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Colloid Transport Code-Nuclear User's Manual

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CTCN : COLLOID TRANSPORT CODE NUCLEAR

A User's Manual

by

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ABSTRACT

This report describes the CTCN computer code, designed to solve the equations of transient colloidal transport of radionuclides in porous and fractured media. This Fortran 77 package solves systems of coupled nonlinear differential equations with a wide range of boundary conditions. The package uses the Method of Lines technique with a special section which forms finite-difference discretizations in up to four spatial dimensions to automatically convert the system into a set of ordinary differential equations. The CTCN code then solves these equations using a robust, efficient ODE solver. Thus CTCN can be used to solve population balance equations along with the usual transport equations to model colloid transport processes or as a general problem solver to treat up to four-dimensional differential systems.

1.0. MODEL DESCRIPTION

1.1. Nature and Purpose

The CTCN code is a baseline version of a comprehensive code for quantifying hydrological colloidal migration of radionuclides for the Yucca Mountain Project. It is designed to solve unsteady population balance equations along with mass, energy and momenta conservation equations in up to four Cartesian axes. The code is designed to incorporate a wide range of boundary conditions and submodels within the main equations and thus can be used for many other colloidal transport problems.

Yucca Mountain is the site for a proposed HLW repository. Earlier reports indicate that colloidal transport plays a significant part in the overall migration of radionuclides through groundwater (Saltelli et al., 1984; Fried et al., 1976; Champ et al., 1982; Travis and Nuttall, 1985; Fried et al., 1975; Ho and Miller, 1986; Means et al., 1978; Champ et al., 1984; Gschwend and Reynolds, 1987;). The population balance model developed to analyze colloid transport requires numerical solution to systems of coupled, nonlinear ordinary differential, partial differential and integro-differential equations. CTCN is designed to solve such systems. In anticipation of future alterations to the model, flexibility and robustness have been a major criteria for development of CTCN.

This manual describes the model, its numerical solution and includes a user's guide with several sample problems.

1.2. Mathematical Model

1.2.1. Governing Equations

The population balance permits complete treatment of the colloid problem including birth, growth, capture, and dissolution (Randolph and Larson, 1988). The idea is to establish a phase space consisting of the three spatial and one temporal coordinates (external coordinates) as well as each property to be tracked as a separate axis (internal coordinates).

The usual transport equations are modified to include the internal axes. The rate of change of the properties is assumed to be continuous thus leading to the definition of a velocity along each property axis corresponding to the growth term. Radioactive decay is treated by assigning a concentration property axis to each species to be tracked. It must be noted that the species will not be conserved along the internal axes and so we have to include 'death' and 'birth' terms into the equations.

The colloid transport model treats the following phenomena,

- (i) hydrology,
- (ii) species balances for all distinct chemical species, and
- (iii) population balances for all distinct colloidal species.

The main contribution of the present work is to solve in a general method the population balance equations for colloidal species. Each component of the overall colloid transport model will now be discussed separately.

(i) Hydrology

Traditional approaches to modeling flow through the subsurface involves using the Darcy equation or modifications thereof and applying it to averaged quantities in porous media. However, in some geological

formations the assumption of a porous media is not viable and flow through fractures in the medium must be considered. There is also the problem of flow through the unsaturated (or vadose zone) as opposed to flow through saturated media.

Site-specific data for hydraulic properties of the fractured and porous media can be incorporated into available numerical codes like TRACR3D in a dual-porosity approach for solving the Richard's equation (Mangold and Tsang, 1991) for flow through the unsaturated zone,

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial x} \left(K(\psi) \frac{\partial \psi}{\partial x} \right) + \frac{\partial}{\partial z} \left(K(\psi) \frac{\partial \psi}{\partial z} - 1 \right)$$

where:

θ = volumetric water content

ψ = pressure head

K = hydraulic conductivity.

An alternate approach is to use models of fracture networks and determine the velocity distribution from those networks as in the FRACNET (Robinson, 1988) code.

(ii) Species Balance

The species balance equations are statements of the conservation of mass for each distinct chemical species. For fractured media, they are of the general form (Mangold and Tsang, 1991),

$$\frac{\partial c_i}{\partial t} + (\vec{v} \cdot \nabla) c_i = \nabla \cdot (D_i \nabla c_i) - \lambda_i c_i - \text{sink terms} + \text{source terms}$$

where,

c_i = concentration of species 'i'

λ_i = radioactive decay constant for species 'i'

D_i = effective diffusivity

t = time

v = velocity of the fluid.

For porous media, the conservation equation in unsaturated flow with sorption and decay is (Bear and Verrujit, 1987),

$$\frac{\partial(\theta R_d(\theta) c_i)}{\partial t} = -\nabla \cdot \theta (c_i V - D_h \cdot \nabla c_i) - \theta k_f \left(1 + \frac{\theta_s \rho_s f_a(\theta) k_s K_d}{\theta k_f} \right) c_i + \sum_{(m)} R^{(m)}(x^{(m)}, t) \delta(x - x^{(m)}) c_{i,R}^{(m)}(x^{(m)}, t) - \sum_{(r)} P^{(r)}(x^{(r)}, t) \delta(x - x^{(r)}) c_i(x^{(r)}, t)$$

where

θ = moisture content

For saturated flow, $\theta = n$ = porosity

c_i = concentration of pollutant

V = velocity vector at a particular point

D_h = coefficient of hydrodynamic dispersion

θ_s = solid's volumetric fraction = $1-n$ (for saturated flow)

ρ_s = solid's density

$f_a(\theta)$ = area of solid-liquid interface/total area of solid

k_s = degradation rate constant of the decaying species

k_f = degradation rate constant in water (not differ from k_s)

K_d = distribution coefficient (linear sorption isotherm)

$\sum_{(m)} R^{(m)}(x^{(m)}, t) \delta(x - x^{(m)}) c_{i,R}^{(m)}(x^{(m)}, t)$ = artificial recharge at rates $R^{(m)}$

at points $x^{(m)}$ with concentration $c^{(m)}$.

$\sum_{(r)} P(r) (x(r), t) \delta(x - x(r)) c_i(x(r), t) = \text{water withdrawn at pumping rates } P(r)$

at points $x(r)$

$$R_d(\theta) = 1 + \frac{\theta_s \rho_s f_a(\theta) K_d}{\theta} = \text{coefficient of retardation}$$

If the isotherm used for sorption is not the linear isotherm, the structure of $R_d(\theta)$ will change.

Here we have included radioactive processes into the equations and assumed that other processes can be written as source or sink terms or boundary conditions for these equations. The development of submodels is an area of active research. Speciation in solution at a given point in space can be determined through standard geochemistry software packages (Mangold and Tsang, 1991).

(iii) Population balance for each colloidal species 'i',

$$\frac{\partial \psi_{ii}}{\partial t} + \nabla \cdot (\vec{v} \psi_{ii}) - \nabla \cdot (D_b \nabla \psi_{ii}) + \sum_{j=1}^m \frac{\partial (v_{ji} \psi_{ii})}{\partial \xi_j} + D_i - B_i = 0$$

where,

ψ_{ii} = number density of colloid type 'i'

ξ_j = property axis for property type 'j'

$v_{ji} = \frac{d \xi_j}{d t}$ = property growth rate

D_b = Brownian diffusion coefficient

B_k = colloid birth function

D_k = colloid death function

1.2.2. Submodels

The model requires submodels for the following phenomena:

Birth (heterogeneous and homogeneous nucleation) rate

Death rate

Growth Rate

Agglomeration rate

De-agglomeration rate

Adsorption/desorption of radionuclides

Decay of Nuclei within or on a colloid

Randolph and Larson give birth mechanisms. H. van Olphen points out specific mechanisms for clay colloids. Jantzen and Bibler proposed that iron and glass waste canisters react under geological conditions to produce iron silicate colloids.

Capture models have been given by McDowell-Boyer et al. for three types of removal: filter caking, straining, and physico-chemical removal (Brownian motion, inertia, interception, hydrodynamic and sedimentation).

Agglomeration is treated by the birth and death rate terms in the population balance. Smoluchowski first developed a diffusion limited agglomeration model for monodispersed particles. Hidy and Brock reviewed his work and extensions by Swift and Friedlander to polydisperse size distributions of agglomerating particles.

Recent work by Hurd included charge effects in a Witten-Sander model and showed that the resulting fractal-like particle has a fractal dimension of two but the number of calculations required make this model useless for now.

Since these submodels are in various stages of development at LANL, the code has been designed to incorporate them easily in later versions.

