MC. TRAD – 2 D
A multiple coordinate computer code for calculation of transport by diffusion in two dimensions

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February 1985
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This report was prepared as an account of work sponsored by Nagra. The viewpoints presented and conclusions reached are those of the author(s) and do not necessarily represent those of Nagra.
A computer code for the modelling of heat conduction or diffusive mass transport has been produced for use in the safety analysis of radioactive waste repositories.

MC.TRAD-2D (Multi-Coordinate Transport by Diffusion in 2-Dimensions) solves the diffusion equation in rectangular, cylindrical or polar plane coordinates. The code has been used in the analysis of heat dissipation from radioactive waste and in the study of near field nuclide migration.

The present report contains a technical description of the code, a user's manual, describing input requirements and the full range of options and a verification study whereby the code's performance in solving a number of (thermal) test problems is compared with analytical solutions to the same problems.
Für die mathematische Modellierung von Wärmeleitungs- und Diffusions­
prozessen wurde ein Computerprogramm zur Verwendung in Sicherheitsana­
lysen von Lagern radioaktiven Abfalls erstellt.

MC.TRAD-2D (Multi-Coordinate Transport by Diffusion in 2 Dimensions)
 löst die Diffusionsgleichung in rechtwinkligen, zylindrischen oder
Polarkoordinaten. Das Programm wurde verwendet, um die Ausbreitung der
von radioaktivem Abfall abgegebenen Wärme sowie die Nuklidausbreitung im
Nahfeld zu untersuchen.

Der vorliegende Bericht enthält eine Beschreibung des Programms, ein
Benutzerhandbuch, das die Anforderungen bezüglich einzugebender Daten
und die zur Verfügung stehenden Optionen beschreibt sowie eine Verifi­
zierungsstudie, in welcher für eine Reihe von (Wärmeleitungs-)Problemen
die mit dem Programm erhaltenen Resultate mit analytischen Lösungen
verglichen werden.
RESUME

En vue de la modélisation mathématique de processus de conduction thermique et de diffusion, un programme pour ordinateur a été élaboré en vue de l'utilisation, dans des analyses de sécurité, de dépôts de déchets radioactifs.

MC. TRAD-2D (Multi-Coordinate Transport by Diffusion in 2 Dimensions) résout l'équation de diffusion en coordonnées cartésiennes, cylindriques ou polaires. Le programme a été utilisé pour analyser la propagation de la chaleur qui se dégage du déchet radioactif ainsi que celle des nucléides dans le champ proche.

Le présent rapport renferme une description du programme, un manuel d'utilisation qui décrit les exigences concernant les données d'entrée et les options à disposition, ainsi qu'une étude de vérification dans laquelle, pour une série de problèmes (de conduction thermique), on compare les résultats obtenus avec le programme aux solutions analytiques.
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1. INTRODUCTION

The program family TRAD has been designed to provide codes for the solution of a wide variety of diffusion problems. Originally the programs were intended for use in heat transfer modelling, but have since been successfully extended to the domain of mass diffusion. This extension of the range of application of TRAD is possible because of the fundamental similarity of the governing equation.

For heat diffusion in 2-dimensional Cartesian coordinates the equation of conservation of thermal energy takes the form:

\[
\frac{\partial}{\partial t} (\rho CT) = \frac{\partial}{\partial y} (k \frac{\partial T}{\partial y}) + \frac{\partial}{\partial z} (k \frac{\partial T}{\partial z}) + S \tag{1.1}
\]

The equation of conservation of mass diffusing in a porous medium appears thus:

\[
\frac{\partial}{\partial t} (\varepsilon pRN) = \frac{\partial}{\partial y} (\varepsilon pD \frac{\partial N}{\partial y}) + \frac{\partial}{\partial z} (\varepsilon pD \frac{\partial N}{\partial z}) + S \tag{1.2}
\]

The algebraic symbols introduced by these equations are defined in the general nomenclature (Chapter 4) and, where necessary, described at appropriate points in Chapter 2. Derivations of the equations can be found in numerous works on diffusion and heat conduction, in particular Bird, Stewart and Lightfoot [1] or Carslaw and Jaeger [2].

The similarities between the two equations are clear. Each can be considered as a particular interpretation of a general conservation equation in which the parameters and the dependent variable are to be interpreted according to the nature of the problem being modelled. At the same time this general form can be written in other 2-dimensional coordinate systems by a straightforward transformation of the independent space variables. The present version of TRAD-2D incorporates cylindrical geometry as well as rectangular.

The general form of the governing equation for the transport of a general scalar, \( \phi \), may therefore take any one of the following forms:
In planar Cartesian coordinates:

\[
\frac{\partial}{\partial t} \phi \left( \mathbf{c}, \mathbf{p} \right) = \frac{\partial}{\partial y} \left( D \frac{\partial \phi}{\partial y} \right) + \frac{\partial}{\partial z} \left( D \frac{\partial \phi}{\partial z} \right) + S \tag{1.3a}
\]

In cylindrical coordinates:

\[
\frac{\partial}{\partial t} \phi \left( \mathbf{c}, \mathbf{p} \right) = \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial \phi}{\partial r} \right) + \frac{\partial}{\partial z} \left( D \frac{\partial \phi}{\partial z} \right) + S \tag{1.3b}
\]

In polar plane coordinates:

\[
\frac{\partial}{\partial t} \phi \left( \mathbf{c}, \mathbf{p} \right) = \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial \phi}{\partial r} \right) + \frac{1}{r^2} \frac{\partial}{\partial \theta} \left( r^2 \frac{\partial \phi}{\partial \theta} \right) + S \tag{1.3c}
\]

Figure 1-1 contains sketches of the three types of coordinate systems treated.

Apart from permitting calculations in any of the three coordinate systems noted above, the code allows time-dependence of the sources (\(S\) in equations 1.1 or 1.2) and a number of alternative boundary condition treatments.

Internally, the code carries out all computations assuming S.I. units. However, for certain problems a time base unit other than seconds may be more appropriate (e.g. geological processes where one year is a convenient time unit). In such cases certain input parameters are expressed in the specified time base unit, as are relevant output values. Conversions are carried out internally where necessary using the supplied timescale factor.

The TRAD code thus provides a flexible tool for diffusive transport calculations.
a) $y-z$ rectangular

b) $r-z$ cylindrical

c) $r-\theta$ polar

FIGURE 1-1: The alternative coordinate systems showing typical domains
2. SPECIAL FEATURES

2.1 The Domains Which Can Be Modeled

The calculational domain comprises one of the three spatial zones shown in Figure 1-1. These domains may be of any aspect ratio. The following points should be noted:

- The coordinate directions are always referred to in the terminology of equations (1.3), namely:
  a) $y - z$
  b) $r - z$
  c) $r - \theta$

The positive $z$-direction is vertically upwards in all cases where vertical planes or cylinder axes are modelled. This allows vertical temperature gradients or simplified natural convection phenomena to be considered, as in [3].

- The $y$-$z$ domain is a slab of unit thickness

- The $r$-$z$ domain is a 1 radian segment of a right, circular cylinder.

- The $r$-$\theta$ domain is a slab of unit thickness, forming part of a circular disc. The solution method does not allow the material to be considered as continuous in the circumferential ($\theta$) direction. Thus, a complete disc could only be a true model of a domain with imposed temperatures or concentrations, or perfect insulation, along one radius. This radius would represent simultaneously both extremes of the domain in the $\theta$-direction. In the radial direction, the extremes of the domain are the outer circumference on the one hand and the centre of the circular domain - a single point - on the other.
2.2 Alternative boundary conditions

In the numerical finite difference scheme used in the TRAD codes, each node on the edge of the calculational domain may be treated separately to conform with one or other of the following four types of boundary conditions:

- Insulated boundary:

  expressed by \( \frac{\partial \phi}{\partial x_j} = 0 \) in the \( x_j \)-direction;

- Imposed constant boundary values:

  Up to 9 different fixed values may be used in different parts of the boundary for any one problem.

- Imposed time-varying boundary values:

  whereby a boundary value time-history may be imposed on any one or any group of boundary nodes. The numerical scheme operates on discrete time intervals. If this boundary option is used, a new value is read from an input file for each new timestep.

- Linear exchange with a constant background expressed by:

\[
\dot{q}'' = h (\phi_S - \phi_\infty)
\]  

(2.1)

where:

- \( h \) local surface transfer coefficient [W m\(^{-2}\) K\(^{-1}\)] or [kg m\(^{-2}\) s\(^{-1}\)]
- \( \dot{q}'' \) specific surface flux [W m\(^{-2}\)] or [moles m\(^{-2}\) s\(^{-1}\)]
- \( \phi_S \) local domain surface value [°C] or [moles kg\(^{-1}\)]
- \( \phi_\infty \) background value [°C] or [moles kg\(^{-1}\)]
Both the background value and the transfer coefficient must be known in this case. This type of surface transfer may be used also under certain circumstances to simulate radiation exchange with the surroundings, as indicated by Hopkirk et al. [3].

