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DISCRETE FORMULATION OF HEAT CONDUCTION AND DIFFUSION EQUATIONS

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Abstract—Temperature or concentration at a fixed point may be predicted for a subsequent moment $(t+\tau)$ by similar values at the adjacent points at a given time moment t and previous moments $(t-j\cdot\tau)$.
This predicted quantity is found as a mean one for its actual and previous values at all space points. Space–time countable set averaging is made by an averaging matrix. The normalization condition of averaging matrix coefficients results in parabolic or hyperbolic transfer equations involving relaxation terms. In the case of a polynomial averaging matrix the transfer equation does not contain lower powers of the differential Laplace operator.

NOMENCLATURE

- T, temperature or concentration;
- t, time;
- x, abscissa;
- τ, free path time, time quantum;
- h, free path, distance quantum;
- j, k, p, q, m, natural numbers;
- Γ_{kj}, coefficients of averaging matrix;
- C_{2m}^{q}, number of $2m$ combinations q;
- s, 0 or 1;
- τ_q, relaxation time;
- Q, energy or substance flow;
- c, heat capacity;
- ∇, Hamilton operator;
- ∇^2, Laplace operator;
- a_{2m+s}^{2p+s}, transfer parameters.

IN WORKS [1–9] the diffusion equations for energy and substance were proposed which contain relaxation addends. The experiments on reciprocal diffusion in alloys [10] confirm the presence of large relaxation addends in the diffusion equation which at the beginning of a process exceed those for the rate of a concentration growth.

The equation for heat conduction or diffusion may be obtained assuming temperature or concentration T at a moment $(t+\tau)$ at a point x to be a mean quantity

$$T(x,t+\tau) = \sum_{j=0}^{\infty}\sum_{k=-\infty}^{+\infty}\Gamma_{kj}T(x+kh;t-j\tau) \qquad (1)$$

of temperatures or concentration at the adjacent points

$$x_k = x+kh;\quad k=0;\quad \pm1;\quad \pm2; \qquad (2)$$

at given t and previous time moments

$$t_j = t-j\tau;\quad j=0;\quad 1;\quad 2. \qquad (3)$$

Distance quantum h between two adjacent points is some free path [13] which is covered for free path time τ, being a time quantum of a transfer process.

Coefficients Γ_{kj} of the averaging matrix Γ satisfy the normalization condition

$$\sum_{j=0}^{\infty}\sum_{k=-\infty}^{+\infty}\Gamma_{kj} = 1 \qquad (4)$$

which shows that if T is unchangeable at all points during the whole process

$$T(x+kh;t-j\tau) = T_0 = \text{const}, \qquad (5)$$

then the predicted function of T at a point x in time τ does not change

$$T(x,t+\tau) = T_0. \qquad (6)$$

Relation (1) predicts the quantity T at x at moment $(t+\tau)$ following t as an arithmetic mean of quantities $T(x_k, t_j)$ which are observed at a given moment t and were observed during previous moments $(t-j\cdot\tau)$ at all points x_k of the straight line x.

There is no ground to consider that the effect of symmetrical points appears to be different, and, therefore, for the numbers of the averaging matrix the condition

$$\Gamma_{k;j} = \Gamma_{-k;j} \qquad (7)$$

is satisfied, that allows a temperature at the points equidistant from x to be singled out in relation (1)

$$T(x;t+\tau) = \sum_{j=0}^{\infty}\Gamma_{0j}T(x;t-j\tau) + \sum_{j=0}^{\infty}\sum_{k=1}^{\infty}\Gamma_{kj}[T(x+kh;t-j\tau) + T(x-kh;t-j\tau)]. \qquad (8)$$

