

## NOTATION

$\rho$ , gas density;  $P$ , pressure;  $\rho_0$ , gas density at pressure  $P_0$ .

## LITERATURE CITED

1. H. N. Temperley et al. (eds.), *Physics of Simple Liquids*, Elsevier (1968).
2. A. V. Chelovskii, A. A. Antanovich, M. A. Plotnikov, and R. A. Chernyavskaya, "Possibility of using the molecular dynamics method for determination of thermodynamic properties of gases at high pressures and temperatures," in: *Thermophysical Properties of Gases* [in Russian], Nauka, Moscow (1973), pp. 96-98.
3. D. S. Tsiklis, *Dense Gases* [in Russian], Khimiya, Moscow (1977).
4. S. S. Tsimmerman and V. M. Miniovich, "Simple equation of state for highly compressed gases," *Zh. Fiz. Khim.*, 51, No. 1, 208-209 (1977).
5. V. M. Cheng, "Table 5.7," in: D. S. Tsiklis, *Dense Gases* [in Russian], Khimiya (1977), pp. 112-113.
6. R. L. Miles, D. H. Liebenberg, J. C. Bronson, "Sound velocity and equation of state of  $N_2$  to 22 kbar," *J. Chem. Phys.*, 63, 1198-1204 (1975).
7. D. S. Tsiklis and E. V. Polyakov, "Measurement of gas compressibility by the displacement method. Nitrogen compressibility at pressures to 10,000 atm and temperatures to 400°K," *Dokl. Akad. Nauk SSSR*, 176, No. 2, 307-311 (1967).
8. S. L. Robertson and S. L. Babb, "Isotherms of nitrogen to 400°C and 10,000 bar," *J. Chem. Phys.*, 50, 4560-4564 (1969).
9. P. Malbrunot and B. Vodar, "Experimental PVT data and thermodynamic properties of nitrogen up to 1000°C and 5000 bar," *Physica*, 66, 351-363 (1973).
10. A. A. Antanovich and M. A. Plotnikov, "Study of thermodynamic properties of nitrogen at pressures to 8 kbar and temperatures to 1800°K," *Inzh.-Fiz. Zh.*, 33, No. 2, 280-286 (1977).

## APPLICATION OF STATISTICAL APPROACHES TO SOLVE IMPURITY

### PROPAGATION PROBLEMS

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The Cauchy problem for an equation of hyperbolic type describing impurity diffusion at a finite velocity is solved by the Monte Carlo method.

In connection with the appearance of high-speed electronic computers, interest in the Monte Carlo method has increased considerably at the present time. Its simplicity and universality permit extension of the circles of problems that can be solved by this method. In particular, this refers to problems allowing probabilistic treatment.

Let us examine a problem associated with impurity propagation in an unbounded space.

As is known, the description of passive impurity propagation processes in a turbulent medium by a semiempirical turbulent diffusion equation has the disadvantage that the velocity of impurity propagation is infinite. Hence, it can be detected at any instant at any distance from the source. This results in substantial errors when determining the impurity concentration near a cloud boundary.

Certain authors ([1] and the bibliography therein) proposed extensions of the diffusion equations by giving them a hyperbolic character (in this case the impurity propagation velocity is finite). In this connection, the stochastic models based on the random walk method merit special attention.

Let us consider the simplest one-dimensional model of continuous motion of impurity par-

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ticles in a turbulent flow. Let us assume that the instantaneous velocity of particles moving randomly at the constant velocity  $v$  exists almost everywhere and is bounded, and the ordinate of each particle and the direction of its motion jointly form a Markov process.

During each time interval  $dt$  a probability  $adt$  exists for the change in particle motion direction because of its collisions with other particles.

The distribution of the number of collisions  $N(t)$  which a particle experienced to the time  $t$  is a Poisson distribution [2]

$$P\{N(t) = k\} = \frac{(at)^k}{k!} \exp(-at).$$

Taking into account that the particle velocity changes sign with each collision, the velocity at the time  $t$  equals  $v(t) = v(-1)^{N(t)}$  and its position is

$$x(t) = \int_0^t v(\tau) d\tau = vt^*,$$

where

$$t^* = \int_0^t (-1)^{N(\tau)} d\tau \quad (1)$$

( $t^*$  is the so-called "randomized time").