In addition, defined regions within the modelled domain may be fixed at a constant temperature or concentration to simulate certain types of sources.

This feature has mainly been used in mass diffusion models to represent a solubility limit controlled source. It may also be used to represent a source or sink of latent heat (e.g. melting ice).

2.3 Sources

The general source term $S$ in equations 1.3 represents the injection (or extraction) of the transported variable. Thus, for thermal problems $S$ is interpreted as a specific heat source [$J m^{-3} s^{-1}$] while in mass diffusion problems it is a specific mass source [moles $m^{-3} s^{-1}$]. Of use in some mass transport problems is the possibility to define a total mass source [moles $s^{-1}$] representing a known local injection rate.

Either constant or time-varying sources may be treated. A single specific or total source rate may be specified at any one time during a problem. However, any number of discrete cells in the finite difference computational grid (see Chapter 3) may be heat or mass generating at the specified rate, thus enabling distributed or repeated sources to be modelled.

Some flexibility in the specification of the time varying source rate has been introduced. The source strength is always expressed as a polynomial:

$$Q = f(t) = a_1 + a_2 \theta + a_3 \theta^2 + a_4 \theta^3 + a_5 \theta^4 + a_6 \theta^5$$  \hspace{1cm} (2.2)
where:

\[ Q = \dot{q}'' \text{ or } \log(\dot{q}'') \]
\[ \theta = (t + t_{\text{sh}}) \text{ or } \log(t + t_{\text{sh}}); \text{ and} \]
\[ t_{\text{sh}} \text{ is a timeshift, allowing a parametric study of the effects} \]
\[ \text{of shifting the time origins of the problem and of the source} \]
\[ \text{relative to each other.} \]

The permutations of linear and logarithmic scales thus made available
and the freedom to choose up to six polynomial terms in equation 2.2
permit a wide range of situations to be modelled.

Sources whose strengths are stationary in time are modelled by employing
the first coefficient only for equation 2.2, so that:

\[ f(\theta) = a_1 \]

For mass diffusion problems an extra source term may be introduced to
represent loss of mass by radioactive decay. The specification of a
decay constant \( \lambda \) \( (= \ln(2.0)/\text{Half-life}) \) \( [s^{-1}] \) adds the term:

\[ -\varepsilon \rho \lambda N \]

(2.3)

to the term \( S \) in equations 1.3.

2.4 Material Properties

For thermal problems, the conductivity of each of the (up to 9) mate­
rials in the modelled domain may be treated as temperature-dependent
according to a polynomial expression of the type:

\[ k_i = c_{i1} + c_{i2}T^r + c_{i3}T^{2r} + c_{i4}T^{3r} + c_{i5}T^{4r} \]

(2.4)

where:
\( k_i \) \hspace{1cm} \text{thermal conductivity of material } i \ [W \text{ m}^{-1} \text{ K}^{-1}]

\( r \) \hspace{1cm} \text{a (real) exponent scaling factor (normally } -1 \leq r \leq +1)\)

The availability of up to five coefficients permits the modelling of most material types. In particular, for a material whose conductivity may be regarded as fixed, the first coefficient alone should be used, so that:

\[ k_i = c_{i1} \]

The same feature may also be used in mass diffusion problems to give a concentration-dependent diffusivity.

The formulation of equation 1.2 assumes that mass diffusion is taking place in water resident in some saturated porous medium. The diffusion constant \( D \) represents the diffusivity in this situation and may be substantially less than the molecular diffusivity in water, due to the tortuosity and constrictivity of the connected pore space within the medium.

The retention factor \( R \) in equation 1.2 is introduced to represent the effects of equilibrium sorption of the diffusing material on to the surface of the porous medium. At any point, sorption will result in a certain quantity of the diffusing material being immobilised. This quantity can be expressed as a concentration in the solid part of the porous medium \( N_s \) [moles kg\(^{-3}\)]. Therefore, the total quantity per unit volume \( (N_t) \) at any point is given by the sum of the liquid and solid concentrations, thus:

\[ N_t = \varepsilon \rho N_L + (1-\varepsilon) \rho N_s \]

Assuming that the mobile and immobile concentrations are in equilibrium and that this equilibrium can be expressed as a constant ratio between \( N_L \) and \( N_s \) (usually termed \( K_d \)), the above expression may be reformulated:
The term in square brackets is known as the retention factor $R$, and is a constant property of the medium together with the diffusing material.

Because sorbed radionuclides are subject to decay the constant $R$ also appears in the decay source term (2.3).
3. NUMERICAL SOLUTION

The diffusion equations presented in the previous sections are solved in MC-TRAD-2D by a finite difference technique. The planar calculation domain is subdivided by a rectangular grid into a number of cells. The spacing of the grid lines may be irregular, to obtain finer or coarser discretisation in more or less sensitive parts of the domain. Each resulting rectangular cell represents the control volume around a geometrically central node.

Material properties are defined at the node and are assumed constant across the control volume.

Figure 3-1 shows how the cells are numbered in the two-dimensional domain and Figure 3-2 indicates the nomenclature employed in this section to describe the difference forms of expressions and equations. The subscripts P, E, W, N, S are used for the particular control volume and its central node under consideration and for its four neighbours: "East", "West", "North" and "South". Lower case subscripts denote positions on the cell boundary and the subscript/superscript o indicates the "old" value from the previous timestep. Using this nomenclature, equation (1.1) describing heat conduction in rectangular coordinates, selected as the simplest alternative to employ as an example, may be rewritten in discretised form as follows:

\[
\frac{\rho C}{\Delta t} \left( T_P - T_P^0 \right) = \frac{1}{\Delta y_P} \left( \frac{k_E}{\delta y_e} (T_E - T_P) - \frac{k_W}{\delta y_w} (T_P - T_W) \right) \\
+ \frac{1}{\Delta z_P} \left( \frac{k_N}{\delta z_n} (T_N - T_P) - \frac{k_S}{\delta z_s} (T_P - T_S) \right) + S_P
\]  

(3.1)

It will be noted that the thermal conductivities, k, in this formulation may be anisotropic within any control volume, but that the principle axes of the diffusion tensor are aligned with the geometrical axes. An alternative, more general formulation is presented later in equation 3.4.
In order to maintain flux continuity across the faces of the control volumes it is necessary to define the diffusive coefficients on the e, w, n and s cell boundaries as the harmonic means of the conductivities for each pair of neighbouring cells.

Thus, for example:

\[ k_e = \frac{2\delta y_k k_p}{\delta y_k + \delta y_k} \quad \text{in the y-direction, or} \]

\[ k_e = \frac{\delta r k_k k_p}{\ln(\frac{r}{r})k_p + \ln(\frac{r}{r})k_p} \quad \text{in the r-direction} \]

for the cylindrical or polar coordinate cases.

If now the various components of the source term \( S_p \) are collected and represented by the linear expression in \( T \):

\[ S_p = S_{i_p} + S_{d_p}T_p \]

a number of possible non-linearities may be treated reliably and it becomes possible to express equation 3.1 in the following form:

\[
(A_E + A_W + A_N + A_S + A_O - S_d)T_p = A_{T_E} + A_{T_W} + A_{T_N} + A_{T_S} + A_{T_O} + S_i
\]

(3.2)

Such an equation being written for each control volume it becomes possible to solve the resulting array, as soon as the domain boundaries are defined. The array of equations may be written as a single matrix equation:

\[
\{A\} \{T\} = \{B\}
\]

(3.3)
where:

\[ A_{ii} \] are the coefficients of \( T_p \)

\[ A_{ij} \] are the coefficients of the neighbouring nodal temperatures

\[ B_i = S_i + A_0 T^0_p + (A_{\text{boundary}} \times T_{\text{boundary}}) \]

The first method of solution available for the 2-dimensional version of TRAD uses the Alternating Direction Implicit [4] method. The domain is swept alternately and iteratively by a sequence of row-by-row and column-by-column one-dimensional solutions. For each of these line solutions the temperatures in the two neighbouring lines are fixed at their latest values leaving a tri-diagonal coefficient matrix to be handled by Gaussian elimination.

Some problems converge slowly using the ADI method. Such slow convergence occurs, for instance, when large material property discontinuities occur in the field, when floating boundary values are required or where temperature dependent properties introduce non-linearities in the problem. For such cases, a direct inversion of the banded matrix equation 3.3 is included as an alternative solution method.

This method uses more computer core storage, but in general, less processing time to arrive at a converged solution.

However, the authors wish to avoid dictating which method to use on which occasion as this will depend on the computer used and on problem size and nature.
If material anisotropy is such that the principle axes of the conductivity tensor are inclined to the space coordinates then a third method of solution must be used.

