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NUMERICAL CALCULATION OF THREE DIMENSIONAL TRANSPORT OF HEAT BY CONDUCTION

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Abstract

The programme has been developed for investigation of the dynamical behaviour of calorimetric equipments and permits a numerical calculation of the equation of the heat conduction for arbitary initial and boundary conditions and an arbitary distribution of heat sources. In order to derive a set of discrete linear difference equations from the partial differential equation, which is necessary for the numerical calculation, the sample is considered as a network of points, which are connected to each other by conducting rods. Although a rectangular lattice has been chosen as a network, curved surfaces can be treated. It has been taken care, that the number of input data is as low as possible. The programme is written in STANDARD FORTRAN and takes 45 K and 0,2 sec for calculating the shape of temperature at 1100 points.

1. Introduction

A detailed understanding of the dynamical behaviour of calorimetric measuring equipments requires investigating transport of heat inside those systems, because this is the way by which the information about a thermal event in the sample propagates to that place, where it is measured. Thus a computer programme applying a well known method of numerical calculation (Dusinberre,1949, Schneider, 1957, Grigull, Sandner, 1979)

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has been developped in combination with other auxiliary programmes,which help to reduce the large number of input data or check the solution with respect to criteria of symmetry or refer to a graphical evaluation.

Most programmes are written in STANDARD FORTRAN, so they will be suitable for a great deal of computers.

2. Algorithm of numerical calculation of transport

Before explaining the algorithm we shall briefly derive the equation of heat conduction, because this will lead to an easier understanding of the structure of the programme and why auxiliary programmes are necessary.

2.1 Equation of heat conduction

We start by the balance equation refering to a certain region i of a medium

$$\oint_{A_i} \underline{j}\, d\,\underline{A} + \int_{V_i} \dot{q}\ (\underline{r},t)\ dV = \int_{V_i} c\ (\underline{r})\ \frac{\partial T\ (\underline{r},t)}{\partial t}\ dV \qquad (2,1)$$

where A_i, V_i denote the surface area and the volume of the region i, respectively, $\underline{j}$ the flow density of heat, $\dot{q}\ (\underline{r},t)$ the density of heat production describing the distribution of heat sources and $c\ (\underline{r})$ the(volume) specific heat capacity. Inserting the well-known phenomenological equation (1. Fourier's law)

$$\underline{j} = \underline{\underline{\lambda}} \cdot \nabla T \qquad (2,2)$$

yields with the help of the lemma of Gauss

$$\nabla\ (\lambda \nabla T) + \dot{q}\ (\underline{r},t) = c\ (\underline{r})\ \frac{\partial T\ (\underline{r},t)}{\partial t} \qquad (2,3)$$

This leads to the well known equation of heat conduction

$$\lambda \nabla^2 T(\underline{r},t) + \dot{q}(\underline{r},t) = c(\underline{r}) \frac{\partial T(\underline{r},t)}{\partial t} \qquad (2,4)$$

provided that the medium is homogeneous, otherwise the expression

$$\nabla \lambda(\underline{r}) \cdot \nabla T(\underline{r},t) + \lambda \nabla^2 T(\underline{r},t) + \dot{q}(\underline{r},t) = c(\underline{r}) \frac{\partial T(\underline{r},t)}{\partial t} \qquad (2,5)$$

is obtained.

2.2 Algorithm of numerical solution

A numerical method is not able to resolve (2,4), (2,5) directly - instead of the partial differential equation a set of corresponding discrete difference equation is resolved. Thus the continuous medium is supposed to be replaced by a network of points i (i = 1,...,M) having the capacity of the cell i, which are connected with the neighboured points by conducting rods i, k (i = 1,...,M, k neighboured to i) each having the coefficient of conductivity L_{ik}. The network chosen here is a rectangular lattice. The set of discrete difference equations is obtained immediately from the balance equation (2,1), if one replaces the partial derivative $\partial T/\partial t$ by ratio

$$\frac{\partial T(\underline{r},t)}{\partial t} \approx \frac{T_i^{N+1} - T_i^N}{\Delta t} \qquad (2,6)$$

where the subscript, denotes the i-th cell and the superscript N, N+1 refer to the actual time t and the following time $t + \Delta t$, respectively. Thus the set of difference equation

$$\sum_{\substack{k \text{ neighboured} \\ \text{to } i}} J_{ik}^N + \dot{Q}_i^N = C_i \cdot \frac{T_i^{N+1} - T_i^N}{\Delta t} \qquad (2,7)$$