It is natural to consider that the effect of far distant points is weaker than that of the adjacent ones, and with an increase in k, the matrix numbers decrease monotonically

$$|\Gamma_{k,j}| \geqslant |\Gamma_{k+1;j}|. \qquad (9)$$

It is obvious that a contribution of the previous temperatures to temperature formation $T(x,t+\tau)$ is the less, the earlier these temperatures were observed and thus:

$$|\Gamma_{k,j}| \geqslant |\Gamma_{k,j+1}| \qquad (10)$$

that is quite analogous to the previous inequality. It may be expected that the points infinitely far along the abscissa and in time do not affect a temperature change at a point, and the asymptotic equalities

$$\lim_{k\to\infty}\Gamma_{kj} = \lim_{j\to\infty}\Gamma_{kj} = 0 \qquad (11)$$

are therefore valid. In particular, such an equality holds in the case of a finite averaging matrix. In [5] Γ consists only of two non-zero elements

$$\Gamma_{-1;0} = \Gamma_{1;0} = 0.5. \quad (12)$$

Due to a small length h and time τ of a free path each temperature in equation (8) may be expanded into a Taylor series with respect to kh and $(-j\tau)$:

$$T(x+kh; t-j\tau) = T+\frac{1}{1!}\left[\frac{\partial T}{\partial x}kh-\frac{\partial T}{\partial t}j\tau\right] +\frac{1}{2!}\left[\frac{\partial^2 T}{\partial x^2}k^2h^2-2\frac{\partial^2 T}{\partial x\partial t}khj\tau+\frac{\partial^2 T}{\partial t^2}j^2\tau^2\right] +\frac{1}{n!}\left[\frac{\partial^n T}{\partial x^2}k^nh^n-C_n^1\frac{\partial^n T}{\partial x^{n-1}\partial t}(kh)^{n-1}j\tau + C_n^2\frac{\partial^n T}{\partial x^{n-2}\partial t^2}(kh)^{n-2}(j\tau)^2+\ldots+(-1)^q \times C_n^q\frac{\partial^n T}{\partial x^{n-q}\partial t^q}(kh)^{n-q}(j\tau)^q+\ldots+(-1)^n\frac{\partial^n T}{\partial t^n}(j\tau)^n\right] \quad (13)$$

and the same expansion may be performed for a predicted temperature

$$T(x, t+\tau) = T+\frac{\partial T}{\partial t}\frac{\tau}{1!}+\frac{\partial^2 T}{\partial t^2}\frac{\tau^2}{2!}+\ldots+\frac{\partial^q T}{\partial t^q}\frac{\tau^q}{q!}+\ldots. \quad (14)$$

Of course, all partial derivatives are taken at a point x at a moment t, i.e. at $k = j = 0$.

If all these expansions are substituted into relation (8), then in the R.H.S. all odd coordinate derivatives cancel out, and it may be written as:

$$T+\frac{\partial T}{\partial t}\frac{\tau}{1!}+\frac{\partial^2 T}{\partial t^2}\frac{\tau^2}{2!}+\ldots+\frac{\partial^q T}{\partial t^q}\frac{\tau^q}{q!}+\ldots = \sum_{j=0}^{\infty}\Gamma_{0j}\left[T-\frac{\partial T}{\partial t}\frac{\tau}{1!}j+\frac{\partial^2 T}{\partial t^2}\frac{\tau^2}{2!}j^2+\ldots +(-1)^q\frac{\partial^q T}{\partial t^q}\frac{\tau^q}{q!}j^q+\ldots\right]+2\sum_{j=0}^{\infty}\sum_{k=1}^{\infty}\Gamma_{kj} \times\left\{T-\frac{\partial T}{\partial t}\frac{\tau}{1!}j+\frac{1}{2!}\left[\frac{\partial^2 T}{\partial x^2}h^2x^2+\frac{\partial^2 T}{\partial t^2}\tau^2j^2\right] -\frac{1}{3!}\left[3\frac{\partial^3 T}{\partial x^2\partial t}h^2k^2\tau j+\frac{\partial^3 T}{\partial t^3}\tau^3j^3\right]+\ldots +\frac{1}{2m!}\left[\frac{\partial^{2m} T}{\partial x^{2m}}h^{2m}k^{2m}+C_{2m}^2\frac{\partial^{2m} T}{\partial x^{2m-2}\partial t^2} \times h^{2m-2}k^{2m-2}\tau^2j^2+\ldots+C_{2m}^{2p}\frac{\partial^{2m} T}{\partial x^{2m-2p}\partial t^{2p}} \times h^{2m-2p}k^{2m-2p}\tau^{2p}j^{2p}+\ldots+\frac{\partial^2 mT}{\partial t^{2m}}\tau^{2m}j^{2m}\right] -\frac{1}{(2m+1)!}\left[C_{2m}^1\cdot\frac{\partial^{2m+1} T}{\partial x^{2m}\partial t}h^{2m}k^{2m}\tau j+C_{2m}^3\frac{\partial^{2m+1} T}{\partial x^{2m-2}\partial t^3} \times h^{2m-2}k^{2m-2}\tau^3j^3+\ldots+C_{2m+1}^{2p+1}\frac{\partial^{2m+1} T}{\partial x^{2m-2p}\partial t^{2p+1}} \times h^{2m-2p}k^{2m-2p}\tau^{2p+1}j^{2p+1}+\ldots+\frac{\partial^{2m+1} T}{\partial t^{2m+1}} \times\tau^{2m+1}j^{2m+1}\right]+\ldots\right\}. \quad (15)$$