This method involves not only the direct neighbour cells, but also the diagonal neighbours in a nine-point differencing scheme. Equation 3.1 is replaced by:

\[
\frac{\partial C}{\partial t} [T_p - T_p^0] = \frac{1}{\Delta y_p} \left\{ \frac{k_{yy}}{\delta y_e} (T_E - T_F) - \frac{k_{yy}}{\delta y_w} (T_P - T_W) \right\} \\
+ \frac{1}{\Delta z_p} \left\{ \frac{k_{zz}}{\delta z_n} (T_N - T_P) - \frac{k_{zz}}{\delta z_s} (T_P - T_S) \right\} \\
+ \frac{k_{yx}}{\Delta z_p \Delta y_p} (T_{ne} - T_{nw}) + \frac{k_{yx}}{\Delta z_p \Delta y_p} (T_{se} - T_{sw}) \\
+ \frac{k_{xy}}{\Delta y_p \Delta z_p} (T_{ne} - T_{se}) - \frac{k_{xy}}{\Delta y_p \Delta z_p} (T_{nw} - T_{sw}) + S_p \tag{3.4}
\]

Again, the same matrix equation (3.3) may be assembled, although now the elements of the coefficient matrix \([A]\) involve the NE, SE, SW and NW links as well.

The same banded matrix inversion scheme is used here as for the second solution method, with appropriate modifications for the broader bandwidth implied by the nine-point formulation.

In view of the nature of problems which have been met most frequently by the authors this third solution method has been developed only for the cartesian coordinate option.
FIG. 3-1: FINITE-DIFFERENCE GRID SHOWING CELL NUMBERING SCHEME
FIG. 3-2: DETAIL OF A CALCULATION CELL AND ITS NEIGHBOURS
To improve stability and convergence in non-linear problems an under-relaxation technique is employed in the iterative, implicit solutions. If an iteration by any of the 3 alternative methods (for a line with method 1 or for the whole field with methods 2 and 3) yields a set of temperatures \( (T') \), the values allocated are:

\[
T = vT' + (1-v)T^p
\]

where:

- \( v \) is the relaxation factor \( 0 < v \leq 1 \)
- \( p \) indicates the value of \( T \) from the previous iteration

For perfectly linear problems the value \( v = 1 \) can be used. The stronger the non-linearity, the smaller must be the relaxation factor.
4. NOMENCLATURE

Parameters and Variables

A  Coefficients in the implicit, canonical finite difference form of the conservation equation and in the matrix equation 3.3
a  Coefficients in the expression for time-dependent source strength
B  Constant vector in the matrix equation 3.3
C  Specific heat [J kg\(^{-1}\) K\(^{-1}\)]
D  Diffusivity of the transported material in the pore water [m\(^2\) s\(^{-1}\)]
\(c_{ij}\)  Coefficients in the expression for temperature dependent thermal conductivity
\(\varepsilon\)  Porosity [-] [m\(^3\)/m\(^3\)]
h  Linear surface heat or mass transfer coefficient [W m\(^{-2}\) K\(^{-1}\)] or [kg m\(^{-2}\) s\(^{-1}\)]
\(K_d\)  Equilibrium sorption concentration ratio [kg m\(^{-3}\)]
k  Thermal conductivity [W m\(^{-1}\) K\(^{-1}\)]
\(\lambda\)  Radioactive decay constant [s\(^{-1}\)]
N  Concentration of diffusing material [moles kg\(^{-1}\)]
\(\nu\)  Under-relaxation coefficient
\(\dot{q}''\)  Surface heat or mass flux [W m\(^{-2}\)] or [moles m\(^{-2}\) s\(^{-1}\)]
\(\dot{q}'''\)  Heat or mass source intensity [W m\(^{-3}\)] or [moles m\(^{-3}\) s\(^{-1}\)]
R  Retention factor [-]
r  Distance in the radial coordinate direction [m]
\(r\)  Global scaling factor for the exponents in the polynomial expression for temperature dependent thermal conductivity
\(\rho\)  Material density [kg m\(^{-3}\)]
S  Source terms in conservation equation [W m\(^{-3}\)] or [moles m\(^{-3}\) s\(^{-1}\)]
\(S_d\)  "Directly" temperature- or concentration-dependent portion of linearised source term [W m\(^{-3}\) K\(^{-1}\)] or [kg m\(^{-3}\) s\(^{-1}\)]
\(S_i\)  "Indirect" portion of linearised source term [W m\(^{-3}\)] or [moles m\(^{-3}\) s\(^{-1}\)]
T  Temperature [°C]
t  Time [s]
\(\phi\)  The value of a general scalar variable
\( t_{sh} \) Timeshift for examining the effect of moving the phase of a
time-dependent source relative to the timescale of the problem
[s]

\( \theta \) Time-based variable of the polynomial expression for time de­
dependent source strength [\( \dot{q}' \) or \( \log(\dot{q}'') \)]

\( \theta \) Angular distance in the circumferential coordinate direction
[rad.]

\( y, z \) Distances in the linear coordinate directions [m]

**Subscripts/Superscripts**

\( i \) Refers to material \( i \)

\( j \) Identifies a general coordinate direction \( x_j \)

\( N, S, E, W \) The direct neighbours of node \( P \) in the domain

\( n, s, e, w \) The mid-points of the faces of the control volume
for node \( P \)

\( l \) refers to the value (of the concentration) in pore
water

\( NE, SE, SW, NW \) The diagonal neighbours of node \( P \) in the domain

\( ne, se, sw, nw \) The corner points of the control volume for node \( P \)

\( o \) Refers to the "old" situation - the previous time­
step

\( P \) A general node in the calculation domain for which a
thermal energy conservation equation is written

\( p \) Refers to the "previous" iteration

\( s \) Refers to conditions on a surface at the domain
boundary

\( s \) refers to the value (of the concentration) in the
porous solid

\( \infty \) Refers to conditions outside the domain

\( t \) Refers to the total quantity (solid plus liquid) per
unit volume
5. BIBLIOGRAPHY


APPENDIX I

INPUT DATA DESCRIPTION FOR TRAD-2D

A sample input listing is included in Table A1-1 at the end of this Appendix.

Data in the input string is arranged into a sequence of five blocks as follows:

BLOCK 1: specifies the general nature of calculation.

BLOCK 2: specifies the time and space discretisations to be used in the model.

BLOCK 3: specifies the detailed nature of the calculation and the output.

BLOCK 4: contains all physical parameters necessary for the definition of the problem.

BLOCK 5: contains the flag array for defining the geometric and material properties and the boundary conditions.

A line-by-line explanation of the individual items of data is given here. This may be compared with Table A1-1, which contains the input necessary for running one of the cases described in Appendix II.

It should be noted that grid and variable arrays are dimensioned in this version to accommodate problems of the following sizes:

- up to 39 finite difference cells in the horizontal direction
up to 39 finite difference cells in the vertical direction
up to 9 different material types

The following input/output files are required:

TAPE 1 Restart file
TAPE 2 Input data for the time dependent boundary
   (if needed)
TAPE 3 Temperature or concentration time histories (if needed)
TAPE 4 Heat or mass flux time histories (if needed)
TAPE 5 Input data
TAPE 6 Iteration control and spatial distribution outputs
BLOCK 1 - Type of Calculation

Variables Input:

1. RCODE, JTITLE A8, A72
2. KOORD, KVAR, KBOUND, KSURF, KSOURC, NONISO, KSOLVE 10I4

Explanation:

RCODE
= START A new calculation (creates restart file).
= RESTART A restart run (restart file is read and will be rewritten).

JTITLE
72 character job name, which is reproduced at the start of each output table.

KOORD
= 1 Rectangular coordinate system with (y-z) coordinates.
= 2 Cylindrical coordinate system with (r-z) coordinates.
= 3 Cylindrical coordinate system with (r-θ) coordinates.

The orientations of the alternative coordinate pairs, presented in the tabulated output listings are indicated in the sketches.

N.B.: KOORD = 1

KOORD = 2
KOORD = 3

KVAR = 1  The independent variable is temperature.

= 2  The independent variable is a mass concentration.

= 3  The independent variable is a decaying radionuclide concentration.

KBOUND = 1  Time-dependent boundary condition is applied at the edges of the domain at nodes for which 10 < PFLAG ≤ 19. The boundary values are read step-by-step from TAPE2 with a format defined by THFORM.

= 0  No time-dependent boundary condition. (Refer to the note at the end of this block).

KSURF = 1  Convective exchange with background is treated by the transfer coefficient HCR at the boundary from cell surfaces where the boundary node has been flagged with 20 < PFLAG ≤ 29.

= 0  No convective exchange. (Refer to the note at the end of this block).

KSOURC = 1  Source polynomial will be interpreted as a total source.