1.3. Numerical Model

In spite of the great importance of these equations to particulate system dynamics, solutions have been difficult to obtain. Analytical solutions are available only for a few simple forms of the initial conditions and submodel formulations. Numerical solutions have been reported but the optimum method for solving the equations has not been determined. One promising class of methods for solving the resulting equations is collocation on finite elements (Gelbard and Seinfeld, 1978). It is a widely used method but there is considerable doubt and a large degree of arbitrariness in the placement of collocation points. Traditional collocation methods are not accurate since, due to large variations in magnitude of the size variable, a single high-order polynomial fit is not feasible.

Marchal et al.(1988) present an effective argument for the use of finite-difference techniques in the solution of the population balance equations. They note that the methods using decomposition of the dependent variable(s) on a set of orthogonal functions suffer from a number of disadvantages. For example, the choice of the set of orthogonal functions is arbitrary, and the ways to achieve the mathematical transformation are different from one problem to another. Despite successes with these techniques, a degree of arbitrariness always remains. Moreover their result is the PSD as a continuous function whereas experimental data using particle counters is a histogram because of the inherent lumping of the PSD in measurement. The theoretical message is here stronger than the experimental measurements (while the moments transformations approach yields less information than the experimental data); the model is too precise for a computational adjustment of kinetic parameters.

Thus we use finite-differencing techniques to solve the resulting equations. Due to uncertainties in the submodels at this point, the code has

been designed to handle a general system of coupled, nonlinear PDEs, ODEs and integro-differential equations. The Method of Lines is a handy, reliable tool to numerically approximate the solution of systems of differential-algebraic equations. The PDEs are converted into sets of coupled first order ODEs by discretizing all but the temporal axis. Thus we get an ODE for each spatial point. These ODEs are then solved using a robust, adaptive ODE solver. This idea was first applied by E. Rothe in 1930 (Liskovets, 1965) to equations of parabolic type and indeed is a 'natural' method for parabolic PDEs. It has been seen to be a very robust method for a variety of problems, notably the 'driven cavity' problem using the streamline-vorticity formulation of the Navier-Stokes equations where it outperformed the ADI method (Painter, 1981). Most general PDE software uses the method of lines (Melgaard and Sincovec, 1981; Scheisser, 1971; Sincovec and Madsen, 1974; Loeb, 1974; Carver, 1973; Hyman, 1976). Until recently, most of these packages addressed problems in one or two spatial dimensions. However, recent advances in solving large systems of ODEs accurately and economically allow solution of large systems (up to four dimensions) feasible.

If a survey is made of general purpose solvers for differential systems (Machura and Sweet, 1980), it is seen that despite the emergence of many new methods for the solution of such systems, the method of choice continues to be the method of lines. It has been used in a variety of codes. The user implements this method by discretizing the spatial derivatives etc. with a choice from an array of finite difference methods available in the code and choosing from two general purpose ODE solvers.

To accommodate many yet to be defined submodels, constitutive relationships, and boundary conditions, the CTCN code is designed to be a

general differential systems solver. It is capable of solving equations of the form,

$$\frac{\partial u_i}{\partial t} = g \left(u_i, x, y, z, r, t, \frac{\partial u_i}{\partial x}, \frac{\partial u_i}{\partial y}, \frac{\partial u_i}{\partial z}, \frac{\partial u_i}{\partial r}, \frac{\partial^2 u_i}{\partial x^2}, \frac{\partial^2 u_i}{\partial y^2}, \frac{\partial^2 u_i}{\partial z^2}, \frac{\partial^2 u_i}{\partial r^2}, \frac{\partial(xf)_i}{\partial x}, \frac{\partial(yf)_i}{\partial y}, \frac{\partial(zf)_i}{\partial z}, \frac{\partial(rf)_i}{\partial r} \right)$$

Here, the subscript 'i' indicates the different dependent variables, x, y, z, and r are the four independent spatial axes and xf, yf, zf, and rf are terms comprising of flux expressions which may be differenced as a whole. These flux variables can also be differenced directionally, i.e. forward or backward differencing depending on the direction of the characteristics oriented into the axes. Thus we have four such terms, one corresponding to each of the four independent axes, along which its first derivative is to be taken. These terms themselves can be functionals of the form,

$$xf(i) = g \left(u_i, x, y, z, r, t, \frac{\partial u_i}{\partial x}, \frac{\partial u_i}{\partial y}, \frac{\partial u_i}{\partial z}, \frac{\partial u_i}{\partial r}, \frac{\partial^2 u_i}{\partial x^2}, \frac{\partial^2 u_i}{\partial y^2}, \frac{\partial^2 u_i}{\partial z^2}, \frac{\partial^2 u_i}{\partial r^2} \right)$$

and similarly for yf(i), zf(i) and rf(i).

Apart from the equations, we need grid specifications, and boundary and initial conditions. The equations are solved on a finite, Cartesian, equispaced, orthogonal grid and with specific initial conditions specified by the user. Initial conditions need not be consistent with the boundary conditions.

A wide variety of boundary conditions can be incorporated into the problem domain. In general, the following types of boundary conditions are used,

$$a_i u_i + b_i \frac{\partial u_i}{\partial x} = c_i \quad \text{at the } x - \text{boundaries}$$

and similarly for the other boundaries. CTCN incorporates boundary conditions by using fictitious points and cubic interpolation. It is sometimes necessary to impose a boundary condition that should actually be enforced at infinity but is enforced numerically at a large distance from the last

meaningful grid point. CTCN obviates the use of such artificial and error-prone procedures. This kind of condition is handled by setting all coefficients (a, b and c) for that boundary condition to be set to zero. The code then interpolates the values of the dependent variables as required into the fictitious points.

The code offers many options for the type of finite-difference spatial discretizations to be performed. It incorporates these into the equations along with the boundary conditions to form a set of ordinary differential equations. If there are NPDE dependent variables on $(NX * NY * NZ * NR)$ grid points in the four axes respectively, then we get $(NPDE * NX * NY * NZ * NR)$ ODEs. As can be seen, the design of the code is geared towards flexibility and generality. This version of CTCN should be seen as a research version designed to be able to incorporate submodels, equations and boundary conditions under development and also to assist the development of these very submodels. Once these parameters have been set, the code can be 'fixed' in the sense that the user would only have to input a data file giving values for the parameters entering the equations etc. There would be no need for user-specified subroutines and consequently CTCN could be set up so that only the output and input data files would be visible to the user.

The ODEs resulting from any MOL (method of lines) discretization are stiff, i.e. components of the solution have time constants that vary in orders of magnitudes. This inherent stiffness is compounded by stiff features within the original system of equations (e.g. reactions with drastically different rate constants, diffusion etc.). There has been a lot of work on solving huge systems of stiff ODEs largely motivated by the generality and effectiveness of the MOL approach. Hindmarsh consolidated these efforts

into his set of codes ODEPACK at LLNL. Of these codes, experience has shown the code LSODES to be the most effective package for the problems under consideration. However, even LSODES is not efficient for large problems (> 20-40,000 ODEs). Recent research by Hindmarsh and Brown resulted in the development of an experimental solver LSODPK which has so far proved to be more effective than LSODES.

The code is designed to accommodate either solver with minimal modifications.

2.0. CODE DESCRIPTION

2.1. Files and Operating Parameters

CTCN operates on any UNIX/VMS workstation or mainframe as well as on CRAY supercomputers under the UNICOS operating system. CTCN is written in Fortran 77 and efforts have been made to make the code as machine-independent as possible. A working knowledge of Fortran 77 is necessary to use the code. The workspace required depends on the dimensionality of the problem so a two-dimensional run could be performed on a workstation while bigger problems would require about thirty minutes of cpu time on a mainframe or a few minutes on a CRAY Y/MP. For two and three-dimensional problems, post-processing options are available to create input files for the NCSA Imagetool graphics package or the Spyglass Dicer package, respectively.

The package consists of the following files and subroutines:

<u>Files</u>	<u>Routines</u>
makefile	
inc.for	include file
dims.h	include file

user.f	main program, subroutines eqn, func and bound.
face.f	subroutine face.
setup.f	subroutines bset, bcal, fder, dercal and set.
lsodpk.f	ODE solver LSODPK.

These files have counterparts for VMS systems.

2.2. Subroutines and their description

See fig. 1 for a structural overview of CTCN. A list of the tasks performed by the various subroutines follows.

1. **main program** sets up choice of options for CTCN and the ODE solver. Defines the grid points and initial conditions.
2. **subroutine eqn** defines the equations for the dependent variables.
3. **subroutine func** defines the flux terms.
4. **subroutine bound** defines the boundary conditions.