is obtained. $\dot{Q}_i$, C_i denote the total production of heat

$$\dot{Q}_i^N = \int_{V_i} \dot{q}\ (\underline{r},t)\ \ dV \qquad (2,8$$

and the total capacity

$$C_i = \int_{V_i} c\ (\underline{r})\ \ dV \qquad (2,9$$

respectively. J_{ik}^N are the actual flows from k to i - they are described by the phenomenological expression

$$J_{ik}^N = L_{ik}\ (T_k^N - T_i^N), \qquad (i = 1,\ldots,M;\ k \text{ neighboured to } i) \qquad (2,1$$

where the symmetrical matrix $\underline{\underline{L}}$ denotes the coefficients of conductivity of the rods of the network. According to the symmetry already mentioned L_{ik} is represented by the conductivity coefficients L_i, L_k of the cells i,k

$$L_{ik} = \frac{\mathfrak{L}_i - \mathfrak{L}_k}{\mathfrak{L}_i + \mathfrak{L}_k} \qquad (2,11$$

Inserting into (2,7) yields the algorithm

$$\frac{\Delta t}{C_i} \sum_{k \text{ neighboured to } i} L_{ik}\ T_k^N + T_i^N\ (1 - \frac{\Delta t}{C_i} S_i) + \frac{\Delta t}{C_i}\ \dot{Q}_i = T_i^{N+1} \qquad (2,12$$

$(i = 1,\ldots,m;\ N = 0,\ldots)$

m denotes all points, the temperatures of which have to be calculated (consequently there are M-m points, the temperatures of which are given as boundary condition), and S_i is the sum

$$S_i = \sum_{k \text{ neighboured to } i} L_{ik} \qquad (i = 1,\ldots,m) \qquad (2,13$$

3. Programmes and Subroutines

The logical structure of the programme can be devided into three parts. The first one is concerned with reading the input data such as the material properties, the geometrical form of the surface and of the inhomogeneities, the initial and boundary conditions. In the second part all those quantities, which do not depend on time, are calculated. Finally the third part determines the numerical solution. According to the algorithm (2,12) it consists of a loop, which is interrupted after having reached a value of N sufficiently large. Fig. 1 is a flow chart of the logical structure.

3.1 Subroutines PROBE TBEGIN, QUELL, TBEK

The subroutinies TBEGIN . TBEK determine the initial and boundary conditions. QUELL the positions and strengths if the heat sources. PROBE is a special subroutine concerning the geometrical form of the sample. It permits reducing the number of input data in order to economize the user's work and to avoid errors. The data (positions and material parameters) of the surface cells are read at first, then the properties of all cells in the bulk are determined and finally inner inhomogeneities are read. Thus only the data of the surface have to be given, which are less than those of the whole sample. This subroutine operates in combination with additional auxiliary programmes, which permit an additional reduction.

3.2 Subroutines DELTIM, MATRIX, OUTPUT, NACHBR, REKURS

DELTIM calculates the limit of stability of the numerical solution (Dusinberre 1949, Schneider 1957). This is the maximum