= 0  Source polynomial will be interpreted as a specific source [per m³].
<table>
<thead>
<tr>
<th>NONISO</th>
<th>Value</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td></td>
<td>All materials have isotropic properties.</td>
</tr>
<tr>
<td>1</td>
<td></td>
<td>At least one material in the problem domain has anisotropic thermal conductivity or mass diffusivity aligned with the geometrical coordinate axes.</td>
</tr>
<tr>
<td>2</td>
<td></td>
<td>At least one material in the problem domain has anisotropic thermal conductivity or mass diffusivity, for which the principal axes of the conductivity tensor are inclined to the coordinate axes. This value may only be selected if KOORD=1.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>KSOLVE</th>
<th>Value</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td></td>
<td>The ADI (Alternating Direction Implicit) solver is to be used. Not valid if NONISO=2.</td>
</tr>
<tr>
<td>2</td>
<td></td>
<td>The 5-point differencing direct matrix inversion solver is to be used. Not valid if NONISO=2.</td>
</tr>
<tr>
<td>3</td>
<td></td>
<td>The 9-point differencing direct matrix inversion solver is to be used. This may only be selected if KOORD=1 and if NONISO=2.</td>
</tr>
</tbody>
</table>

**Note:**

Constant value and zero flux boundary conditions are treated independently. See INPUT, BLOCK 4.
**BLOCK 2 - Problem Discretisation**

Variables Input:

<table>
<thead>
<tr>
<th>Line</th>
<th>Variables</th>
<th>Format</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>NSTEPS, NITERS, TSCALE, ESCALE, TUNIT, EUNIT</td>
<td>$3I4,4X,2F8.2,2(1X,A3)$</td>
</tr>
<tr>
<td>2</td>
<td>TIMAX, TIMEX, DT, DTMAX, EX</td>
<td>8F8.2</td>
</tr>
<tr>
<td>3</td>
<td>NI, NJ</td>
<td>10I4</td>
</tr>
<tr>
<td>4</td>
<td>DZ(I) or DTHETA(I)</td>
<td>10F8.2</td>
</tr>
<tr>
<td></td>
<td>(according as KOORD is set to 1, 2 or 3 respectively)</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>dummy line</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>DY(J) or DR(J)</td>
<td>10F8.2</td>
</tr>
<tr>
<td></td>
<td>(according as KOORD is set to 1, 2 or 3 respectively)</td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>ZMIN, YMIN</td>
<td>10F8.2</td>
</tr>
</tbody>
</table>

Explanation:

**NSTEPS**  
Number of timesteps to be calculated.

- $= 0$  
  Steady state calculation.

- $> 0$  
  Time dependent calculation.

**NITERS**  
Maximum number of iterations per timestep.

**TSCALE**  
Multiplication factor to convert chosen time units to seconds (the number of seconds in the chosen time units). (Refer to note 1 at the end of this Block).

**ESCALE**  
Multiplication factor to convert Joules to chosen energy units. (Number of Joules per chosen energy unit).
TUNIT

Abbreviation for chosen time units to be used in outputs (e.g. YR).

EUNIT

Abbreviation for chosen energy units to be used in outputs (e.g. KWH).

TIMAX

Time limit of calculation (in chosen units). (Refer to Note 1 at the end of this Block). The calculation will cease either after NSTEPS timesteps or at problem time TIMAX, whichever is reached first.

TIMEX

Time at which timestep expansion starts. (Refer to Note 1 at the end of this Block).

DT

Length of initial timestep. (Refer to Note 1 at the end of this Block).

DTMAX

Maximum desired timestep length. (Refer to note 1 at the end of this Block).

EX

Timestep expansion factor (ratio of successive steps).

NI

≤ 39 Number of finite difference cells in the z- or θ-direction. (DZ(I) or DTHETA(I)).

NJ

≤ 39 Number of finite difference cells in y-or r-direction (DY(J) or DR(J)).

DZ(I)

Array, length NI of finite difference cell "widths" in [m] or in [radian/π], as applicable. (Refer to Note 2 at the end of this Block).

DY(J)

Array, length NJ of finite difference cells widths [m]. (Please refer to Note 2 at the end of this Block).

ZMIN

z- or θ-coordinate of domain origin [m] or [radian/π].
YMIN y- or r-coordinate of domain origin [m].

Note 1:

Time units in the time step definitions and in output tables may be selected at will (e.g. seconds, days, years).

A new calculation always starts at problem time zero. A restart calculation will read the current problem time from the restart file.

Material properties, coefficients and parameters and the strengths of sources/sinks must be input in S.I. units, unless otherwise indicated.

Note 2:

A total of NI values of DZ(I) and NJ values of DY(J) will be required.

The first and last values of each must be 0.0 corresponding to the zero volume cells at the domain boundaries.
BLOCK 3 - Run Details

Variables Input:

line 1 CRIT, RELAX 10F8.2
line 2 ITJUMP, IOJUMP, NTJUMP, NOJUMP, ISKIP, JSKIP, INITO, NTYP 20I4
line 3 ITYP(16) 20I4
line 4 JTYP(16) 20I4

Explanation:

CRIT In each timestep the iteration process will stop automatically when the normalised change of the dependent variable, summed over the whole domain (i.e. the residual change) is less than CRIT.

RELAX The relaxation factor used in the iterative solution scheme.

ITJUMP Timestep jump factor for the iteration control output.

IOJUMP Iteration jump factor for 2-D result output tables. The arrays indicated by IPRINT will all be output every IOJUMP iterations. This feature should only be used for checking problem convergence when it is strictly necessary. To suppress this output set, IOJUMP > NITERS.

NTJUMP Timestep jump factor for time history outputs.

NOJUMP Timestep jump factor for those 2-D result output tables specified by IPRINT.

ISKIP Column skip factor for 2-D(I,J) result output tables.

JSKIP Row skip factor for 2-D (I,J), result output tables.
INITIO

The initial contents of arrays specified by IPRINT to be printed in the results tables will be output prior to any further computation.

NTYP

Number of typical cells (see ITYP, JTYP below), for which parameter values are collected into the time history file in time dependent calculations and/or presented in the iteration control output.

ITYP(16)

I-locations of up to 16 "typical" cells.

JTYP(16)

J-locations of up to 16 "typical" cells.
BLOCK 4 - Physical Data

Variables Input:

<table>
<thead>
<tr>
<th>Line</th>
<th>Variables</th>
<th>Format</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>HCR(9)</td>
<td>10F8.2</td>
</tr>
<tr>
<td>2</td>
<td>LINLOG, NRCF, QSCALE, TSHIFT</td>
<td>10F8.2</td>
</tr>
<tr>
<td>3</td>
<td>ASOURC(6)</td>
<td>6F20.12</td>
</tr>
<tr>
<td>4</td>
<td>NRCON(9)</td>
<td>10I8</td>
</tr>
<tr>
<td>5</td>
<td>RCON(9)</td>
<td>10F8.2</td>
</tr>
<tr>
<td>6</td>
<td>ACON1(9,5)</td>
<td>10F8.2</td>
</tr>
<tr>
<td>7</td>
<td>ACON2(9,5)</td>
<td>10F8.2</td>
</tr>
<tr>
<td>8</td>
<td>PSICON(9)</td>
<td>10F8.2</td>
</tr>
<tr>
<td>9</td>
<td>ROCF(9)</td>
<td>10F8.2</td>
</tr>
<tr>
<td>10</td>
<td>EPS(9)</td>
<td>10F8.2</td>
</tr>
<tr>
<td>11</td>
<td>ALAM</td>
<td>10F8.2</td>
</tr>
<tr>
<td>12</td>
<td>FBOUND(9)</td>
<td>10F8.2</td>
</tr>
<tr>
<td>13</td>
<td>FFIELD(9)</td>
<td>10F8.2</td>
</tr>
<tr>
<td>14</td>
<td>FINIT, FGRAD, FAMB</td>
<td>10F8.2</td>
</tr>
</tbody>
</table>

Explanation:

**HCR**
An array of up to 9 values of the surface transfer coefficient $[W m^{-2} K]$ or $[kg m^{-2} s^{-1}]$

**LINLOG**
Index to determine the type of relationship between source strength and time (source units are $W m^{-3}$ or moles $m^{-3} s^{-1}$ if KSOURC = 0 and $W$ or moles $s^{-1}$ if KSOURC = 1).

- $= 0$ No source
- $= 1$ $\dot{q}''' = f(t) * QSCALE$
- $= 2$ $\log(\dot{q}''') = f(t) * QSCALE$
- $= 3$ $\log(\dot{q}''') = f(\log(t)) * QSCALE$
where \( t \) is in the chosen units of time. See TSHIFT below for its definition.

**NRCF**

\[ \leq 6 \]

Number of coefficients of the polynomial expression \( f(t) \) or \( f(\log(t)) \). See under ASOURC below for the description of the polynomial.

**QSCALE**

Scaling and conversion factor for use when manipulating source strengths:

- for converting the base function \( f(t) \) or \( f(\log t) \) to \( W \, m^{-3} \, W \), moles \( m^{-3} \, s^{-1} \) or moles \( s^{-1} \).

- for modifying the source intensity in parametric studies.

**TSHIFT**

Time shift value in the specified time units for source calculation, such that in the function \( f(t) \) or \( f(\log(t)) \):

\[ t = \text{TIME} + \text{TSHIFT} \]

where \text{TIME} is the current problem time; thus enabling phase shifts of the source function relative to the problem timescale to be introduced.