Fig. 1 : Structural Overview of CTCN

5. subroutine face	incorporates boundary conditions into the initial data. Calls the ODE solver for the different output times, prints data for CTCN and some of the ODE solver's outputs, allocates array sizes for the ODE solver and may be used to change some of the other optional inputs to the ODE solver.
6. subroutine set	calculates the right hand side of the ODEs for the ODE solver.
7. subroutine dercal	evaluates the spatial derivatives of the dependent variables.
8. subroutine fder	evaluates the first derivatives of the flux terms.
9. subroutine bset	evaluates the values of the dependent variables at the fictitious points to incorporate the boundary conditions into the discretization.
10. subroutine bcal	calculates the boundary values.
11. subroutine lsodpk	driver routine for the ODE solver package LSODPK

2.3. Step-wise Operation

For any particular problem the user has to modify files 'user.f', 'inc.for' and possibly 'face.f' according to the step-wise procedure detailed below.

Step 1 : Enter the dimensions of the system in file 'inc.for'. This is a one-line file of the form,

parameter (npde=1, nx= 101, ny=1, nz=1,nr=1).

Set the unused axes to have at least one grid point and that for a one-dimensional problem, the x-axis has to be the independent axis for correct results. For two-dimensional problems, the x and y axes have to be used (and not the x and z axes or the y and z axes etc.) and so on. Also, once the axes are chosen, they must be set so that the number of points is in the order $NX \leq NY \leq NZ \leq NR$. This does not include the dummy axes and is essential for maximum efficiency when using the LSODES solver.

Step 2 : Modify the MAIN program in file 'user.f'. Set the following variables (see example problems),

(i) output times - tout, tint, tlast, nout.

(ii) ODE solver options - itol, rtol, atol, mf.

(iii) Evaluation flags for the derivatives - meth.

(iv) Grid points and initial conditions - x, y, z, r and u.

Step 3 : Modify subroutine EQN in file 'user.f'. Enter the equations for the system using either the one grid point form or the one call form.

Step 4 : Modify subroutine FUNC in file 'user.f'. Enter the flux terms, if any, for the system using either the one grid point form or the one call form.

Step 5 : Modify subroutine BOUND in file 'user.f' so as to reflect the boundary conditions for the system.

Step 6 : Modify the block data module BDAT in file 'user.f'. Here, one only needs to make the dimensions of variable meth in the main program consistent with the number of zero's entered in the data statement in BDAT.

Once these steps have been completed, the code is ready to use. It may be necessary to modify subroutine FACE in file 'face.f' if the memory allocation for work arrays or optional inputs to the ODE solver or the solver itself need to be changed.

The operation of the code for UNIX machines is as follows (commands to be typed in are in italics) :

- (1)The user modifies files 'inc.for' and 'user.f' according to his problem as detailed later.
- (2)If the ODE solver needs to be changed or the memory allocations or optional inputs to the solver need to be modified, the user may modify file 'face.f'.
- (3)The user types in the *make* command and an executable file 'ctcx' is created.
- (4)Typing in the filename for the executable *ctcx* begins execution. The output file 'ctcn.out' is created at the end of the run.

The operation of the code for VMS machines is as follows:

- (1)The user modifies files 'inc.for' and 'user.for' according to his problem as detailed later.
- (2)If the ODE solver needs to be changed or the printing and/or code timing calls need to be modified, the user may modify file 'face.for'.
- (3)The command *@make* has to be executed once before using a third-party make. This executes the file 'make.com'. This is necessary only once after each fresh login since this file links with a script containing default rules and software for the make command.

(4)The user types in the *make* command and an executable file 'ctcn.exe' is created.

(5)Typing in the command *run ctcn* begins execution. The output file 'ctcn.out' is created at the end of the run.

.c. 2.4. Common Errors

The ODE solver LSODPK or alternative routines from the ODEPACK package have an excellent diagnostic routine built-in. It is recommended that the user read the documentation for the particular package he may be using. This will also be useful if the user wants to use the full capabilities of these powerful, versatile packages by using the more advanced options. These can be set from the subroutine face.

Although LSODPK has been as good as, if not better than LSODES for our test problems, it is conceivable that it may not converge to a solution for certain problems. In such a case, LSODPK will print out warnings indicating this fact to the user. An alternative solver should then be used and LSODES would be the most logical choice. The calling sequence and usage of these two packages is almost exactly the same, so the user can very easily replace one for the other by reading the comment lines for these subroutines.

Another common glitch would involve subroutine face printing out a diagnostic message saying that the ODE solver needs more memory for its real and/or integer workspace(s). It also gives values for the current memory allocation(s) and the required memory allocation(s). In such a case, the user would modify the dimensions for variable(s) *rwork* and/or *iwork* to the value required for the memory allocation(s) for the workspace. Also the value(s) of variable(s) *lrw* and/or *liw* should be set to the same number(s).

Another common error is setting the values for the number of grid points for any axis to zero. This will cause a floating overflow. Even if a particular axis is not going to be used, the number of grid points for it should be set to 1.

3.0. EXAMPLE PROBLEMS

In this section a complete description of the code is given by showing its usage for solving two example problems. The first problem is a simple diffusion equation in one dimension while the second one is a two-dimensional fracture problem that uses the population balance approach in its most elementary form but is readily extensible to a complete model with aggregation, birth terms etc.

3.1. Example 1 : Conduction in a Semi-infinite Medium

A semi-infinite medium, $x \geq 0$, is initially at zero temperature. For times $t > 0$, the boundary surface at $x = 0$ is subjected to a temperature $T_0 (= 1.0)$. We wish to calculate the temperature distribution at any given time. The equation is ,

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2}$$

Initial Conditions : $u = 0$.

Boundary Conditions :

at $x = 0$, $u = 1.0$ and at $x = \text{infinity}$, $u = 0$.

We use a grid of 51 points distributed evenly in $0 \leq x \leq 1.0$ taking $\alpha = 0.005$ and seek the solution for $t = 5$.

The analytical solution is

$$T = T_0 \operatorname{erfc} \left(\frac{x}{\sqrt{4 \alpha t}} \right)$$

Detailed below is the complete procedure for solving the first example equations.

Step 1 : Modify file 'inc.for' to reflect the dimensionality of the problem.

We will solve this one-dimensional PDE on a grid of 51 points. In this case file 'inc.for' is written as,

parameter (npde = 1, nx = 51, ny = 1, nz = 1, nr = 1)

Note that we must set the unused axes to have at least one grid point and that for a one-dimensional problem, the x-axis has to be the independent axis for correct results.

Step 2: Modify the main program. The following variables are to be set,

(i) output times : Set the number and values of the output times where the solution is to be calculated. For our problem we want output at $t = 5.0$ s. The integration must begin at $t = 0$ and end at $t = 5.0$. The following variables are to be set,

1. dimension TOUT as TOUT(1) since we need output at just one time.

2. TINT - Integration starts at $t = \text{TINT}$ and initial values are given at this time. Set $\text{TINT} = 0$.

3. TOUT(NOUT) - array of size NOUT. Contains the values for the output times. Set $\text{TOUT}(1) = 5.0$.

4. TLAST - Integration ends at $t = \text{TLAST}$. Set $\text{TLAST} = 5.0$.

5. NOUT - number of output times. Set $\text{NOUT} = 1$.

(ii) ODE solver options : Four parameters are to be set. Three are concerned with error tolerances for solving the ODEs. Relative and absolute error tolerances can be specified in scalar or vector form, i.e. for the whole system of equations or for any number of subsystems (e.g. for each dependent variable etc.). ITOL, RTOL and ATOL are these three parameters. If RTOL(relative error tolerance) and/or ATOL(absolute error tolerance) are vectors they must be dimensioned accordingly and ITOL(flag) must be set to two, otherwise it should be set to one. The tolerances may be set as vectors if one of the dependent variables differs significantly in magnitude with the others and so would require a different level of accuracy during integration. A good rule for choosing the tolerances is that if the data requires precision of 10^{-n} then RTOL should be set to $10^{-(n+1)}$ and ATOL should be two orders of magnitude less than RTOL.