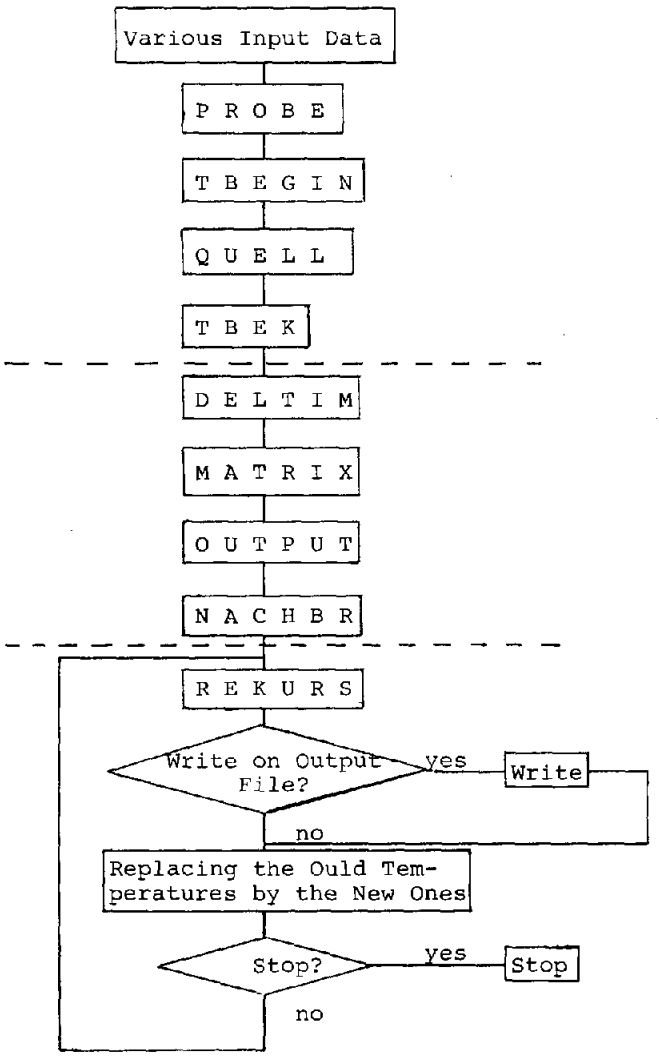

Fig. 1: Flow chart of the main programme. The names in capital letters refer to the subroutines

value of Δt, where the numerical solution still converges. It is given by

$$\Delta t_{max} = \max \left\{ \frac{C_i}{S_i} \right\} \qquad (3,1)$$

MATRIX determines the diagonal and the off-diagonal elements of (2,12), OUTPUT is necessary for controlling the output, NACHBR stores the indices of the neighbours of each cell. These four subroutines are not really required for a solution but they help reducing the time of calculation. REKURS calculates the new temperatures from the old ones by (2,12).

3.3. Auxilary programmes

As already mentioned the network representing the continuous sample has been chosen as a rectangular lattice. This lattice, however, is not very suitable, if there are surfaces which are not planes but which are curved. The capacity is given by the integral (2,9) the conductivity coefficient $\mathcal{L}_i^{x,y,z}$ by a similar integral, which is derived by the following consideration: Suppose that the curved surface is given by an equation

$$x_s = x_s\,(y,z) \qquad (3,2)$$

In fig. 2 a general case of a surface cell is shown. In order to get the coefficient of conductivity $\mathcal{L}_i^{x}$, we now assume a steady temperature T_s being at the surface (3,2) and T_1 being at the left wall $i \cdot \Delta x$. The phenomenological equation is according to (2,2)

$$j_x = \lambda \cdot \frac{\partial T}{\partial x} \qquad (3,3)$$

Integration yields with the help of stationarity

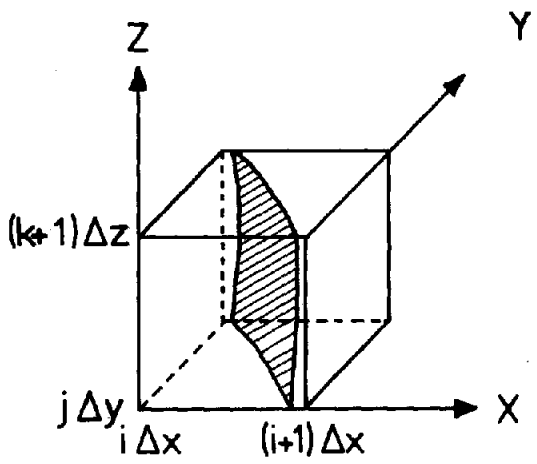

Fig. 2: Surface cell, which is intersected by a curved surface $x_s(y,z,)$.

$$\int_{i \cdot \Delta x}^{x_s(y,z)} j_x dx = j_x \cdot (x_s(y,z) - i \cdot \Delta x) = \lambda \cdot \frac{(T_s - T_1)}{\Delta T} \qquad (3,4)$$

$$j_x = \lambda \cdot \Delta T \cdot \frac{1}{x_s(y,z) - i \cdot \Delta x} \qquad (3,5)$$

The flow across the total left wall is given by

$$J_x = \lambda \iint \frac{dydz}{x_s\,(y,z) - i \cdot \Delta x} \cdot \Delta T \qquad (3,6)$$

Consequently α_i^x is obtained as

$$\alpha_i^x = \lambda \cdot \iint \frac{dydz}{x_s\,(y,z) - i \cdot \Delta x} \qquad (3,7)$$

The conductivity coefficients refering to the other directions are calculated by an analogous method.

An analytical evaluation of the integrals (2,9), (3,7) has been carried out for a cylindrical surface. It leads to complicated expressions, which have been programmed in the subroutine OBERFL required for generating the input data of the subroutine PROBE.