In this sum mixed time derivatives of an even order have a plus sign and those of an odd one, a minus sign. Matrix coefficients Γ_{kj} tend to zero rather quickly, and the averaging matrix Γ may be, on the whole, finite so that transposition of summation order is possible. Taking into account the main property of averaging matrix coefficients [4] or its equivalent

$$\sum_{j=0}^{\infty}\Gamma_{0j}+2\sum_{j=0}^{\infty}\sum_{k=1}^{\infty}\Gamma_{kj} = 1 \quad (16)$$

it directly follows from symmetry condition (7), and equation (15) does not contain an unknown function $T(x, t)$.

Determination of a relaxation time spectrum [6–8]

$$\tau_q^q = \frac{\tau^q}{q!}\left[1-(-1)^q\left(\sum_{j=0}^{\infty}\Gamma_{0j}j^q+2\sum_{j=0}^{\infty}\sum_{k=1}^{\infty}\Gamma_{kj}j^q\right)\right] \quad (17)$$

and a kinematic parameter of internal transfer of even $(0 \leqslant p \leqslant m-1)$

$$a_{2m}^{2p} = C_{2m}^{2p}\frac{h^{2m-2p}\tau^{2p}}{(2m)!}\sum_{j=0}^{\infty}\sum_{k=1}^{\infty}\Gamma_{kj}k^{2m-2p}j^{2p} \quad (18)$$

and odd orders

$$a_{2m+1}^{2p+1} = -2C_{2m+1}^{2p+1}\frac{h^{2m-2p}\tau^{2p+1}}{(2m+1)!} \times\sum_{j=0}^{\infty}\sum_{k=1}^{\infty}\Gamma_{kj}k^{2m-2p}j^{2p+1} \quad (19)$$

allows the heat conduction or diffusion equation to be given in a canonic form

$$\sum_{q=1}^{\infty}\tau_q^q\frac{\partial^q T}{\partial t^q} = \sum_{p=0}^{m-1}\sum_{m=1}^{\infty}\sum_{s=0}^{1}a_{2m}^{2p+s}\frac{\partial^{2m+s} T}{\partial x^{2m-2p}\partial t^{2p+s}}, \quad (20)$$

and when the field is multidimensional, the R.H.S. is a series expansion of the differential Laplace operator ∇^2

$$\sum_{q=1}^{\infty}\tau_q^q\frac{\partial^q T}{\partial t^q} = \sum_{s=0}^{1}\sum_{p=0}^{m-1}\sum_{m=1}^{\infty}a_{2m+s}^{2p+s}\frac{\partial^{2p+s}}{\partial t^{2p+s}}\nabla^{2m-2p}T. \quad (21)$$

In all previously published works [1–9] consideration was made of simultaneous averaging when the effect of the previous states is not taken into account, and according to formula (1) temperature is predicted only by its actual values

$$T(x, t+\tau) = \sum_{k=-\infty}^{+\infty}\Gamma_{k0}T(x+kh; t) \quad (22)$$

but not by the previous values of the function $T(x, t)$. Such erasing of inheritance is satisfied by the averaging matrix with zero values of the coefficients in all lines

$$\Gamma_{kj} = 0; \quad j \geqslant 1 \quad (23)$$

except the first one

$$\Gamma_{k0} \neq 0 \quad (24)$$

which is satisfied by the normalization condition

$$\sum_{k=-\infty}^{+\infty}\Gamma_{k0} = 1 \quad (25)$$

or owing to symmetry condition (7)