Under the assumptions mentioned, the particle concentration  $S(x, t)$  satisfies the known telegraph equation [1]

$$\frac{1}{v^2} \frac{\partial^2 S}{\partial t^2} + \frac{2a}{v^2} \frac{\partial S}{\partial t} = \frac{\partial^2 S}{\partial x^2}, \quad (2)$$

which, in the limit as  $a \rightarrow \infty$ ,  $v \rightarrow \infty$ ,  $v^2/2a \rightarrow D$ , goes over into the ordinary parabolic turbulent diffusion equation.

Let us consider the Cauchy problem for (2). The initial conditions are

$$S(x, 0) = \varphi(x), \quad \left. \frac{\partial S}{\partial t} \right|_{t=0} = 0. \quad (3)$$

It can be shown [2] that the solution of the problem (2), (3) is expressed by the formula

$$S(x, t) = \frac{1}{2} [\langle \varphi(x + vt^*) \rangle + \langle \varphi(x - vt^*) \rangle], \quad (4)$$

where  $t^*$  is defined by (1), and  $\langle \dots \rangle$  is the mathematical expectation. In the particular case  $a = 0$ , when the probability of a change in particle motion direction is zero, the solution (4) goes over into the known D'Alembert solution of the Cauchy problem for string vibrations [3].

It can be shown that  $t^* \leq t$ ; hence, the particle concentration  $S(x, t)$  can only be propagated the distance  $x = vt^* \leq vt$  in a time  $t$ .

We therefore obtain for the realization with number  $i$

$$S_i(x, t) = \frac{1}{2} [\varphi(x + vt_i^*) + \varphi(x - vt_i^*)].$$

The arithmetic mean

$$\bar{S}(x, t) = \frac{1}{K} \sum_{i=1}^K S_i(x, t) \quad (5)$$

can be used as an estimate for the quantity  $S(x, t)$ .

The modeling of particle motion for arbitrary  $x, t$  is performed multiply to obtain a statistically stable value of the desired function  $\bar{S}(x, t)$ .

Selection of the quantity of realization  $K$  depends on what requirements are imposed on  $S(x, t)$ . The estimate  $\bar{S}(x, t)$  obtained for the function  $S(x, t)$  differs from  $S(x, t)$  because of random reasons in the general case, it is consequently expedient to examine the question of the accuracy and confidence of the obtained values  $\bar{S}(x, t)$  in greater detail.

The accuracy of the estimate  $\bar{S}(x, t)$  can be characterized by the quantity  $\epsilon$  such that

$$|S(x, t) - \bar{S}(x, t)| < \epsilon, \quad (6)$$

and its confidence, by the probability  $\beta$  that inequality (6) would be satisfied [4], i.e.,

$$P(|S(x, t) - \bar{S}(x, t)| < \epsilon) = \beta.$$

Let us determine the quantity of realizations  $K$  needed to obtain the estimate  $\bar{S}(x, t)$  with accuracy  $\epsilon$  and confidence  $\beta$ .

Let the random variable  $\bar{S}(x, t)$  have the mathematical expectation  $S(x, t)$  and the variance  $\sigma^2$ . Because of the central limit theory of probability theory, for sufficiently large values of  $K$  the quantity  $\bar{S}(x, t)$  has an almost normal distribution with mathematical expectation  $S(x, t)$  and variance  $\sigma^2/K$ . Hence, for each value of  $\beta$  a quantile magnitude  $t_\beta$  can be selected from the normal distribution table such that  $\epsilon = t_\beta \sigma / \sqrt{K}$ , from which follows

$$K = t_\beta^2 \sigma^2 / \epsilon^2. \quad (7)$$

Taking into account that the value of  $\sigma^2$  is ordinarily unknown, the quantity mentioned is taken equal to the variance  $\sigma_{K^*}^2$  determined over  $K^*$  realizations in modeling practice, where  $K^* = 100-200$ . Then  $K$  is determined by means of (7) under the condition  $\sigma^2 = \sigma_{K^*}^2$ .