Additional plot programmes have been worked out, the first one of which concerns a graphical representation of the input data. This is necessary because there is a lot of possibilities of making errors in calculating the capacities and the conductivity coefficients, if the structure of the sample is complicated. The second one plots the numerical solution T(t) of a number of points, which can be chosen arbitarily.

4. Transport of heat in a model of calorimetric measuring equipment

As an example of numerical solution a sample shown in fig. 3, which represents one fourth of a model of a calorimetric measuring equipment, is treated. Since the planes y = x = o are mirror planes with respect to the complete sample, these planes have to be mirror planes with respect to the solution too. Thus it is

sufficient to calculate one fourth of the whole sample, which i adiabatically isolated at x = y = o. This symmetry consideratio helps to save time of calculation and to reduce the amount of storage. The sample consists of two parts: a heater of cement w a pot of aluminium upon it. The heater is heated by a pulse of 100 W lasting 1 s. The coefficient of heat transition between t heater and the bottom of the pot amounts to 400 W K^{-1} m^{-2}. On t bottom of the pot is lying a cover consisting of aluminium its corresponding coefficient of heat transition amounts to 100 W K^{-1} m^{-2}.

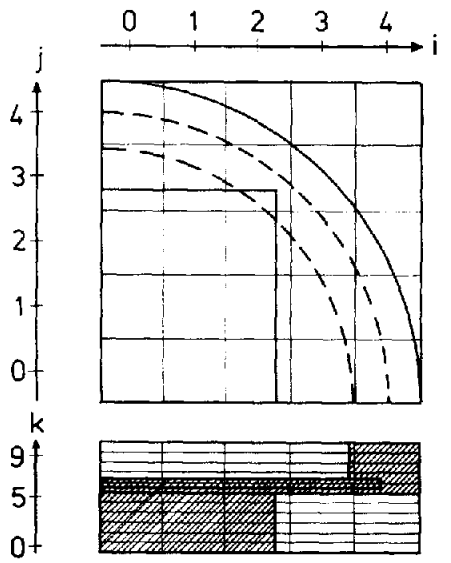

Fig. 3: One fourth of a model of calorimetric measuring equipme
All numbers are given in mm. The model is ten times as large as a realistic original equipment.

The following figures show diagrams of the solution at various points. It should be realized that the result does not reveal a surprising properties - the behaviour is quite plausible.

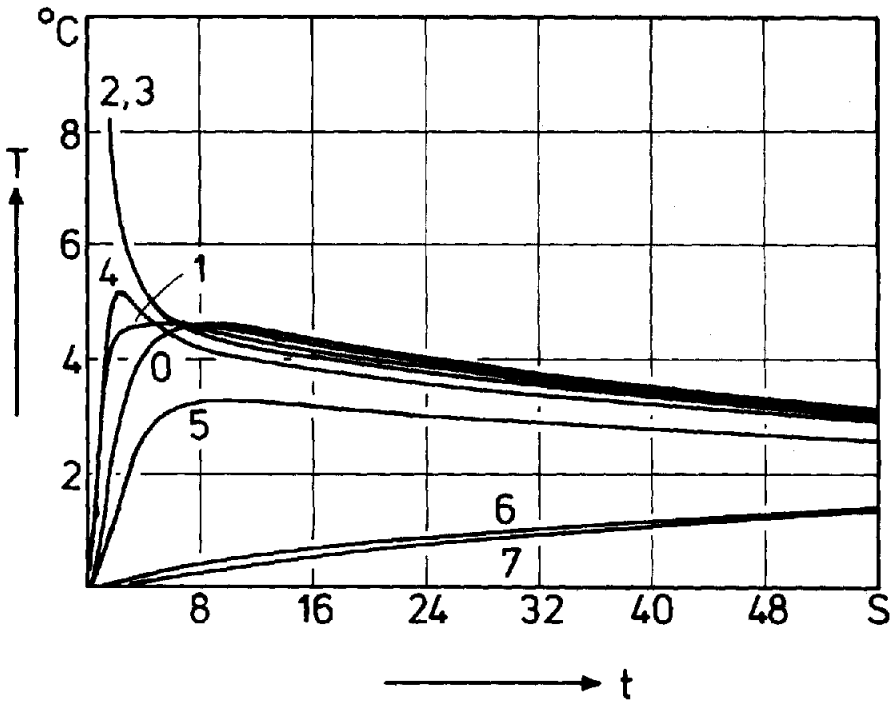

Fig. 4: Temperatures at the center (i = o, j = o) of the heater. The numbers of the curves denote the value of the vertical coordinate k. k = o for example is the ground of the block of cement, the layers k = 2, k = 3 contain the electrical heater, k = 6 is the bottom of the pot, k = 7 the cover