**ASOURC(6)**

An array of NRCF coefficients \( (a_j) \) to be inserted in a user-definable function for the time dependence of the strength of the sources in the domain, of the form:

\[ f(\theta) = a_1 + a_2 \theta + a_3 \theta^2 + \ldots + a_{\text{NRCF}} \theta^{\text{NRCF}-1} \]

where \( \theta = t \) or \( \log(t) \).
NRCON(9) An integer array containing the number of coefficients (\( \leq 5 \)) of polynomial expressions for the temperature dependence of the principal thermal conductivities or concentration dependence of principal mass diffusivities for zones of each of up to 9 material types.

RCON(9) An array of real factors used to scale the exponents of the terms in the polynomial expressions for principal thermal conductivities or mass diffusivities of each material type. (See factor \( r \) in polynomial under ACON1, below).

ACON1(9,5) 2-D array, whereby each of up to five lines contains up to 9 coefficients \( c_{ij} \) for the polynomial type expressions:

\[
 k_i \text{ or } D_i = c_{i1} + c_{i2}T^r + c_{i3}T^{2r} + \ldots
\]

thereby defining the temperature dependence of that principal thermal conductivity (or concentration dependence of mass diffusivity) for each material type (i) associated with the y- or r-axis. The number of lines of input data required is equal to the largest value of NRCON(i).

ACON2(9,5) Only to be input if NONISO \( \neq 0 \). 2-D array, identical in organisation to ACON1, defining the other principal conductivity or diffusivity for each material type, i.e. that one associated with the z- or \( \theta \)-direction.

N.B.: It is assumed that the number of polynomial coefficients and the exponent scaling factors are identical for both principal components of the conductivity/diffusivity tensor.
PSICON(9) Only to be input if NONISO = 2 (and KOORD = 1). An array giving the inclination of the principal tensorial component of conductivity or diffusivity, defined by the ACON1 array, to the y-axis for each material type. PSICON is input in degrees according to the convention sketched below:

![Diagram](image)

ROCP(9) Thermal capacity of the solid material for each material type [J/m³ K].

EPS(9) Only required if KVAR > 1. An array of up to 9 values of the porosity in each material zone [-].

ALAM Only required if KVAR = 3. The decay constant of a radionuclide [TUNIT⁻¹].

FBOUND(9) An array of the temperatures [°C] or retention factor for each material type [-] or concentrations [moles kg⁻¹] for use as fixed boundary conditions at the domain boundaries as specified by the value(s) of PFLAG on the boundary.

FFIELD(9) An array of temperatures or concentrations for use as fixed values within the domain as specified by the PFLAG array.

FINIT A value for use in initialising the temperature [°C] or concentration [moles kg⁻¹] field over the interior of the domain.
The imposed gradient (for instance, geothermal temperature gradient), if it is to be considered [°C m⁻¹] or [moles kg⁻¹ m⁻¹]. If FGRAD ≠ 0.0, FINIT is placed along the bottom edge of the domain and the field is initialised according to the desired gradient:

\[ F(I,J) = FINIT - FGRAD \times Z(I) \]

where \( Z(I) \) is the distance of the \( I \)'th row of cell nodes from the domain edge, \( I = 1 \). If, however, FGRAD = 0.0, the program places appropriate values from the FBOUND array around the edges of the domain and allots the initial value FINIT to the cells within the domain.

**N.B.**: Not relevant with r-θ coordinates.

The background temperature or concentration.
The flag array defines the desired boundary conditions and the spatial distributions of important variables and material types.

The block of flags occupies a space of NI columns and NJ rows of format 40I2.

<table>
<thead>
<tr>
<th>Line</th>
<th>Description</th>
<th>Format</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>dummy line</td>
<td>A10</td>
</tr>
<tr>
<td>2</td>
<td>dummy line</td>
<td>A10</td>
</tr>
<tr>
<td>3 (lines)</td>
<td>PFLAG (NI,NJ)</td>
<td>40I2</td>
</tr>
<tr>
<td>4</td>
<td>THFORM (only if KBOUND = 1)</td>
<td>3A10</td>
</tr>
</tbody>
</table>

**Explanation:**

**PFLAG**

**Inside the Domain:**

- **= 1 - 9**  
  Indicates which one of up to 9 different user definable materials exists in the cell.

- **= 10, 20, 30, .... 90**  
  Source in the cell is to be treated. The first digit indicates the material of the cell.

- **> 10**  
  The cell will be maintained at a fixed temperature or concentration. The first digit specifies the material of the cell, the second digit specifies the element of the array FFIELD in which the fixed value is defined.

**On Domain Boundaries:**

- **= -1**  
  Zero gradient boundary condition (insulating boundary).
Fixed values are to be imposed on the boundary at this point corresponding to FBOUND (1 - 9).

A time-dependent boundary condition is applied at this point. The second digit indicates the column on File TAPE2 in which the boundary value is to be found.

KBOUND must be =1 and TAPE2 must be available (see note below).

Linear exchange is treated at this point between the boundary and the background. The second digit indicates which of the 9 HCR values is to be used at this point.

Alphanumeric variable in the form of a conventional FORTRAN FORMAT specification, set in brackets, which defines the format of the data file TAPE2 to be read in if KBOUND=1. (Must be set only if KBOUND = 1).

The first 3 lines of TAPE2 (for table headings) are skipped over.

The file must consist of 2-10 columns, the first column being the time, in the specified time units and the subsequent column, numbered 1-9 for reference by PFLAG, the boundary values at that time.

Note:

When using TAPE2 to specify boundary values the time discretisation specified in the input is overridden by the time data read from TAPE2. The time specified in the first active line of TAPE 2 (i.e. line 4) must be greater than zero.
START

1 1 0 0 1 0 1
500 99 60.0 3.6E+6 MIN KWH
360.0 0.0 0.1 1.00 1.10
13 20
0.00 .010 .015 .020 .040 .080 .120 .135 .200 .200
.170 .010 0.00
0.00 .010 .015 .025 .040 .080 .120 .130 .160 .180
.190 .300 .750 1.00 2.00 5.00 19.8 70.0 200.0 0.00
0.0 0.0
1.0E-10 1.0
60 999 10 60 1 1 0 4
12 12 12 12
6 9 12 20
5.0
0 1 1.000 0.0
 0.00
 0.0 1.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
0.00 180.0 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
0.00 3.0E+6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
1.0 0.00 0.0
1 2 3 4 5 6 7 8 9 0 1 2 3 4 5 6 7 8 9 0 1 2 3
(*J)

Table A1-1: Sample Input Data File
APPENDIX II

SAMPLE PROBLEM OUTPUT

A sample input listing is included in Table A2-1. It will be noted that this is the same table as presented in Appendix I. This second appendix gives a brief description of the problem for which this input was generated and shows extracts from the output generated by TRAD in its solution.

The problem is incidentally also that which is presented in the code verification analysis in Appendix III as Problem No. 1. It concerns heat conduction in a semi-infinite rectangular domain:

\[ 0 < y < 21; \quad z > 0 \]

Figure A2-1 is a sketch of this domain with \( l = 1.0 \) m, showing also the initial and boundary conditions. The initial temperature of the domain is \( 1.0 \) °C. At time \( t = 0 \), the outer edges of the domain are suddenly fixed at zero temperature. The problem consists in calculating the time-dependent temperature distribution at times up to 6 hours after the sudden change.

Figure A2-2 is a plot of the extremity of the finite difference grid. It is to be noted that, in this plot, the z-axis represents one of the side edges of the rectangle, the y-axis the near (finite) edge of the rectangle. Fixed temperature (zero) boundary conditions are applied to both of these edges. The model examines only one half of the specified rectangle, taking advantage of symmetry. Thus, the centreline forms the other boundary parallel to the z-axis.
The infinite extremity is modelled by extending the domain in coarse steps out to 300 m. Both of these latter boundaries are treated as zero gradient (insulated).

Extracts from the results are contained in two further tables. Table A2-2, a page of output, contains the temperature distribution over the whole domain for timestep no. 60 together with the iteration output for the next timestep selected for presentation, no. 120. The 2-D output table is selected by NOJUMP, the iteration control output by IOJUMP. Both have been set to 60.

The output for step 60 starts with a summary of the timestep:

SMAX indicates the maximum proportional temperature change, $\Delta T/T$, in any cell in the field in the last iteration during the timestep, indicating the poorest degree of convergence in any individual cell.

SUMD is the domain temperature residual:

$$\frac{\sum_{i,j} |\Delta T_{ij}|}{\sum_{i,j} T_{ij}}$$

presented to give the degree of convergence over the whole field in the last iteration.

TIME is the time at the end of the timestep in the selected time units [minutes].

DT is the length of the timestep in the selected time units.