$$\Gamma_{00}+2\sum_{k=1}^{\infty}\Gamma_{k0} = 1. \qquad (26)$$

For such averaging the relaxation time spectrum degenerates, and all quantities τ_q coincide with free path time except for a constant multiplier

$$\tau_q = \tau/\sqrt[q]{(q!)}. \qquad (27)$$

It is important that all τ_q do not depend on averaging matrix elements. All higher and odd kinematic parameters for internal transfer are equal to zero:

$$a_{2m+s}^{2p+s} = 0; \quad p > 0; \quad s \geqslant 0 \qquad (28)$$

and only pure geometric parameters

$$a_{2m}^{0} = \frac{2h^{2m}}{(2m)!}\sum_{k=1}^{\infty}\Gamma_{k0}\cdot k^{2m}; \quad 1 \leqslant m < \infty \qquad (29)$$

differ from zero which are proportional to even powers of the free path h and depend mainly on the coefficients Γ_{k0} of the first line of the averaging matrix Γ.

Relaxation times (27) with an increase of their order and power decrease monotonically

$$\tau_q > \tau_{q+1}; \quad \lim_{q\to\infty}\tau_q = 0 \qquad (30)$$

and thus heat conduction equation (20) which corresponds to simultaneous averaging or, i.e. to complete erasing of inheritance

$$\sum_{q=1}^{\infty}\tau_q^q\frac{\partial^q T}{\partial t^q} = \sum_{m=1}^{\infty}a_{2m}^{0}\frac{\partial^{2m}T}{\partial x^{2m}} \qquad (31)$$

has small relaxation times at higher time temperature derivatives. These equations have been considered in [1–9].

Attention should be paid to the fact that there may exist different modes of simultaneous averaging even on the finite section $2ph$ wide

$$x_k = x+kh; \quad -p \leqslant k \leqslant p. \qquad (32)$$

For example, for the averaging coefficients

$$\Gamma_{k0} = 1/(2p+1) \quad |k| < p; \qquad \Gamma_{k0} = 0; \quad |k| > p; \quad \Gamma_{kj} = 0 \quad j \geqslant 1, \qquad (33)$$

in terms of which linear smoothing [11–12] or averaging by means of the arithmetic mean is expressed

$$T(x;t+\tau) = \frac{1}{2p+1}\sum_{k=-p}^{\infty}T(x+kh;t) \qquad (34)$$

at a moment t, the kinematic, more precisely geometric transfer parameters

$$a_{2m}^{0} = \frac{2h^{2m}}{(2p+1)(2m)!}\sum_{k=1}^{p}k^{2m}; \quad 1 \leqslant m < \infty \qquad (35)$$

become infinitely small with a decrease of their order

$$\lim_{m\to\infty}a_{2m}^{0} = 0 \qquad (36)$$

and may be described by a monotonic decrease. Thus, we have:

$$\sqrt[m]{(a_{2m}^{0})} > \sqrt[m+1]{(a_{2m+2}^{0})}. \qquad (37)$$

Therefore, heat conduction equation (31) in the R.H.S. has also small parameters at higher coordinate temperature derivatives.

However, the situation becomes essentially complicated if simultaneous averaging is made not only by linear relation (34) but by the parabolic law

$$\Gamma_{k0} = \begin{vmatrix} 1 & S_2 & ..S_{2n} \\ k^2 & S_4 & ..S_{2n+2} \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ k^{2n} & S_{2n+2} & ..S_{4n} \end{vmatrix} : \begin{vmatrix} S_0 & S_2 & ..S_{2n} \\ S_2 & S_4 & ..S_{2n+2} \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ S_{2n} & S_{2n+2} & ..S_{4n} \end{vmatrix}. \qquad (38)$$