The fourth parameter is the ODE integration flag MF. Usually it should be set to 10 for a non-stiff problem and 22 for a stiff problem if LSODPK is to be used. For more details see the documentation for the solver. The changes to be made are,

1. ITOL - Set ITOL = 1 (RTOL and ATOL are scalars).

2. RTOL - Set RTOL = 10^{-4} (need a precision of 10^{-3}).

3. ATOL - Set ATOL = 10^{-6} .

4. MF - Set MF = 22 (the problem is stiff and the solver is LSODPK).

(iii) Evaluation flags for the derivatives : For every dependent variable we must indicate which spatial and/or flux derivatives are to be calculated and by what methods. Since there are two spatial and one flux derivatives for each of the four axes, there are $(2+1) \times 4 = 12$ flags for each dependent variable. Total number of flags = $12 * \text{NPDE}$. Thus we allocate integers for a variable METH of dimensions (NPDE, 12). The flag corresponding to each term and the options for its value and their significance are given in the comments in the code.

1. METH - Looking at the equations we see that we need to calculate only the second derivative with respect to x for the one dependent variable. Thus we need only to set a value for METH(1,11). We choose to use centered second order differencing for the derivatives. Thus, we set

meth(1, 11) = 2

(iv) Grid points and initial conditions : The grid points must be given values and the initial conditions for the system must be specified. Since our problem is one-dimensional we need to set DX, X(J) and U(I, J, 1,1,1) as follows,

c grid extends from 0 to 1.0. grid spacing dx = ***

dx=1.0/(nx-1)

do 20 j=1,nx

c set values for x(j) and initial conditions in u(1,j,1,1,1)

$$x(j)=(j-1)*dx$$

$$u(1,j,1,1)=0.0$$

20 continue

Step 3 : Modify subroutine EQN for the problem so as to describe the right-hand side of the equations. The time derivatives of the dependent variables are to be defined in terms of the grid points (x, y, z, r), time t and the spatial (ux -> first derivative of u(1) with respect to x, uxx -> second derivative of u(1) with respect to x etc.) and flux derivatives (fx -> derivative of flux term xf(1) with respect to x) of the dependent variables.

This subroutine may be written in two forms. In the first form the subroutine defines the equations at one spatial mesh point for each call. This form is the most applicable and easy for the user. Sometimes, however, the second form of the subroutine in which the user defines all the equations at all the grid points in one call to subroutine EQN, is more efficient. The second form may be used if the user needs to prescribe special discretizations, use unequal grid spacings, incorporate global integral relationships into the equations or to include ODEs as boundary conditions. This would be essential for any detailed population balance model since terms like the birth of particles into a size region would be given by an integral term involving particles with sizes less than this particular size range (aggregation). The choice of the second form is indicated to CTCN by setting IX > NPDE. We give both forms of the subroutine for our example problem,

Form 1 : One call defines equations at one grid point.

subroutine eqn(ut,u,ux,uy,uz,ur,uxx,uyy,uzz,urr,fx,fy,fz,fr,t,x,y

```

&      ,z,r,ix)
integer ix,npde
include 'inc.for'
real ut(npde),u(npde),ux(npde),uy(npde),uz(npde),ur
&      (npde),uxx(npde),uyy(npde),uzz(npde),urr(npde),
&      fx(npde),fy(npde),fz(npde),fr(npde),t,x,y,z,r
c ***modify the lines below to reflect the equations to be
solved****
    ut(1)=0.005*uxx(1)
c *****no need to set ix*****
c *****end of problem specific part*****
    return
end

```

Form 2 : One call defines equations at all grid points.

```

subroutine eqn(ut,u,ux,uy,uz,ur,uxx,uyy,uzz,urr,fx,fy,fz,fr,t,x,y
&      ,z,r,ix)
integer ix,npde
include 'inc.for'
c *****note changes in dimensioning for this form of the sub.****
    real ut(npde,nx,ny,nz,nr),u(npde,nx,ny,nz,nr),ux(npde,nx,ny,nz,
& nr),uy(npde,nx,ny,nz,nr),uz(npde,nx,ny,nz,nr),ur(npde,nx,ny,
& nz,nr),uxx(npde,nx,ny,nz,nr),uyy(npde,nx,ny,nz,nr),uzz(
& npde,nx,ny,nz,nr),urr(npde,nx,ny,nz,nr),fx(npde,nx,ny,nz,nr)
& ,fy(npde,nx,ny,nz,nr),fz(npde,nx,ny,nz,nr),fr(npde,nx,ny,nz,
& nr),t,x(nx),y(ny),z(nz),r(nr)
c***end of changes in dimensioning for this form of the

```

```

c  subroutine**
c ***modify the lines below to reflect the equations to be
c  solved****
c ***note the do loop for this one dimensional problem involves
c  only the x subscript. All other subscripts are one.*****
      do 10 j = 1, nx
          ut(1,j,1,1,1)=0.005*uxx(1,j,1,1,1)
      10 continue
c***This form is indicated to CTCN by setting ix to be greater than
c  npde*****
      ix = 4
c *****end of problem specific part*****
      return
      end

```

Step 4 : When the equations involve the derivative of a flux function, that function should be defined in subroutine FUNC to retain the divergence form of the equations in the discretizations. These terms can also optionally be differenced by directional differencing. Subroutine FUNC defines four flux terms so as to provide the first derivative with respect to each of the axes. These terms are XF, YF, ZF and RF for the x, y, z and r axes respectively. The structure of the subroutine and the definition of the four terms are analogous with the structure of subroutine EQN and the definition of the time derivatives in it. Again, we may use subroutine FUNC in the same two forms as subroutine EQN except that then CTCN's directional differencing option may not be used to difference the flux terms. For this example we do not use a flux term.

```

      subroutine func(xf,yf,zf,rf,u,ux,uy,uz,ur,uxx,uyy,uzz,urr,t,x,y,z
&      ,r,ix,npde)
      real xf(npde),yf(npde),zf(npde),rf(npde),u(npde),ux
&      (npde),uy(npde),uz(npde),ur(npde),uxx(npde),uyy
&      (npde),uzz(npde),urr(npde),t,x,y,z,r,v,p
      integer ix,npde
      c *****modify this part for the specific problem*****
      c      no flux term
      c *****end of problem-specific part*****
      return
      end

```

Step 5: When the boundary conditions are not defined in subroutine EQN using the second form (define the equations at all grid points in one call), the user must set them in subroutine BOUND. This is done by giving values to the variable B. As mentioned earlier, the general form of the boundary conditions is,

$$a_1 u_1 + b_1 \frac{\partial u_1}{\partial x} = c_1$$

for the x-axis and analogously for the other axes. Thus the variable B is an array consisting of $3 \times 2 \times 4 \times \text{NPDE}$ elements since there are four axes with two boundaries each and three coefficients (a, b and c) for each dependent variable (=NPDE dependent variables) at each boundary. Of these elements we define only the ones relevant to the problem, i.e. for a one-dimensional problem we define only those concerned with the two x-boundaries. If the actual boundary condition is to be enforced at infinity, it is frequently more useful to not impose a boundary condition at an artificially large distance in the grid but to allow cubic interpolation

at that boundary. This option is chosen by setting the coefficients (a, b and c) to zero. We make use of this option for our problem at the boundary $x = 0.2$. Thus for our problem the subroutine BOUND looks as follows,

```

subroutine bound(u,b,x,y,z,r,t)
integer npde
include 'inc.for'
real u(npde),b(npde,24),x,y,z,r,t
c This subroutine defines the boundary conditions -  $a*u + b*$ 
c  $(du/dn) = c$ .  $du/dn$  is the outward normal derivative at the
c boundary. a,b,c are functions of x,y,z,r,t,u(i).
c The a,b and c values are entered in variable b in this way:
c b(i,1), b(i,2) and b(i,3) --> a,b and c at  $x=x(1)$  for the i-th component
c b(i,4), b(i,5) and b(i,6) --> a,b and c at  $x=x(nx)$  for the i-th "
c b(i,7) , b(i,8) and b(i,9) --> a,b and c at  $y=y(1)$  for the i-th "
c b(i,10) , b(i,11) and b(i,12) --> a,b and c at  $y=y(ny)$  for the i-th "
c b(i,13) , b(i,14) and b(i,15) --> a,b and c at  $z=z(1)$  for the i-th "
c b(i,16) , b(i,17) and b(i,18) --> a,b and c at  $z=z(nz)$  for the i-th "
c b(i,19) , b(i,20) and b(i,21) --> a,b and c at  $r=r(1)$  for the i-th "
c b(i,22) , b(i,23) and b(i,24) --> a,b and c at  $r=r(nr)$  for the i-th "
c CAUTION: Enter all values of b. Default values are not zero!
c*****begin problem-specific part. set values for b.*****
c at  $x=0$ ,
c  $u(1) = 1$ 
      b(1,1)=1.0
      b(1,2)=0.0
      b(1,3)=1.0

```

```

c at x=1.0,
c At x = infinity, u = 0.
b(1,1)=0.0
b(1,2)=0.0
b(1,3)=0.0
c*****end problem-specific part*****
return
end

```

Step 6: Modify the block data module BDAT. There is only one line that needs modification and that is the data statement for variable METH. It must be made dimensionally consistent with METH in the main program. As explained before, for this problem METH has dimension 12. Therefore, our modification is,

```

DATA METH/12 * 0/

```

We now give a complete listing of the file USER.F for the first example problem. Comment lines are *italicized*. Actual Fortran code is in plain type and the problem-specific parts of this code are in **bold type**. Modifications are preceded by asterisks in the comment lines.