The temperature table contains the temperatures at the nodal points. The (I,J) addresses of each node are given, as also are its (y,z) coordinates.
The iteration output gives the values of $S_{\text{MAX}}$ and $S_{\text{UMD}}$ for each iteration, together with the addresses of the node corresponding to $S_{\text{MAX}}$. An additional convergence guide is given by $S_{\text{SUM}}$ which is the domain thermal energy residual:

$$\frac{\sum_{i,j} | \Delta z \Delta y (\rho C_T)_{ij} |}{\sum_{i,j} \Delta z \Delta y (\rho C_T)_{ij}}$$

In this example four nodal temperatures from the field have been selected as "typical" values, whose development may be followed in the appropriately labelled columns.

Table A2-3 contains the $(I,J)$ addresses and temperature time histories of the same four "typical" cells at timesteps specified by NTJUMP (set to 10 in this case). The second and third columns of this table give information about the time-dependent heat source, not in fact used for the test problem:

- **SOSUM** is the summed average heat release rate during a timestep in all control volumes in the domain which are flagged as source cells. The units are Joules per selected time unit.

- **WMEAN** is the average heat release rate (in arbitrary units) during a timestep given by the polynomial expression $f(\theta)$ as defined by LINLOG, NRCH, TSHIFT and CHOT, but before the multiplication by $Q_{\text{SCALE}}$, which will yield a specific heat generation rate in $W \text{ m}^{-3}$. 
Table A2-1: Printout of the Input Data File for the Sample Problem
### Table A2-2

One-page extract from output file showing temperature distribution for one timestep and iteration control for the next timestep selected in the sample problem sum.
<table>
<thead>
<tr>
<th>TIME (MIN)</th>
<th>SDSUM (J/TU)</th>
<th>WMEAN (W) / 12, 6/12, 9/12, 12/12, 20/20</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.594E+00</td>
<td>0.0</td>
<td>0.793, 1.000, 1.000</td>
</tr>
<tr>
<td>5.727E+00</td>
<td>0.0</td>
<td>0.490, 0.982, 1.000</td>
</tr>
<tr>
<td>1.483E+01</td>
<td>0.0</td>
<td>0.313, 0.870, 0.989</td>
</tr>
<tr>
<td>2.483E+01</td>
<td>0.0</td>
<td>0.235, 0.735, 0.948</td>
</tr>
<tr>
<td>3.483E+01</td>
<td>0.0</td>
<td>0.187, 0.619, 0.884</td>
</tr>
<tr>
<td>4.483E+01</td>
<td>0.0</td>
<td>0.153, 0.524, 0.808</td>
</tr>
<tr>
<td>5.483E+01</td>
<td>0.0</td>
<td>0.128, 0.446, 0.731</td>
</tr>
<tr>
<td>6.483E+01</td>
<td>0.0</td>
<td>0.108, 0.382, 0.658</td>
</tr>
<tr>
<td>7.483E+01</td>
<td>0.0</td>
<td>0.092, 0.329, 0.589</td>
</tr>
<tr>
<td>8.483E+01</td>
<td>0.0</td>
<td>0.079, 0.285, 0.527</td>
</tr>
<tr>
<td>9.483E+01</td>
<td>0.0</td>
<td>0.068, 0.249, 0.471</td>
</tr>
<tr>
<td>1.048E+02</td>
<td>0.0</td>
<td>0.060, 0.218, 0.421</td>
</tr>
<tr>
<td>1.148E+02</td>
<td>0.0</td>
<td>0.052, 0.191, 0.377</td>
</tr>
<tr>
<td>1.248E+02</td>
<td>0.0</td>
<td>0.046, 0.169, 0.337</td>
</tr>
<tr>
<td>1.348E+02</td>
<td>0.0</td>
<td>0.040, 0.149, 0.302</td>
</tr>
<tr>
<td>1.448E+02</td>
<td>0.0</td>
<td>0.036, 0.132, 0.271</td>
</tr>
<tr>
<td>1.548E+02</td>
<td>0.0</td>
<td>0.032, 0.117, 0.243</td>
</tr>
<tr>
<td>1.648E+02</td>
<td>0.0</td>
<td>0.028, 0.104, 0.218</td>
</tr>
<tr>
<td>1.748E+02</td>
<td>0.0</td>
<td>0.025, 0.093, 0.196</td>
</tr>
<tr>
<td>1.848E+02</td>
<td>0.0</td>
<td>0.022, 0.083, 0.176</td>
</tr>
<tr>
<td>1.948E+02</td>
<td>0.0</td>
<td>0.020, 0.074, 0.158</td>
</tr>
<tr>
<td>2.048E+02</td>
<td>0.0</td>
<td>0.018, 0.066, 0.142</td>
</tr>
<tr>
<td>2.148E+02</td>
<td>0.0</td>
<td>0.016, 0.060, 0.128</td>
</tr>
<tr>
<td>2.248E+02</td>
<td>0.0</td>
<td>0.014, 0.053, 0.115</td>
</tr>
<tr>
<td>2.348E+02</td>
<td>0.0</td>
<td>0.013, 0.048, 0.104</td>
</tr>
<tr>
<td>2.448E+02</td>
<td>0.0</td>
<td>0.011, 0.043, 0.094</td>
</tr>
<tr>
<td>2.548E+02</td>
<td>0.0</td>
<td>0.010, 0.039, 0.085</td>
</tr>
<tr>
<td>2.648E+02</td>
<td>0.0</td>
<td>0.009, 0.035, 0.076</td>
</tr>
<tr>
<td>2.748E+02</td>
<td>0.0</td>
<td>0.008, 0.031, 0.069</td>
</tr>
<tr>
<td>2.848E+02</td>
<td>0.0</td>
<td>0.007, 0.028, 0.062</td>
</tr>
<tr>
<td>2.948E+02</td>
<td>0.0</td>
<td>0.007, 0.025, 0.056</td>
</tr>
<tr>
<td>3.048E+02</td>
<td>0.0</td>
<td>0.006, 0.023, 0.051</td>
</tr>
<tr>
<td>3.148E+02</td>
<td>0.0</td>
<td>0.005, 0.021, 0.046</td>
</tr>
<tr>
<td>3.248E+02</td>
<td>0.0</td>
<td>0.005, 0.019, 0.042</td>
</tr>
<tr>
<td>3.348E+02</td>
<td>0.0</td>
<td>0.004, 0.017, 0.038</td>
</tr>
<tr>
<td>3.448E+02</td>
<td>0.0</td>
<td>0.004, 0.015, 0.034</td>
</tr>
<tr>
<td>3.548E+02</td>
<td>0.0</td>
<td>0.004, 0.014, 0.031</td>
</tr>
</tbody>
</table>

**Table A2-3:** Time history output for four monitor cells from the sample problem
A3.1 INTRODUCTORY REMARKS

Three two-dimensional problems have been selected from Carslaw & Jaeger's book [2], as test cases against which the performance of the numerical code and of its major features might be verified. The analytical solutions to these problems, also presented by Carslaw and Jaeger may be evaluated with high accuracy, thus providing a useful measure for the correctness and precision of TRAD.

Each problem is defined so as to treat the temperature range between 0 and 1 degree, whereby the zero degree reference point may be anywhere on the Kelvin scale.

In this manner the modelling precision can be characterised in each case by the absolute values of the differences between analytical and numerical results.

This Appendix is also published separately under the title "Verification of the two-dimensional version of TRAD - a computer code for the study of diffusive heat transport".
A3.2 PROBLEM 1

This problem, taken from Carslaw and Jaeger is the calculation of the time-dependent temperature distribution in the semi-infinite rectangle:

\[-\ell < y < \ell, \quad z > 0\]

with an (arbitrary) uniform initial temperature, if all edges of the rectangle are suddenly fixed at zero temperature. The thermal diffusivity of the material in the solid domain was taken as

\[\kappa = \frac{k}{\rho C} = 3.6 \times 10^{-3} \text{ m}^2 \text{s}^{-1}\]

where:

- \(C\) the specific heat \([\text{J kg}^{-1} \text{K}^{-1}]\)
- \(k\) the thermal conductivity \([\text{W m}^{-1} \text{K}^{-1}]\)
- \(\rho\) the density \([\text{kg m}^{-3}]\)

The solution, given in § 5.6 (equation 8) is the infinite series:

\[T(y, z, t) = \frac{4}{\pi} \text{erf} \left( \frac{z}{2\sqrt{\kappa t}} \right) \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n + 1)} \left( e^{\frac{-\kappa \phi_n^2 t}{2}} \right) \cos \phi_n y \quad (A3.1)\]

where:

\[\phi_n = \frac{(2n + 1)\pi}{2l}\]

Figure A3.1 shows part of the finite difference cell grid used for the TRAD calculations of this case. The geometrical limits of the problem are symmetrical about the centreline of the rectangular space, where an insulated boundary condition was applied. The origin of the coordinate system for the numerical calculation is one corner of the rectangle at its finite end.
The physical dimensions selected were based on \( l = 1 \text{m} \). Thereby, the calculational domain was extended up to 300 m in steps of increasing coarseness - see sample input and output in Appendix II, which are for this problem - in order to simulate the infinite extent of the rectangle. Figure A3.2 contains plots of the calculated temperature time histories at four points along the symmetry line \((y = 1.0 \text{ m})\) at varying distances from the "finite" end of the rectangular domain \((z = 0.0)\). Here, the continuous curves represent the analytical solutions, while the starred points show the results obtained with TRAD.