Here the sums of even powers are designated [11–12]

$$S_{2q} = \sum_{k=-p}^{p}k^{2q} \qquad (39)$$

and all conditions of expression (33) are surely satisfied. Parabolic-type averaging (38)

$$T(x,t+\tau) = \sum_{k=-p}^{p}\Gamma_{k0}\,T(x+kh,t) \qquad (40)$$

corresponds to smoothing by means of an algebraic second-degree polynomial constructed by the method of least squares for the points [see equation (32)], whose number is greater than a degree of an approximating polynomial

$$p > 0. \qquad (41)$$

For such a simultaneous averaging matrix the first n of geometrical transfer parameters (35) are equal to zero

$$a_{2m}^{0} = 0; \quad m = 1,2,\dots,n \qquad (42)$$

and the heat conduction equation

$$\sum_{q=1}^{\infty}\tau_q^q\frac{\partial^q T}{\partial t^q} = \sum_{m=n+1}^{\infty}a_{2m}^{0}\frac{\partial^{2m}T}{\partial x^{2m}} \qquad (43)$$

does not contain the first $2n$ of coordinate temperature derivatives.

From the energy conservation equation

$$\frac{\partial T}{\partial \tau} = -\frac{1}{c}\operatorname{div}\bar{Q}, \qquad (44)$$

where c is the material heat capacity, it follows that between energy flow Q and temperature gradient there exists the relationship

$$\sum_{q=1}^{\infty}\tau_q^q\frac{\partial^{q-1}\bar{Q}}{\partial t^{q-1}} = -c\,\mathrm{grad}\sum_{p=0}^{m-1}\sum_{m=1}^{\infty}\frac{\partial^{2p}}{\partial t^{2p}}\nabla^{2m-2p-2} \times\left[a_{2m}^{2p}T+a_{2m+1}^{2p+1}\frac{\partial T}{\partial t}\right], \qquad (45)$$

being the Fourier law generalization. If the powers of free path time being higher in the first derivative and those of free path being higher in the second derivative are neglected, i.e. assuming

$$\tau_q = 0; \quad q > 1 \qquad a_{2m+s}^{2p+s} = 0; \quad (m \geqslant 2; s = 0)(m \geqslant 1; s = 1) \qquad (46)$$

then from relation (45) for temperature gradients and its time derivative, the Fourier law follows

$$\tau_1' \bar{Q} = -ca_2^0 \nabla T \quad (47)$$

since thermal conductivity of a substance is

$$a = a_2^0/\tau_1 = \lambda/c. \quad (48)$$

If τ and h being greater than two are neglected, i.e. assuming

$$\tau_q = 0; \quad q > 2, \quad (49)$$

then basic relation (45) results in the equation for Peierls–Cattaneo's heat flux

$$\tau_1 \bar{Q} + \tau_2^2 \frac{\partial \bar{Q}}{\partial t} = -ca_2^0 \nabla T. \quad (50)$$

If all time derivatives are taken into account, i.e.

$$\tau_q \neq 0, \quad (51)$$

then equation (45) reduces to a polyrelaxation expression for a temperature gradient

$$\sum_{q=1}^{\infty} \tau_q^q \frac{\partial^{q-1} \bar{Q}}{\partial t^{q-1}} = -ca_2^0 \nabla T \quad (52)$$

which was proposed by Temkin in 1967 [8].

Of course, a relaxation time spectrum depends strongly on a temperature gradient, and at the same time all relaxation times, besides the first one, tend to zero

$$\tau_q = 0; \quad q \geqslant 2 \quad (53)$$

when

$$\nabla T = 0. \quad (54)$$

Existence of non-zero relaxation times when performing the last equality means that heat flux may take place with no temperature gradient, that contradicts the second law of thermodynamics.

Determination of relaxation times [17] and kinematic internal heat-transfer parameters [18–19] is an interesting field of the study on the inverse internal heat conduction problem, whose solution was proposed [8].