Therefore, to find the numerical result of solving problem (2), (3) to the required accuracy  $\epsilon$  and confidence  $\beta$ , it is necessary to execute  $K$  realizations of the Poisson process, to evaluate  $t^*$  by means of (1), and to find the mean value of the solution of the appropriate wave equation.

For a practical realization of the algorithm considered above for the evaluation of the integral (1), it is more convenient to use the known property of the Poisson process [5] that the time interval between two successive events (in our case two successive collisions, when the direction of particle motion changes) is a random variable that can be represented according to [6], in the form

$$T = -\frac{\ln \alpha}{a}, \quad (8)$$

where  $\alpha$  is a random variable distributed uniformly in the interval  $(0, 1)$ . The evaluation of the integral (1) hence reduces to realization of the sampling of the random variable  $\alpha$ , which is easily accomplished on an electronic computer according to a standard program to obtain "pseudorandom numbers."

Using (8) for each  $r$ -th realization of the random variable  $\alpha_r$ , we find the time interval  $T_r$  between two successive collisions during which the particle did not change the direction of its motion.

The quantity of realizations  $R$  of the sampling process for the random variable  $\alpha$  depends on the time  $t$  and is selected from the condition

$$\min_R \sum_{r=1}^R T_r \geq t.$$

Let us represent this mentioned sum in the form

$$\sum_{r=1}^R T_r = T^+ + T^-,$$

where

$$T^+ = \sum_{r=1}^{R'} T_{2r-1}; \quad T^- = \sum_{r=1}^{R'} T_{2r}. \quad (9)$$

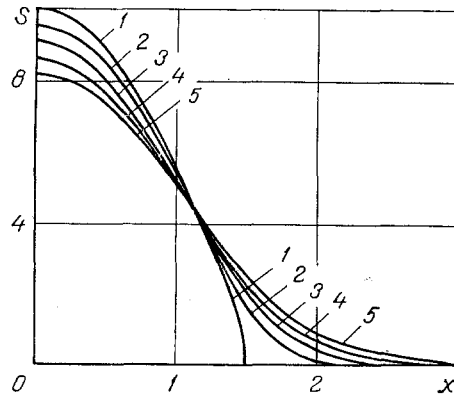


Fig. 1. Impurity concentration profiles  $S(x, t)$  at different times: 1)  $t = 0$ ; 2) 1; 3) 2; 4) 3; 5) 4.

Taking the initial direction of particle motion as positive, and taking into account that for each collision the motion direction will be reversed, we see from (9) that the particle would move in the positive direction during the time  $T^+$ , and in the negative direction during  $T^-$ . The "randomized time"  $t^* = T^+ - T^-$  is determined from known values of  $T^+$  and  $T^-$ .

By using the statistical approach examined above, the problem about impurity propagation in an unbounded two- (or three)-dimensional space can also be solved.

Let the impurity propagation be described by the equation

$$\frac{1}{v^2} \frac{\partial^2 S}{\partial t^2} + \frac{2a}{v^2} \frac{\partial S}{\partial t} = \Delta S, \quad (10)$$

where  $\Delta$  is the two- (or three)-dimensional Laplace operator. The initial conditions are

$$S(M, 0) = \varphi(M), \quad \left. \frac{\partial S}{\partial t} \right|_{t=0} = 0, \quad (11)$$

where  $M$  is a point of two- (or three)-dimensional space.

The solution of the problem (10), (11) is expressed in terms of known solutions (e.g., the integral Poisson (or Kirchhoff) formula [3]) of the appropriate problem for the wave equation (equation (10) with the term  $\frac{2a}{v^2} \frac{\partial S}{\partial t}$ ) omitted: in which the time  $t$  should be replaced by the "randomized time"  $t^*$  according to (1), and the mean value should be found [2].

The considered statistical approach to solve the problem of impurity propagation in an unbounded space by using the Poisson process and a comparatively simple procedure permits a solution to be obtained for the problem in terms of known solutions of simpler problems by avoiding the application of complex and tedious analytical or numerical methods here.