3.1.1. Code Listing for example 1

```

program user
c This program interfaces with CTCN to solve systems of coupled, nonlinear
c differential systems of upto second order in upto four spatial axes and first
c order in time. Thus we solve for u(i,j,k,l,m) where,
c         i = 1 to npde (number of PDEs)
c         j = 1 to nx (number of points in the x axis)
c         k = 1 to ny (number of points in the y axis)
c         l = 1 to nz (number of points in the z axis)

```

```

c          m = 1 to nr (number of points in the r axis)
c The problem should be set up so that the axes are used in the order x,y,z,r.
c thus, a 1-dimensional problem MUST use the x-axis only. A 2-D problem
c must use the x and y as principal axes (not x & z or y & r or y & z etc.).
c Thus for a two dimensional 10 x 61 grid, nr=nz=1, nx=61 , ny=10.
c The basic problem parameters are defined in this main program. The eqn.s
c are written out in subroutine eqn, the boundary conditions in subroutine
c bound and flux terms in subroutine func. Boundary conditions may be of
c the general form, -->  $a*u + b*(du/dn) = c$  --> a,b and c are functions of the
c spatial coordinates,time and other u variables. du/dn is the derivative
c normal to the boundary. Boundary conditions need not be specified at all,
c in which case a cubic extrapolation technique is used.
c For some problems it may be desirable to difference certain terms by
c skewed differences by considering the variation with u of the terms to be
c differenced. in this case, these terms may be entered using subroutine
c func and the appropriate differencing method selected. See subroutine
c func for further details.
c Thus, to solve any given system, the user needs to modify this program
c and include file INC.FOR.
c Include file 'inc.for' sets up the dimensions.
      integer npde,nx,ny,nz,nr,meth,idim
      include 'inc.for'
      double precision u(npde,nx,ny,nz,nr),tol,dx,dy,dz,dr,du,x,y,z,r
      common /c1/ tol,dx,dy,dz,dr,du
      common /c6/ x(nx),y(ny),z(nz),r(nr)
      common /c7/ idim,meth(npde,12)
c This is the user-defined program specific to a particular problem
c and sets up parameters for CTCN.
c tout(i)---> array of output times. nout=i
c tint---> initial value for time.
c tlast---> final value of t. Integration is done upto tlast.
c rtol---> relative tolerance for the ODE integrator.
c atol---> absolute tolerance for the ODE integrator. Can be a vector
c defined for each ODE, if so, set itol(below)=2.
c *****this is where the modifications begin*****
c ***** modification**** dimension tout*****

```

```

double precision tout(1),tint,tlast,rtol,atol
c   nout---> no. of output times. Dimension of the tout array.
c   mf---> ODE integration method flag, the solver LSODPK is used.
c   itol---> 1 or 2 accordingly as atol is a scalar or a vector.
integer nout,mf,itol
c Bdat is the block data subprogram at the end of this file.
external bdat
c Integration starts from t=tint
c ***modification***set tint****
tint=0.d0
c Enter array of times when output is required.
c****modification*****set tout(nout)=*****
tout(1)=5.d0
c Integration stops at t=tlast.
c*****modification*****set tlast*****
tlast=5.d0
c The number of output times=array size for tout=nout
c *****modification*****set nout*****
nout=1
c Itol,rtol and atol are used to specify error tolerances for LSODPK-the ODE
c integrator.
c****modifications****set itol,rtol and atol*****
itol=1
rtol=1.d-4
atol=1.d-6
c ode solvers require an ODE integration flag
c   for LSODPK solver           = mf = 22 for stiff problems, &
c                               = 10 for non-stiff problems.
c*****modification*****set mf*****
mf=22
c The type of differencing for each term is indicated by meth.
c   meth(i,1)= flag for ur(i), i.e. du/dr for the i-th pde.
c   meth(i,2)= flag for urr(i), i.e. d2u/dr2 for the i-th pde.
c   meth(i,3)= flag for fr(i), i.e. d(rf)/dr for the i-th pde.
c   meth(i,4)= flag for uz(i), i.e. du/dz for the i-th pde.
c   meth(i,5)= flag for uzz(i), i.e. d2u/dz2 for the i-th pde.

```



```

c  meth(i,6)= flag for fz(i), i.e. d(zf)/dz for the i-th pde.
c  meth(i,7)= flag for uy(i), i.e. du/dy for the i-th pde.
c  meth(i,8)= flag for uyy(i), i.e. d2u/dy2 for the i-th pde.
c  meth(i,9)= flag for fy(i), i.e. d(yf)/dy for the i-th pde.
c  meth(i,10)= flag for ux(i), i.e. du/dx for the i-th pde.
c  meth(i,11)= flag for uxx(i), i.e. d2u/dx2 for the i-th pde.
c  meth(i,12)= flag for fx(i), i.e. d(xf)/dx for the i-th pde.
c  if meth(*,*) = 2 ---> second order centered differences
c          = 4 ---> fourth order centered differences
c          = -2 ---> second order skewed differences
c          ( only for flux terms written into rf,zf,yf,xf )
c          = -4 ---> third order skewed differences
c          ( only for flux terms written into rf,zf,yf,xf )
c  Default value = 0
c*****modification(s)*****set meth ( *, *) *****
      meth(1,11)=2
c Enter the axes grid sizes, default = 1.d0. dr=delta(r),...etc.
c*****modification(s)*****enter grid sizes****
      dx=1.d0/dble(nx-1)
c Enter grid point values.Input r(i)--> grid points on r axis....etc.
c*****modification(s)*****enter grid values*****
      do 20 j =1,nx
        x(j)=(j-1)*dx
c Enter initial conditions. no default values.
c*****modifications*****enter initial conditions*****
      u(1,j,1,1,1)=0.D0
20 continue
c Call the interfacing subroutine CTCN
      call face(u,rtol,atol,tint,tlast,tout,nout,mf,itol)
      stop
      end

      subroutine eqn(ut,u,ux,uy,uz,ur,uxx,uyy,uzz,urr,fx,fy,fz,fr,t,x,y
&      ,z,r,ix)
c This subroutine is used to enter the PDEs
      integer ix,npde

```

```

include 'inc.for'
c *****optional modifications*****change dimension statement if the
c second form of subroutine EQN is to be used*****
double precision ut(npde),u(npde),ux(npde),uy(npde),uz(npde),ur
&      (npde),uxx(npde),uyy(npde),uzz(npde),urr(npde),
&      fx(npde),fy(npde),fz(npde),fr(npde),t,x,y,z,r
c Input the PDEs in the form ut(i)=f(u(i),x,y,z,r,t,ux(i),uy(i),uz(i),ur(i)
c ,uxx(i),uyy(i),uzz(i),urr(i),fx(i),fy(i),fz(i),fr(i)
c*****modifications*****problem specific equations****
ut(1)=5.d-3*uxx(1)
return
end

subroutine func(xf,yf,zf,rf,u,ux,uy,uz,ur,uxx,uyy,uzz,urr,t,x,y,z
&      ,ix,npde)
c This subroutine defines flux terms for which it is desirable that they be
c differenced as a whole, using centered or skewed differences. Four flux
c terms are defined corresponding to the four axes so that it is possible
c to calculate their first derivatives with respect to the corresponding axes.
c *****optional modifications*****change dimension statement if the
c second form of subroutine func is to be used*****
double precision xf(npde),yf(npde),zf(npde),rf(npde),u(npde),ux
&      (npde),uy(npde),uz(npde),ur(npde),uxx(npde),uyy
&      (npde),uzz(npde),urr(npde),t,x,y,z,r
integer ix,npde
c*****modifications*****enter flux terms for the problem*****
c      no flux term
return
end

subroutine bound(u,b,x,y,z,r,t)
c This subroutine defines the boundary conditions -  $a*u + b*(du/dn) = c$ 
c  $a,b,c$  are functions of  $x,y,z,r,t,u(i)$ .  $du/dn$  is the normal derivative at
c the boundary.
c The  $a,b$  and  $c$  values are entered in variable  $b$  in the following way:
c  $b(i,1)$  ,  $b(i,2)$  and  $b(i,3)$  --->  $a,b$  and  $c$  at  $x=x(1)$  for the  $i$ -th component