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REFERENCES

1. J. Tavernier, Les bases physiques de la transmission de chaleur par conduction dans les solids, *Revue Gén. Thermique* **1**, 19–25 (1962).
2. C. Cattaneo, Sulla conduizione del calore, Seminario matematico e fisico dell, Universita di Modena (1948).
3. J. Tavernier, Communication 1.05, Journees Internationales de Transmission de la Chaleur (1961).
4. A. A. Vlasov, *Statistical Distribution Functions*. Izd. Nauka, Moscow (1966).
5. Y. Taitel, On the parabolic, hyperbolic and discrete formulation of the heat conduction equation, *Int. J. Heat Mass Transfer* **15**(2), 369–371 (1972).
6. A. G. Temkin, *Inverse Heat Conduction Methods*. Izd. Energiya, Moscow (1973).
7. A. G. Temkin, Transfer processes in colloidal capillary-porous bodies with chemical reactions in a force field, in *Heat and Mass Transfer*, Vol. 11, pp. 739–762. Izd. ITMO AN BSSR (1969).
8. A. G. Temkin, Thermal conductivity of p-reverse multilayer medium, in *Mathematical and Physical Problems on Heat and Mass Transfer*, pp. 99–112. Izd. ITMO AN BSSR. Minsk (1973).
9. A. M. Toboltsev, To the theory of the generalized diffusion equations, *Vest. Mosk. Gos. Univ. Ser. Fiz. i. Astronom.* **5**, 597–602 (1973).
10. I. B. Borovsky, K. P. Gurov, I. D. Marchukova and Yu. E. Ugaste, *Reciprocal Diffusion Processes in Alloys*. Izd. Nauka, Moscow (1973).
11. K. Lantsosh, *Practical Methods of Applied Analysis*. Izd. Fizmatgiz, Moscow (1961).
12. A. G. Temkin, *Smoothing and Differentiation of the Experimental Functions*. Izd. Politekhn. In-ta, Riga (1973).
13. B. M. Yavorsky and A. A. Detlaf, *Handbook on Physics*. Izd. Nauka, Moscow (1965).

DISCRETISATION DES EQUATIONS DE LA CONDUCTION THERMIQUE ET DE LA DIFFUSION

Résumé—La température ou la concentration en un point fixé et à un instant futur $(t+\tau)$ peuvent être prévues à partir des valeurs correspondantes aux points voisins à l'instant t donné et aux instants antérieurs $(t-j\cdot\tau)$.

La quantité calculée est obtenue comme moyenne des valeurs présentes et antérieures en tout point de l'espace. La moyenne spatio-temporelle sur une base finie est réalisée par une opération matricielle. La condition de normalisation des coefficients de la matrice de moyenne conduit à des équations de transfert paraboliques ou hyperboliques présentant des termes de relaxation. Dans le cas d'une matrice polynomiale, l'équation de transfert ne contient pas les puissances les plus faibles de l'opérateur différentiel de Laplace.

EINZELFORMULIERUNG DER WÄRMELEITUNGS- UND DIFFUSIONSGLEICHUNGEN

Zusammenfassung—Die zeitabhängige Temperatur oder Konzentration an einer bestimmten Stelle läßt sich für Zeiten $(t+\tau)$ aus den Werten der umliegenden Punkte zu einer gegebenen Zeit t und einer früheren Zeit $(t-j.\tau)$ berechnen. Diese berechnete Größe ergibt sich als Mittelwert aus den eigentlichen und früheren Werten an allen Punkten des Raumes. Eine Raum-Zeitmittelung wurde mit Hilfe einer mittelnden Matrix durchgeführt. Die Normalisierungsbedingung für die Koeffizienten dieser Matrix liefert parabolische oder hyperbolische Übergangsgleichungen mit Relaxationsgliedern. Für eine polynome mittelnde Matrix enthält die Übergangsgleichung keine niedrigen Potenzen des differentiellen Laplace-Operators.

ДИСКРЕТНАЯ ФОРМУЛИРОВКА УРАВНЕНИЙ ТЕПЛОПРОВОДНОСТИ И ДИФФУЗИИ

Аннотация — Температура или концентрация в фиксированной точке могут быть предсказаны для следующего момента $(t+\tau)$ по аналогичным величинам в соседних точках в данный момент t и в предшествующие моменты $(t-j\tau)$.

Эта предсказуемая величина находится как средняя для её актуальных и предыдущих значений во всех точках пространства. Осреднение по пространственно-временному счетному множеству реализуется при помощи матрицы осреднения. Условие нормирования для коэффициентов матрицы осреднения приводит к уравнениям переноса параболического или гиперболического типов, которые содержат релаксационные члены. При полиномиальном построении матрицы осреднения уравнение переноса не включает младшие степени дифференциального оператора Лапласа.