Tabular values of the same time histories are given also in Table A3-1 for both analytical and numerical calculations.

The analytical calculation was performed so that all results are accurate to 12 decimal places. The numerical solution used variable length timesteps. For the results used for comparison with the analytical solution, the initial timestep was 0.1 min., the ratio between successive timesteps expanding in geometric progression was 1.1 and the maximum allowed timestep was 1.0 min. For the 4 time histories displayed, the absolute values of the differences between the two calculations, normalised with respect to the temperature range are given in Table A3-2 below:

<table>
<thead>
<tr>
<th>Position along y-axis [m]</th>
<th>Normalised absolute temperature differences</th>
<th>Time-averaged</th>
<th>Maximum</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>0.0011</td>
<td>0.0180</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.0005</td>
<td>0.0040</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.0028</td>
<td>0.0120</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.0028</td>
<td>0.0100</td>
</tr>
</tbody>
</table>

Figures A3.3 and A3.4 are included to demonstrate the effects of timestep selection upon the precision of the numerical calculation. The
timestep expansion ratio was again 1.1 in both cases. The initial time­steps were both 1.0 minute, but the maximum timestep lengths were 5.0 minutes and 10.0 minutes respectively.

The non-dimensional times:

$$\frac{k_t}{2} \frac{t}{y}$$

for which results may be interpreted for this problem lie in ranges typical of a wide variety of engineering problems.
A3.3. PROBLEM 2

This problem was selected to verify the combination of cylindrical \((r,z)\) coordinates and the treatment of heat generation within the domain. It is to be found in § 8.3 of Carslaw and Jaeger and concerns the steady state temperature distribution developed in a finite cylinder

\[ 0 < z < l, \quad 0 \leq r < R \]

within which heat is generated uniformly and steadily at a specific rate \(\dot{Q}\). The solution is given in § 8.3, equation 38 as:

\[
T(r,z) = C_1 + C_2 \sum_{n=0}^{\infty} \frac{I_0\left[(2n+1)\pi r/l\right]}{(2n+1)^3 I_0\left[(2n+1)\pi R/l\right]} \sin \frac{(2n+1)\pi z}{l}
\]

\[ (A3.2) \]

where:

\[
C_1 = \frac{\dot{Q}z(l-z)}{2k}
\]

\[
C_2 = -\frac{4\dot{Q}}{k}\frac{\pi}{3} \quad \text{and}
\]

\[ I_0(x) \quad \text{the modified Bessel function.} \]

A calculation was performed using the parameters:

\[
R = 1 \text{ m} \\
l = 4 \text{ m} \\
k = 1 \text{ W m}^{-1} \text{ K}^{-1} \\
\dot{Q} = 4 \text{ W m}^{-3}
\]

The graded finite difference cell grid employed for the numerical calculation with TRAD is shown in Figure A3.5.
In Figure A3.6, isotherms derived from the numerical calculation are shown. The comparison between analytical and numerical calculations may be seen in Figures A3.7 and A3.8, which contain respectively two radial and two axial temperature distributions along selected lines. As in Figure A3.2, the continuous lines here represent the analytical solutions and the starred points the numerically computed temperature values.

Output lists of the resulting temperature distributions over the whole calculational domain are given for analytical and numerical solutions respectively in Tables A3-3 and A3-4. In both of these tables the temperature values are given at the positions of the nodal points used for the finite difference computation.

The analytical calculation for this problem was performed so that all results were accurate to 12 decimal places. Table A3-5 below gives the absolute values of average and maximum differences between the two calculations, normalised with respect to the (unit) problem temperature range.

<table>
<thead>
<tr>
<th>Position of section through domain [m]</th>
<th>Absolute error values [K]</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Radial, z = 2.00</td>
<td>0.0039</td>
<td>0.0112</td>
<td></td>
</tr>
<tr>
<td>Radial, z = 0.31</td>
<td>0.0024</td>
<td>0.0060</td>
<td></td>
</tr>
<tr>
<td>Axial, r = 0.00</td>
<td>0.0036</td>
<td>0.0110</td>
<td></td>
</tr>
<tr>
<td>Axial, r = 0.74</td>
<td>0.0024</td>
<td>0.0060</td>
<td></td>
</tr>
</tbody>
</table>

The influence of the selected spatial discretisation of the problem domain has been demonstrated by a calculation using the coarse, uniform finite difference grid shown in Figure A3-9. Figures A3.10 and A3-11 show the reduced quality of the numerical results when compared with Figures A3.7 and A3.8 respectively.
A3.4. PROBLEM 3

The third problem concerns once again a cylindrical \((r,z)\) domain, a steady state problem, but instead of internal heat generation there is surface heat exchange with an ambient environment. The problem is to be found in Carslaw and Jaeger, § 8.3. It specifies a cylindrical solid domain:

\[0 \leq r < R, \quad 0 < z < \ell\]

The plane \(z = 0\) is maintained at a constant temperature \(V\), plane \(z = \ell\) at zero temperature. Heat exchange, according to a linear relationship, takes place from the cylindrical surface \((r=R)\) with a medium which is also at zero temperature. The expression for the steady state temperature distribution, given in § 8.3, equation 10, is as follows:

\[
T(r,z) = V \cdot \sum_{n=1}^{\infty} \frac{2h J_0(\alpha_n) \sinh(\ell-z)\alpha_n}{R(h^2 + \alpha_n^2) J_0(\alpha_n) \sinh \alpha_n} \tag{A3.3}
\]

where:

\[\alpha_n\]

are the roots of the transcendental equation:

\[Ra \cdot J_1(Ra) - Rh J_0(Ra) = 0\]

\(J_0, J_1\)

are Bessel functions.

\(h\)

is the surface heat exchange coefficient defined by the boundary conditions:

\[\frac{\partial T}{\partial r} + hT = 0, \quad 0 < z < \ell, \quad r = R.\]

A calculation was performed using the parameters:
R = 1 m  
\dot{\lambda} = 4 m  
k = 10 W m^{-1} K^{-1}  
h = 5 W m^{-2} K^{-1}  
V = 1 °C

Figure A3.12 shows the finite difference cell grid employed for the TRAD calculation. The isotherm field resulting from this calculation is displayed in Figure A3.13. Figures A3.14 and A3.15 show the temperature distributions along two radial and two axial sections respectively through the domain.

Output lists of the resulting temperature distributions over the whole calculational domain are given for analytical and numerical solutions respectively in Tables A3-6 and A3-7.

For this problem the analytical solution requires the roots, \( \alpha \), of the transcendental Bessel function equation:

\[ \alpha J'_0(\alpha a) + h J_0(\alpha a) = 0 \]  \hspace{1cm} (A3.4)

Using the fact that

\[ J'_0(\alpha a) = -J_1(\alpha a) \]

equation (4.2) can be rewritten as

\[ \alpha a J_1(\alpha a) - h a J'_0(\alpha a) = 0 \]  \hspace{1cm} (A3.5)

This equation has been solved to provide 50 terms for equation (A3.3), yielding accuracies to better than 12 places of decimals except within 1 cm of the temperature discontinuity at the corner \( r = 1, z = 0 \). In this region the numerical solution can be expected to give more reliable results than the analytical.
Table A3-8 below summarises the absolute values of the deviations between analytical and numerical solutions:

**Table A3-8: Absolute error summary for Problem 3**

<table>
<thead>
<tr>
<th>Position of section through domain [m]</th>
<th>Absolute values of deviations [K]</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Radial, z = 0.31 m</td>
<td>0.0016</td>
<td>0.0024</td>
</tr>
<tr>
<td>Radial, z = 1.35 m</td>
<td>0.0019</td>
<td>0.0021</td>
</tr>
<tr>
<td>Axial, r = 0.00 m</td>
<td>0.0008</td>
<td>0.0021</td>
</tr>
<tr>
<td>Axial, r = 1.00 m</td>
<td>0.0011</td>
<td>0.0031</td>
</tr>
</tbody>
</table>
5. SUMMARY

The comparisons presented in the previous sections have demonstrated the essential reliability of the results obtainable with the two-dimensional version of TRAD in applications which include the use of such built-in features as distributed heat sources and surface heat transfer.

Included also has been an indication of the sensitivity of results to the fineness of spatial and temporal discretisation. The version of each calculation selected for comparison with the analytical code has been made with levels of discretisation felt to be useful for typical engineering problems.
A3.6 DETAILED DESCRIPTION OF FIGURES

PROBLEM 1

Figure A3.1  Part of the finite difference cell grid used for the finite difference calculations. This represents half of the tip of the semi-infinite rectangle - the finer discretisation being around the outer edges of the domain.