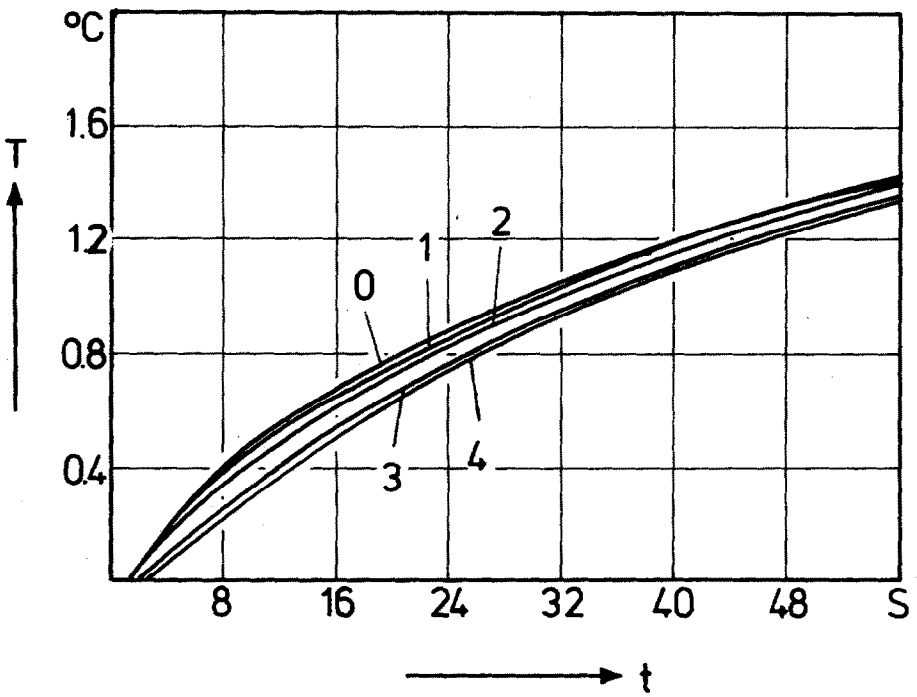

Fig. 5: Temperatures of the bottom of the pot (K=6) in y-direction at i = o. The numbers denote the values of j.

5. Final remarks

Numerical methods of resolving partial differential equations are well known. Nevertheless the programming takes a lot of time and work, because many problems have to be resolved in order to save time of calculation and with respect to an economic use of storage. Thus the number of programmes and subroutines amounts to 30 in the present form of the software package. Additionally the routines should be well understandable by reading the listings, i.e. they should include enough comments - unfortunately we have not yet carried out this work.

A second problem is the great deal of input data concerning the geometrical form of the sample - imagine that only one mistake in the set of data will produce a solution totally wrong. The way of avoiding these errors, we have chosen here is not to type the data directly, but to type programmes which calculate the input data. The reason is simple: it is easier to work out a logical structure and to write the corresponding programme than to type the great amount of data without errors. Errors in typing the programme will be realized by the compiler. Furthermore the concept of giving the position of the surface cells, (subroutine PROBE) helps reducing the number of input data.

The third problem was a suitable handling of a curved surface. Of course choosing sufficiently small lattice constants would be one way of an approximate description of these surfaces but this way is not realistic because of the large time of calculation and the large amount of storage. Another way is the transformation to non-cartesian coordinates, i.e. the use of a curved lattice. Indead this method is mathematically elegant, if these coordinates can be used for the whole sample. If there are several parts of sample, each requiring another kind of coordinates, which was the case for our example, uniform coordinates have to be chosen. For the sake of simplicity we used cartesian ones. Curved surfaces are taken into account by the method previously mentioned.

Finally it should be mentioned that transport by radiation is not negligeably small particularly at higher temperatures. So a realistic treatment of a calorimetric measuring equipment will require extending the programmes to taking into account this phenomenon. Indeed we are preparing this task, which will be no serious problem, since the numerical method is based exclusively to upon

balance equations holding even for nonlinear phenomena of transport.

Acknowledgements

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