```

```

c b(i,4) , b(i,5) and b(i,6) ---> a,b and c at x=x(nx) for the i-th component
c b(i,7) , b(i,8) and b(i,9) ---> a,b and c at y=y(1) for the i-th component
c b(i,10) , b(i,11) and b(i,12) ---> a,b and c at y=y(ny) for the i-th component
c b(i,13) , b(i,14) and b(i,15). ---> a,b and c at z=z(1) for the i-th component
c b(i,16) , b(i,17) and b(i,18) ---> a,b and c at z=z(nz) for the i-th component
c b(i,19) , b(i,20) and b(i,21) ---> a,b and c at r=r(1) for the i-th component
c b(i,22) , b(i,23) and b(i,24) ---> a,b and c at r=r(nr) for the i-th component
c CAUTION: Enter all values of b. Default values are not zero!
integer npde
include 'inc.for'
double precision u(npde),b(npde,24),x,y,z,r,t
c****modification(s)*****enter boundary conditions*****
c at x=0,
c      u(1) = 1
c      b(1,1)=1.d0
c      b(1,2)=0.d0
c      b(1,3)=1.d0
c at x= 0.2,
c      At infinity , u(1) = 0.
c      b(1,4)=0.d0
c      b(1,5)=0.d0
c      b(1,6)=0.d0
c      return
c      end

block data bdat
integer npde,nx,ny,nz,nr,meth,idim,mff
include 'inc.for'
c Include file dims.h sets up all the common blocks.
include 'dims.h'
c****modification***make number of zeros in data statement consistent
with
c      dimensioning of meth for this problem*****
c      data meth/12*0/
c      end

```

File 'inc.for' : parameter(npde=1,nx=51,ny=1,nz=1,nr=1)

Example Problem 1 : Conduction In a Semi-Infinite Medium

3.2. Example 2 :Three-dimensional Fracture Problem

The system consists of a narrow rectangular fracture which contains colloids of various sizes flowing in groundwater at a certain velocity. The colloids are instantly adsorbed into the rock matrix on coming in contact with it. In the principal flow direction, the transport is dominated by the convection term while in the other direction, diffusion is the dominant process. Since the diffusivity is a function of particle size, the PSD (particle size distribution) at the outlet is very different from the PSD at the inlet.

For this example, we are taking a very idealized boundary condition (instantaneous adsorption) and neglecting effects like agglomeration, birth, death, etc. However, as can be seen, these terms are very easily incorporated into this example.

The equation is,

$$\frac{\partial u}{\partial t} = -v_{av} \left(1 - \left(\frac{y}{\delta} \right)^2 \right) \frac{\partial u}{\partial x} + D_x \frac{\partial^2 u}{\partial x^2} + D_y \frac{\partial^2 u}{\partial y^2}$$

The velocity profile above can be derived for a rectangular fracture. Here v_{av} (average velocity) = $2/3 v_{max}$ (maximum velocity). The parameters for the simulation are taken from Rundberg's report (Rundberg et al. 1988).

$$v_{\max} = 0.0024 \text{ cm/s}$$

$$D_x = 0.0011 \text{ cm}^2/\text{s}$$

$$\delta = \text{half-width of the fracture} = 0.0295 \text{ cm}$$

$$\text{Length of fracture} = 12 \text{ cm.}$$

Assuming spherical particles and substituting values for water at 20 °C into the Stokes-Einstein equation, we get

$$D_y = \frac{2.13 \times 10^{-9}}{\text{radius (in microns)}} \text{ cm}^2/\text{s}$$

If we were to include aggregation and other processes, we would use another axis as the size axis. This procedure will be followed here also since it makes data interpretation easier. Thus we have three independent axes. We will use a grid of 11 x 11 x 41 (NX x NY x NZ) where, as indicated in the previous example, we must use the axes as follows,

X —> Size axis. We use a logarithmic scaling from 1 nm to 1 μ.

Thus, $X = \ln(r / 1\mu) / \ln(1\text{nm} / 1\mu)$ where r is the radius of the particle.

Y —> Width of the fracture, $0 \leq Y \leq 0.0259 \text{ cm.}$

Z —> Length of the fracture, $0 \leq X \leq 12 \text{ cm.}$

Initial Conditions : $u = 0$

Boundary Conditions :

at X = 0,	no boundary condition imposed	(size axis).
at X = 1,	no boundary condition imposed	(size axis).
at Y = 0,	$\partial u / \partial y = 0$	(symmetry).
at Y = 0.0295,	$u = 0$	(instant adsorption).
at Z = 0,	$u = 1.0$	(input PSD).
at Z = 12,	$u = 0$ at Z = infinity.	

We seek a solution at $t = 4000 \text{ s.}$ Other simulations in two dimensions (taking particles of one particular size and considering a variety of boundary

conditions at the tuff) for unsaturated and saturated flows have been performed using CTCN.

3.2.1. Code listing for example 2

program user

*c This program interfaces with CTCN to solve systems of coupled, nonlinear
c differential systems of upto second order in upto four spatial axes and first
c order in time. Thus we solve for $u(i,j,k,l,m)$ where,*

c $i = 1$ to npde (number of PDEs)

c $j = 1$ to nx (number of points in the x axis)

c $k = 1$ to ny (number of points in the y axis)

c $l = 1$ to nz (number of points in the z axis)

c $m = 1$ to nr (number of points in the r axis)

c The problem should be set up so that the axes are used in the order x,y,z,r.

c thus, a 1-dimensional problem MUST use the x-axis only. A 2-D problem

c must use the x and y as principal axes (not x & z or y & r or y & z etc.).

c Thus for a two dimensional 10 x 61 grid, nr=nz=1, nx=61 , ny=10.

c The basic problem parameters are defined in this main program. The eqn.s

c are written out in subroutine eqn, the boundary conditions in subroutine

c bound and flux terms in subroutine func. Boundary conditions may be of

c the general form, $--> a*u + b*(du/dn) = c$ $--> a,b$ and c are functions of the

c spatial coordinates,time and other u variables. du/dn is the derivative

c normal to the boundary. Boundary conditions need not be specified at all,

c in which case a cubic extrapolation technique is used.

c For some problems it may be desirable to difference certain terms by

c skewed differences by considering the variation with u of the terms to be

c differenced. in this case, these terms may be entered using subroutine

c func and the appropriate differencing method selected. See subroutine

c func for further details.

c Thus, to solve any given system, the user needs to modify this program

c and include file INC.FOR.

c Include file 'inc.for' sets up the dimensions.

integer npde,nx,ny,nz,nr,meth,idim

include 'inc.for'

double precision u(npde,nx,ny,nz,nr),tol,dx,dy,dz,dr,du,x,y,z,r

```

common /c1/ tol,dx,dy,dz,dr,du
common /c6/ x(nx),y(ny),z(nz),r(nr)
common /c7/ idim,meth(npde,12)
c This is the user-defined program specific to a particular problem
c and sets up parameters for CTCN.
c   tout(i)---> array of output times. nout=i
c   tint---> initial value for time.
c   tlast---> final value of t. Integration is done upto tlast.
c   rtol---> relative tolerance for the ODE integrator.
c   atol---> absolute tolerance for the ODE integrator. Can be a vector
c           defined for each ODE, if so, set itol(below)=2.
c   *****this is where the modifications begin*****
c   ***** modification ***** dimension tout*****
double precision tout(1),tint,tlast,rtol,atol
c   nout---> no. of output times. Dimension of the tout array.
c   mf---> ODE integration method flag, the solver LSODPK is used.
c   itol---> 1 or 2 accordingly as atol is a scalar or a vector.
integer nout,mf,itol
c Bdat is the block data subprogram at the end of this file.
external bdat
c Integration starts from t=tint
c   ***modification***set tint***
tint=0.d0
c Enter array of times when output is required.
c***modification*****set tout(nout)=*****
tout(1)=4.d3
c Integration stops at t=tlast.
c***modification*****set tlast*****
tlast=4.d3
c The number of output times=array size for tout=nout
c   *****modification*****set nout*****
nout=1
c Itol,rtol and atol are used to specify error tolerances for LSODPK-the ODE
c integrator.
c***modifications****set itol,rtol and atol*****
itol=1