As an illustration of the method described above, profiles of the concentration  $S(x, t)$  are shown in Fig. 1 at fixed times  $t$ , as obtained as a result of solving problem (2), (3) for  $v = 1$ ,  $\alpha = 10$ ,  $\epsilon = 0.01$ ,  $\beta = 0.95$ ,  $K^* = 200$ :

$$\varphi(x) = \begin{cases} 10 \cos x & \text{for } |x| \leq \pi/2, \\ 0 & \text{for } |x| > \pi/2. \end{cases}$$

For given values of  $\epsilon$ ,  $\beta$ ,  $K^*$ , there were 2800 tests required (here  $t^*$  was estimated by means of the same realizations for any times not exceeding  $t$ ).

To estimate the quality of the computation, the concentration profiles obtained were compared with concentration profiles computed to the same accuracy ( $\epsilon = 0.01$ ) by means of the exact solution of the problem under consideration which has the form

$$S(x, t) = \frac{1}{2} \exp(-at) \left\{ \varphi(x - vt) + \varphi(x + vt) + \right. \\ \left. + a \int_{x-vt}^{x+vt} \varphi(\xi) \left[ \frac{1}{v} I_0 \left( \frac{a}{v} \sqrt{v^2 t^2 - (\xi - x)^2} \right) + \frac{t I_1 \left( \frac{a}{v} \sqrt{v^2 t^2 - (\xi - x)^2} \right)}{\sqrt{v^2 t^2 - (\xi - x)^2}} \right] d\xi \right\},$$

where  $I_0$ ,  $I_1$  are Bessel functions of imaginary argument of the zeroth and first order, respectively. All the appropriate concentration profiles are here in agreement to 1.5% accuracy, which indicates the efficiency of the computation method examined above.

#### NOTATION

$t$ , time;  $x$ , coordinate;  $P$ , probability;  $\alpha$ , characteristic frequency of turbulent pulsations;  $D$ , coefficient of turbulent diffusion;  $R'$ , integer part of the number  $R/2$ ; and  $R'' = R - R'$ .

#### LITERATURE CITED

1. A. S. Monin, "General survey of atmospheric diffusion," in: Atmospheric Diffusion and Air Pollution [in Russian], IL, Moscow (1962), pp. 44-57.
2. M. Kats, Several Probabilistic Problems of Physics and Mathematics [in Russian], Nauka, Moscow (1967).
3. A. N. Tikhonov and A. A. Samarskii, Equations of Mathematical Physics [in Russian], Nauka, Moscow (1966).
4. N. P. Buslenko, Modeling of Complex Systems [in Russian], Nauka, Moscow (1978).
5. Yu. A. Rozanov, Random Processes [in Russian], Nauka, Moscow (1971).
6. S. M. Ermakov and G. A. Mikhailov, Statistical Modeling Course [in Russian], Nauka, Moscow (1976).

#### SOLUTION OF HEAT-CONDUCTION PROBLEMS IN HETEROGENEOUS MEDIA BY THE INTEGRAL RELATIONS METHOD

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The integral relations method is developed to solve heat-conduction problems in a two-component complex medium and nonstationary filtration for the case of bounded and unbounded domains.

The integral relations method is used sufficiently extensively to solve heat-conduction problems because of the simplicity of the method itself and of the approximate solutions obtained with its use. A detailed survey and application of this method to solve different linear and nonlinear heat-transfer problems in homogeneous bodies can be found in [1]; this method is also applied in other branches of the mechanics of continuous media, e.g., in the theory of nonstationary filtration [2].

The method of integral relations has not been used to solve heat-conduction problems in heterogeneous continuous media; however, its application to filtration problems in binary media has been attempted (the equations of heat propagation in heterogeneous media [3] are analogous to the equations of nonstationary filtration of a homogeneous fluid in porous-cracked media [4, 5]). A completely degenerate system of heat-conduction equations in a two-component continuous medium ( $\varepsilon_1 = 0$ ,  $\varepsilon_2 = 0$ ), reduced to one equation, was taken as the basis in [6]. In such an approach it is required to take account of the singularity in the formulation of the initial and boundary conditions [7, 8], which is inconvenient, and also the domain of application of the method is shrunken (the condition  $\varepsilon_1 \approx 0$  is not always satisfied). Moreover, the dimension of the perturbed zone turns out to be different from zero at the ini-