > 0$, as is seen from Eq. (9).

Thus, solutions for a stationary point source, obtained with the use of the considered closure methods, have vital difference at $x > 0$. The solution of Eqs. (6) at $x < 0$ and $C_1C_3 < 1/2$ diminishes faster that the solution of the semiempirical equation closed with the gradient hypothesis (2).

In case of an instantaneous point source, the change of variables $z = x - t$ and $\tau = t$ is convenient. To obtain the solution, cast out the diffused term of 3-order infinitesimal relative to the above-mentioned time scales in Eq. (6). The resulting system is

$$\frac{\partial \overline{C}}{\partial \tau} + \frac{\partial q_x}{\partial z} = 0,$$
$$\frac{\partial q_x}{\partial \tau} + C_3 q_x + I^2 \frac{\partial \overline{C}}{\partial z} = 0. \quad (10)$$

The following system of initial and boundary conditions corresponds to the preset source:

$$\overline{C}(\pm\infty, \tau) = q_x(\pm\infty, \tau) = 0,$$
$$\overline{C}(z = 0) = \delta(z); \;\; q_x(z, 0) = 0.$$

The problem can be solved by the Laplace over-time transform method. For that, differentiate the second equation with respect to z and substitute the first equation of Eqs. (10) into the obtained expression. Then

$$\frac{\partial^2 \overline{C}}{\partial \tau^2} + C_3 \frac{\partial \overline{C}}{\partial \tau} - I^2 \frac{\partial^2 \overline{C}}{\partial z^2} = 0. \quad (11)$$

In view of the equation following from the first equation of the system and the initial conditions $\left.\frac{\partial \overline{C}}{\partial \tau}\right|_{\tau=0} = -\left.\frac{\partial q_x}{\partial z}\right|_{\tau=0} = 0$, we obtain

$$\overline{C}(z, \tau) = \exp\left(-\frac{C_3 \tau}{2}\right)\left\{\frac{1}{2}\delta(z + I\tau) + \frac{1}{2}\delta(z - I\tau) + \right.$$
$$\left. + \frac{C_3}{4I}\left[I_0(\frac{C_3}{2}M) + \frac{\tau}{M} I_1(\frac{C_3}{M})\right]\right\}; \;\; M = \left(\tau^2 - \frac{z^2}{I^2}\right)^{1/2};$$
$$q_x(z, \tau) = \exp\left(-\frac{C_3 \tau}{2}\right)\left[\frac{1}{2}\delta(z + I\tau) - \frac{1}{2}\delta(z - I\tau) + \right.$$
$$\left. + \frac{C_3}{4I}\frac{z}{M} I_1\left(\frac{C_3}{2}M\right)\right]; \;\; I^2\tau^2 - z^2 > 0, \quad (12)$$

where I_0 and I_1 are the Bessel functions of an imaginary argument.

The solutions obtained are solutions of the telegraph equation, found by Monin in Ref. 1; in contrast to the semiempirical equation, closed with Eq. (2), it describes the impurity propagation with a finite speed. That is, an impurity cloud produced by a source has clearly pronounced boundaries, which move in the transformed coordinate system with the speed $\pm I$; here "+" corresponds to the right boundary of the cloud and "–" to the left one. The redirecting frequency of impurity particles $a = C_3/2$ (it has been introduced by Monin in deriving the telegraph equation) and the average absolute speed of the particles $W = I$ (see Ref. 1). The solution of Eq. (1) closed with Eq. (2) is well known and in this case has the following form[1]:

$$\overline{C}(z, \tau) = \left(\frac{C_3}{4\pi I^2 \tau}\right)^{-1/2} \exp\left(-\frac{C_3 z^2}{4 I^2 \tau}\right). \quad (13)$$

According to Eq. (2), the impurity flow

$$q_x(z, \tau) = \frac{z}{2\tau}\overline{C}(z, \tau).$$

Solutions (12) and (13) for different values of a and W is compared in details in Ref. 1.

An analysis of a formal solution of the one-dimensional impurity flow equation is of interest. For that, consider the set of equations (6) with the initial and boundary conditions set for Eqs. (10). Excluding the advective terms via the change of variables $z = x - t$ and $\tau = t$ and performing the change $q_x = q\exp(-C_3\tau)$, we obtain the equation

$$\frac{\partial q}{\partial \tau} - 2C_1 I^2 \frac{\partial^2 q}{\partial z^2} + I^2 \frac{\partial^2 \overline{C}(z, \tau)}{\partial z}\exp(C_3 \tau) = 0, \quad (14)$$

which can be solved using the Green's function[8]:

$$q(z, \tau) =$$
$$= -I^2 \int_0^{\tau}\int_{-\infty}^{+\infty} G(z - \xi; \tau - \tau_0)\exp\left[C_3(\tau - \tau_0)\right]\frac{\partial \overline{C}(\xi, \tau_0)}{\partial \xi} d\xi\, d\tau_0;$$
$$G(z - \xi; \tau - \tau_0) =$$
$$= \left[8\pi C_1 I(\tau - \tau_0)\right]^{-1/2} \exp\left[-\frac{(z - \xi)^2}{8C_1 I(\tau - \tau_0)}\right]. \quad (15)$$

As is follows from analysis of Eq. (15), turbulent flow of impurity at the point z at the time τ is determined by values of impurity concentration taken at all points of the axis at all previous time points. That is, when closing with the second order methods, impurity flow is not a locally defined variable contrary to Eq. (2). The nonlocal properties are to manifest at small propagation times or at large values of the time scale considered above.

The Green's function with an exponential multiplier in Eq. (15) is a pulse characteristic of some spatiotemporal filter, which provides transformation of the concentration expectancy of impurity to its turbulent flow. An expression in the similar form has been obtained by Voloshchuk[9] but using different approaches. Series of papers devoted to nonlocal properties of turbulence impurity flows have been published in Ref. 10. However, the level of development of nonlocal closure methods is insufficient yet for practical use.

Thus, consideration of the simplest solutions of the semiempirical turbulent diffusion equation (1) shows that second order closure methods provide more informative description of atmospheric impurities propagation from physical standpoint in comparison with traditional closure methods based on the gradient hypothesis (2).

When propagation times are much greater than characteristic time scales, the second order closure methods give virtually the same results as compared with solutions obtained with the gradient hypothesis (2).

Presence of a diffused term in turbulent flow equations results in the general case in nonlocal dependence of the flows on concentration. Such nonlocality is negligible under restrictions mentioned in the above paragraph. Mathematical expectancy transforms to values of turbulent flows as a result of spatiotemporal filtering. This is pointed out by the convolution integral in Eq. (15).

The solution of the semiempirical Eq. (1) closed using the gradient hypothesis (2) has such characteristic that within an arbitrary small time interval after acting of an impurity source, small but finite impurity concentrations are to be observed at an arbitrary large distance of the source. This contradicts the fact that speed of particles cannot be infinite. Therefore, the obtained solution with a finite speed of impurity cloud boundaries is of practical importance.

Hence, study of fundamental principals and use of second order closure methods are of principal importance today, especially in view of the assumption of nonlocal properties of turbulent exchange and development of approaches describing turbulent diffusion with finite propagation speed.

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