```



```

      rtol=1.d-4
      atol=1.d-6
c ode solvers require an ODE integration flag
c   for LSODPK solver      = mf = 22 for stiff problems, &
c                           = 10 for non-stiff problems.
c*****modification*****set  mf*****
      mf=22
c The type of differencing for each term is indicated by meth.
c   meth(i,1)= flag for ur(i), i.e. du/dr for the i-th pde.
c   meth(i,2)= flag for urr(i), i.e. d2u/dr2 for the i-th pde.
c   meth(i,3)= flag for fr(i), i.e. d(rf)/dr for the i-th pde.
c   meth(i,4)= flag for uz(i), i.e. du/dz for the i-th pde.
c   meth(i,5)= flag for uzz(i), i.e. d2u/dz2 for the i-th pde.
c   meth(i,6)= flag for fz(i), i.e. d(zf)/dz for the i-th pde.
c   meth(i,7)= flag for uy(i), i.e. du/dy for the i-th pde.
c   meth(i,8)= flag for uyy(i), i.e. d2u/dy2 for the i-th pde.
c   meth(i,9)= flag for fy(i), i.e. d(yf)/dy for the i-th pde.
c   meth(i,10)= flag for ux(i), i.e. du/dx for the i-th pde.
c   meth(i,11)= flag for uxx(i), i.e. d2u/dx2 for the i-th pde.
c   meth(i,12)= flag for fx(i), i.e. d(xf)/dx for the i-th pde.
c   if meth(*,*) = 2 ---> second order centered differences
c                       = 4 ---> fourth order centered differences
c                       = -2 ---> second order skewed differences
c                           ( only for flux terms written into rf,zf,yf,xf )
c                       = -4 ---> third order skewed differences
c                           ( only for flux terms written into rf,zf,yf,xf )
c   Default value = 0
c*****modification(s)*****set meth ( *, *) *****
      meth(1,4)=2
      meth(1,5)=2
      meth(1,8)=2
c Enter the axes grid sizes, default = 1.d0. dr=delta(r),...etc.
c*****modification(s)*****enter grid sizes*****
      dx=1.d0/dble(nx-1)
      dy=2.95d-2/dble(ny-1)
      dz=1.2d1/dble(nz-1)

```

c Enter grid point values. Input r(i)--> grid points on r axis....etc.

*c*****modification(s)*****enter grid values******

do 10 i=1,nx

x(i)=(i-1)*dx

10 continue

do 20 i=1,ny

y(i)=(i-1)*dy

20 continue

do 30 i=1,nz

z(i)=(i-1)*dz

30 continue

c Enter initial conditions. no default values.

*c*****modifications*****enter initial conditions******

do 50 l=1,nz

do 50 k=1,ny

do 50 j=1,nx

u(1,j,k,l,1)=0.D0

50 continue

c Call the interfacing subroutine CTCN

call face(u,rtol,atol,tint,tlast,tout,nout,mf,itol)

stop

end

subroutine eqn(ut,u,ux,uy,uz,ur,uxx,uyy,uzz,urr,fx,fy,fz,fr,t,x,y

& ,z,r,ix)

c This subroutine is used to enter the PDEs

integer ix,npde

include 'inc.for'

*c *****optional modifications*****change dimension statement if the*

*c second form of subroutine EQN is to be used******

double precision ut(npde),u(npde),ux(npde),uy(npde),uz(npde),ur

& (npde),uxx(npde),uyy(npde),uzz(npde),urr(npde),

& fx(npde),fy(npde),fz(npde),fr(npde),t,x,y,z,r

c Input the PDEs in the form ut(i)=f(u(i),x,y,z,r,t,ux(i),uy(i),uz(i),ur(i)

c ,uxx(i),uyy(i),uzz(i),urr(i),fx(i),fy(i),fz(i),fr(i)

*c*****modifications*****problem specific equations******

```

ut(1) = - 2.4d-3*(1.d0-(y/2.95d-2)**2)*uz(1)+1.1d-3*uzz(1)+2.13d-9/
&      (exp(x*6.90776) *1.d-3)*uyy(1)
c**** 6.90776 = ln ( 1 micron / 1 nm ) = ln (1000) ****
return
end

```

```

subroutine func(xf,yf,zf,rf,u,ux,uy,uz,ur,uxx,uyy,uzz,urr,t,x,y,z
&      ,ix,npde)
c This subroutine defines flux terms for which it is desirable that they be
c differenced as a whole, using centered or skewed differences. Four flux
c terms are defined corresponding to the four axes so that it is possible
c to calculate their first derivatives with respect to the corresponding axes.
c *****optional modifications*****change dimension statement if the
c second form of subroutine func is to be used*****
double precision xf(npde),yf(npde),zf(npde),rf(npde),u(npde),ux
&      (npde),uy(npde),uz(npde),ur(npde),uxx(npde),uyy
&      (npde),uzz(npde),urr(npde),t,x,y,z,r
integer ix,npde
c*****modifications*****enter flux terms for the problem*****
return
end

```

```

subroutine bound(u,b,x,y,z,r,t)
c This subroutine defines the boundary conditions -  $a*u + b*(du/dn) = c$ 
c  $a,b,c$  are functions of  $x,y,z,r,t,u(i)$ .  $du/dn$  is the normal derivative at
c the boundary.
c The  $a,b$  and  $c$  values are entered in variable  $b$  in the following way:
c  $b(i,1)$  ,  $b(i,2)$  and  $b(i,3)$  --->  $a,b$  and  $c$  at  $x=x(1)$  for the  $i$ -th component
c  $b(i,4)$  ,  $b(i,5)$  and  $b(i,6)$  --->  $a,b$  and  $c$  at  $x=x(nx)$  for the  $i$ -th component
c  $b(i,7)$  ,  $b(i,8)$  and  $b(i,9)$  --->  $a,b$  and  $c$  at  $y=y(1)$  for the  $i$ -th component
c  $b(i,10)$  ,  $b(i,11)$  and  $b(i,12)$  --->  $a,b$  and  $c$  at  $y=y(ny)$  for the  $i$ -th component
c  $b(i,13)$  ,  $b(i,14)$  and  $b(i,15)$  --->  $a,b$  and  $c$  at  $z=z(1)$  for the  $i$ -th component
c  $b(i,16)$  ,  $b(i,17)$  and  $b(i,18)$  --->  $a,b$  and  $c$  at  $z=z(nz)$  for the  $i$ -th component
c  $b(i,19)$  ,  $b(i,20)$  and  $b(i,21)$  --->  $a,b$  and  $c$  at  $r=r(1)$  for the  $i$ -th component
c  $b(i,22)$  ,  $b(i,23)$  and  $b(i,24)$  --->  $a,b$  and  $c$  at  $r=r(nr)$  for the  $i$ -th component
c CAUTION: Enter all values of  $b$ . Default values are not zero!

```

```

integer npde
include 'inc.for'
double precision u(npde),b(npde,24),x,y,z,r,t
c****modification(s)*****enter boundary conditions*****
c at x=0,
c   no boundary condition imposed
b(1,1)=0.d0
b(1,2)=0.d0
b(1,3)=0.d0
c at x=1,
c   no boundary condition imposed
b(1,4)=0.d0
b(1,5)=0.d0
b(1,6)=0.d0
c at y=0,
c    $\partial (u(1)) / \partial y = 0$ 
b(1,7)=0.d0
b(1,8)=1.d0
b(1,9)=0.d0
c at y= 0.0295 ,
c    $u(1) = 0$ 
b(1,10)=1.d0
b(1,11)=0.d0
b(1,12)=0.d0
c at z=0,
c   enter the input psd as a function of size(=x).  $u = \text{function}(x)$ 
b(1,13)=1.d0
b(1,14)=0.d0
b(1,15)=1.d0
c at z=12,
c   boundary condition at infinity
b(1,16)=0.d0
b(1,17)=0.d0
b(1,18)=0.d0
return
end

```

```

block data bdat
  integer npde,nx,ny,nz,nr, meth,idim,mff
  include 'inc.for'
c Include file dims.h sets up all the common blocks.
  include 'dims.h'
c***modification***make number of zeros in data statement consistent
with
c   dimensioning of meth for this problem*****
  data meth/12*0/
end

```

Include file 'inc.for' : **parameter(npde=1, nx=11, ny=11, nz=41, nr=1)**

Output for Example Problem 2

4.0. TEST CASES

4.1. Simple ODE

This is a simple ordinary differential equation of the form,

$$du / dt = -u .$$

The dimensionality of this problem is zero. The initial condition is taken to be, $u_0 = 1.0$. The analytical solution is $u = u_0 \exp(-t)$.