Figure A3.2  Temperature time histories at four different locations along the line $y = 1.0$ m, (the axis of symmetry of the semi-infinite rectangle) where the continuous curves represent the analytical solution, while the starred points show the numerical results at discrete times. The initial timestep of 0.1 minute was extended up to 1 minute in geometric progression.

Figure A3.3  Temperature time histories presented as in Figure A3.2, where the initial timestep of 1 minute was extended up to a maximum of 5 minutes in geometric progression.

Figure A3.4  Temperature time histories as in Figures A3.2 and A3.3, where the initial timestep of 1 minute was extended up to a maximum of 10 minutes in geometric progression.

PROBLEM 2

Figure A3.5  The finite difference cell grid employed for the numerical calculations.

Figure A3.6  Isotherms derived from the numerical calculations.

Figure A3.7  Radial temperature profiles at two different axial positions. The analytical results are given by the continuous lines, while the starred points show the numerical results at the nodal points.
Figure A3.8  Axial temperature profiles at two different radii. The analytical and numerical results are presented again as for Figure A3.7.

Figure A3.9  A coarse finite difference cell grid used for additional numerical calculations to demonstrate the influence of the spatial discretisation upon the numerical results.

Figure A3.10  Radial temperature profiles at two different axial positions calculated by analytical and numerical methods, where the coarse grid was employed. Presentation is as in Figure A3.7.

Figure A3.11  Axial temperature profiles at two different radii. Presentation as in Figure A3.8.

PROBLEM 3

Figure A3.12  The finite difference cell grid used for the numerical calculations.

Figure A3.13  Isotherms derived from the finite difference calculations.

Figure A3.14  Radial temperature profiles at two different axial positions calculated by analytical and numerical method. Presentation as in Figure A3.7.

Figure A3.15  Axial temperature profiles at two different radii. Presentation as in Figure A3.8.
<table>
<thead>
<tr>
<th>Time (mins.)</th>
<th>Analytical Solution</th>
<th>Numerical Solution</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1.</td>
<td>2.</td>
</tr>
<tr>
<td>1.594E+00</td>
<td>.775</td>
<td>1.000</td>
</tr>
<tr>
<td>5.727E+00</td>
<td>.478</td>
<td>.986</td>
</tr>
<tr>
<td>1.483E+01</td>
<td>.308</td>
<td>.870</td>
</tr>
<tr>
<td>2.483E+01</td>
<td>.233</td>
<td>.735</td>
</tr>
<tr>
<td>3.483E+01</td>
<td>.186</td>
<td>.619</td>
</tr>
<tr>
<td>4.483E+01</td>
<td>.153</td>
<td>.524</td>
</tr>
<tr>
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<td>.127</td>
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<td>.108</td>
<td>.382</td>
</tr>
<tr>
<td>7.483E+01</td>
<td>.092</td>
<td>.330</td>
</tr>
<tr>
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<td>.286</td>
</tr>
<tr>
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<td>.069</td>
<td>.249</td>
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<td>.060</td>
<td>.218</td>
</tr>
<tr>
<td>1.148E+02</td>
<td>.052</td>
<td>.192</td>
</tr>
<tr>
<td>1.248E+02</td>
<td>.046</td>
<td>.169</td>
</tr>
<tr>
<td>1.348E+02</td>
<td>.040</td>
<td>.149</td>
</tr>
<tr>
<td>1.448E+02</td>
<td>.036</td>
<td>.132</td>
</tr>
<tr>
<td>1.548E+02</td>
<td>.032</td>
<td>.117</td>
</tr>
<tr>
<td>1.648E+02</td>
<td>.028</td>
<td>.104</td>
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<tr>
<td>1.748E+02</td>
<td>.025</td>
<td>.093</td>
</tr>
<tr>
<td>1.848E+02</td>
<td>.022</td>
<td>.083</td>
</tr>
<tr>
<td>1.948E+02</td>
<td>.020</td>
<td>.074</td>
</tr>
<tr>
<td>2.048E+02</td>
<td>.018</td>
<td>.064</td>
</tr>
<tr>
<td>2.148E+02</td>
<td>.016</td>
<td>.059</td>
</tr>
<tr>
<td>2.248E+02</td>
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<td>2.348E+02</td>
<td>.013</td>
<td>.047</td>
</tr>
<tr>
<td>2.448E+02</td>
<td>.011</td>
<td>.042</td>
</tr>
<tr>
<td>2.548E+02</td>
<td>.010</td>
<td>.038</td>
</tr>
<tr>
<td>2.648E+02</td>
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<tr>
<td>2.748E+02</td>
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<td>.031</td>
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<tr>
<td>2.848E+02</td>
<td>.007</td>
<td>.028</td>
</tr>
<tr>
<td>2.948E+02</td>
<td>.007</td>
<td>.025</td>
</tr>
<tr>
<td>3.048E+02</td>
<td>.006</td>
<td>.022</td>
</tr>
<tr>
<td>3.148E+02</td>
<td>.005</td>
<td>.020</td>
</tr>
<tr>
<td>3.248E+02</td>
<td>.005</td>
<td>.018</td>
</tr>
<tr>
<td>3.348E+02</td>
<td>.004</td>
<td>.016</td>
</tr>
<tr>
<td>3.448E+02</td>
<td>.004</td>
<td>.015</td>
</tr>
<tr>
<td>3.548E+02</td>
<td>.004</td>
<td>.013</td>
</tr>
</tbody>
</table>

Table A3-1: Problem 1. Temperature time histories at four monitoring points 1, 2, 3 and 4 on the centre line of the infinite rectangle at z = 0.13, 0.50, 1.20 and 300 m respectively.
Problem 2. Distribution of temperatures at the nodal points used in the numerical solution, but computed by the analytical method.
| \( j \) | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 |
| 1 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| 2 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| 3 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| 4 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| 5 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| 6 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| 7 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| 8 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| 9 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| 10 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| 11 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| 12 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| 13 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| 14 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| 15 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| 16 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| 17 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| 18 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| 19 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| 20 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |

**Table A3-4:** Problem 2. Distribution of temperatures computed by the numerical method
Table A3-6: Problem 3. Distribution of temperatures at the nodal points used in the numerical solution, but computed by the analytical method.
Table A3-7: Problem 3. Distribution of temperatures computed by the numerical method.
Z-DIRECTION  10. CM  WINDOW ON
GEOMETRICAL BOUNDARY  GRID OF CELL EDGES
SEMI-INFINITE RECTANGLE
TEMPERATURE TIME HISTORIES ON A SEMI-INFINITE RECTANGLE (DT=0.1-1 MIN)
TEMPERATURE TIME HISTORIES ON A SEMI-INFINITE RECTANGLE (DT=1-5 MIN)
TEMPERATURE TIME HISTORIES ON A SEMI-INFINITE RECTANGLE (DT=1-10 MIN)
Z-DIRECTION

10. CM

GEOMETRICAL BOUNDARY

GRID OF CELL EDGES

FINITE CYLINDER WITH HEAT PRODUCTION ( R=1 M; L=4 M; K=1 W/MK; Q=4 W/M3 )

FIGURE A3.5
TEMPERATURE, CONTOUR INTERVAL = .100E+01 C

FINITE CYLINDER WITH HEAT PRODUCTION ( R=1 M ; L=4 M ; K=1 W/MK ; Q=4 W/M3 )

FIGURE A3.6
RADIAL TEMPERATURE PROFILES IN A CYLINDER WITH HEAT PRODUCTION

FIGURE A3.7
AXIAL TEMPERATURE PROFILES IN A CYLINDER WITH HEAT PRODUCTION
Finite cylinder with heat production (\(R=1\,\text{m}\), \(L=4\,\text{m}\), \(K=1\,\text{W/mK}\), \(Q=4\,\text{W/m}^3\))

GEOMETRICAL BOUNDARY

GRID OF CELL EDGES

FIGURE A3.9
RADIAL TEMPERATURE PROFILES IN A CYLINDER WITH HEAT PRODUCTION

FIGURE A3.10
Figure A3.11

Axial temperature profiles in a cylinder with heat production.
FINITE CYLINDER WITH SURFACE HEAT LOSS ( R=1 M; L=4 M; K=10 W/MK; H=5 W/M2K )
TEMPERATURE CONTOUR INTERVAL = \(100 \times 10^1 \, \text{C}\)

FINITE CYLINDER WITH SURFACE HEAT LOSS (\( R=1 \, \text{M}; \, L=4 \, \text{M}; \, K=10 \, \text{W/MK}; \, H=5 \, \text{W/MK} \))

FIGURE A3.13
Radial temperature profiles in a cylinder with surface heat loss

Figure A3.14

$Z = 0.31 \text{ m}$

$Z = 1.35 \text{ m}$
AXIAL TEMPERATURE PROFILES IN A CYLINDER WITH SURFACE HEAT LOSS

FIGURE A3.15