Code listing for the problem is given below. The comment lines have been omitted and the modifications are in bold type. This will be the format for all test case listings.

File 'user.for'

```
program user
  integer npde,nx,ny,nz,nr,meth,idim
  include 'inc.for'
  double precision u(npde,nx,ny,nz,nr),tol,dx,dy,dz,dr,du,x,y,z,r
  common /c1/ tol,dx,dy,dz,dr,du
  common /c6/ x(nx),y(ny),z(nz),r(nr)
  common /c7/ idim,meth(npde,12)
  double precision tout(11),tint,tlast,rtol,atol
  integer nout,mf,itol
  external bdat
  tint=0.d0
  do 10 i=1,11
    tout(i)=1.d-1*(i-1)
10  continue
  tlast=tout(11)
  nout=11
  itol=1
  rtol=1.d-7
  atol=1.d-9
  mf=22
  u(1,1,1,1,1)=1.D0
  call face(u,rtol,atol,tint,tlast,tout,nout,mf,itol)
  stop
```

end

```
subroutine eqn(ut,u,ux,uy,uz,ur,uxx,uyy,uzz,urr,fx,fy,fz,fr,t,x,y
&      ,z,r,ix)
integer ix,npde
include 'inc.for'
double precision ut(npde),u(npde),ux(npde),uy(npde),uz(npde),ur
&      (npde),uxx(npde),uyy(npde),uzz(npde),urr(npde),
&      fx(npde),fy(npde),fz(npde),fr(npde),t,x,y,z,r
ut(1) = - u(1)
return
end
```

```
subroutine func(xf,yf,zf,rf,u,ux,uy,uz,ur,uxx,uyy,uzz,urr,t,x,y,z
&      ,r,ix,npde)
double precision xf(npde),yf(npde),zf(npde),rf(npde),u(npde),ux
&      (npde),uy(npde),uz(npde),ur(npde),uxx(npde),uyy
&      (npde),uzz(npde),urr(npde),t,x,y,z,r
integer ix,npde
return
end
```

```
subroutine bound(u,b,x,y,z,r,t)
integer npde
include 'inc.for'
double precision u(npde),b(npde,24),x,y,z,r,t
return
end
```

```
block data bdat
integer npde,nx,ny,nz,nr,meth,idim,mff
include 'inc.for'
include 'dims.h'
data meth/12*0/
end
```


Include file 'inc.for' : parameter(npde=1, nx=1, ny=1, nz=1, nr=1)

4.2. Euler Equations of Gas Dynamics (Hyman,1976)

Three variables, density, momentum and energy, of a gas are described by the following equations,

$$\frac{\partial w}{\partial t} + \frac{\partial}{\partial x} F(w) = \delta \frac{\partial^2 w}{\partial x^2} \quad \text{where} \quad w = \begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix} \quad \text{and} \quad F(w) = v w + \begin{pmatrix} 0 \\ p \\ p v \end{pmatrix}$$

Here, u_1 = mass density, u_2 = momentum, u_3 = total energy per unit volume. Therefore, v = velocity = u_2 / u_1 and p = pressure = $2/3 (u_3 - 1/2 u_1 v^2)$.

$\delta = 0.006$ = artificial dissipation coefficient.

Initial Conditions :

For $0 \leq x \leq 3/4$

$$u_1 = 1.0$$

$$u_2 = 0.0$$

$$u_3 = 1.5$$

For $3/4 \leq x \leq 2$

$$u_1 = 0.125$$

$$u_2 = 0.0$$

$$u_3 = 0.15$$

Boundary Conditions :

At both boundaries ($x = 0$ and $x = 2$), they are

$$(u_1)_x = 0, \quad u_2 = 0.0, \quad (u_3)_x = 0.$$

File 'user.for' :

```

program user
  integer npde,nx,ny,nz,nr,meth,idim
  include 'inc.for'
  double precision u(npde,nx,ny,nz,nr),tol,dx,dy,dz,dr,du,x,y,z,r
  common /c1/ tol,dx,dy,dz,dr,du
  common /c6/ x(nx),y(ny),z(nz),r(nr)
  common /c7/ idim,meth(npde,12)
  double precision tout(1),tint,tlast,rtol,atol
  integer nout,mf,itol
  external bdat
  tint=0.d0
  tout(1)=5.d-1

```

```

tlast=5.d-1
nout=1
itol=1
rtol=1.d-5
atol=1.d-7
mf=22
    meth(1,11)=2
    meth(1,12)=4
    meth(2,11)=2
    meth(2,12)=4
    meth(3,11)=2
    meth(3,12)=4
dx=2.d0/dble(nx-1)
do 10 i=1,nx
    x(i)=(i-1)*dx
10 continue
do 50 j=1,nx
    u(2,j,1,1,1)=0.D0
    if ((7.5d-1-x(j)).gt.tol) then
        u(1,j,1,1,1)=1.d0
        u(3,j,1,1,1)=1.5d0
    else
        u(1,j,1,1,1)=1.25d-1
        u(3,j,1,1,1)=1.5d-1
    endif
50 continue
    call face(u,rtol,atol,tint,tlast,tout,nout,mf,itol)
stop
end

subroutine eqn(ut,u,ux,uy,uz,ur,uxx,uyy,uzz,urr,fx,fy,fz,fr,t,x,y
&          ,z,r,ix)
integer ix,npde
include 'inc.for'
double precision ut(npde),u(npde),ux(npde),uy(npde),uz(npde),ur
&          (npde),uxx(npde),uyy(npde),uzz(npde),urr(npde),

```

```

&      fx(npde),fy(npde),fz(npde),fr(npde),t,x,y,z,r
ut(1) = - fx(1)+6.d-3*uxx(1)
ut(2) = - fx(2)+6.d-3*uxx(2)
ut(3) = - fx(3)+6.d-3*uxx(3)
return
end

```

```

subroutine func(xf,yf,zf,rf,u,ux,uy,uz,ur,uxx,uyy,uzz,urr,t,x,y,z
&      ,ix,npde)
double precision xf(npde),yf(npde),zf(npde),rf(npde),u(npde),ux
&      (npde),uy(npde),uz(npde),ur(npde),uxx(npde),uyy
&      (npde),uzz(npde),urr(npde),t,x,y,z,r
double precision v,p
integer ix,npde
v = u(2)/u(1)
p = 6.67d-1*(u(3)-5.d-1*u(1)*v*v)
xf(1)=u(2)
xf(2)=v*u(2)+p
xf(3)=v*(u(3)+p)
return
end

```

```

subroutine bound(u,b,x,y,z,r,t)
integer npde
include 'inc.for'
double precision u(npde),b(npde,24),x,y,z,r,t
b(1,1)=0.d0
b(1,2)=1.d0
b(1,3)=0.d0
b(2,1)=1.d0
b(2,2)=0.d0
b(2,3)=0.d0
b(3,1)=0.d0
b(3,2)=1.d0
b(3,3)=0.d0
b(1,4)=0.d0

```

```

b(1,5)=1.d0
b(1,6)=0.d0
b(2,4)=1.d0
b(2,5)=0.d0
b(2,6)=0.d0
b(3,4)=0.d0
b(3,5)=1.d0
b(3,6)=0.d0
return
end

```

```

block data bdat
integer npde,nx,ny,nz,nr,meth,idim,mff
include 'inc.for'
include 'dims.h'
data meth/36*0/
end

```

Include file 'inc.for' : parameter(npde=3, nx=101, ny=1, nz=1, nr=1)

Sample Output :

TIME = 0.5000000000000000

X	U(1)	U(2)	U(3)
0e+0	0.974730D+00	0.000000D+00	0.148188D+01
1e-1	0.949876D+00	0.618173D-01	0.137971D+01
2e-1	0.879697D+00	0.141869D+00	0.122416D+01
3e-1	0.795870D+00	0.224727D+00	0.105921D+01
4e-1	0.710293D+00	0.294661D+00	0.912709D+00
5e-1	0.629001D+00	0.346409D+00	0.792575D+00
6e-1	0.557051D+00	0.379321D+00	0.700354D+00
7e-1	0.503231D+00	0.395335D+00	0.639187D+00
8e-1	0.478539D+00	0.399605D+00	0.613507D+00
9e-1	0.473509D+00	0.398955D+00	0.609422D+00
1e+0	0.468591D+00	0.394974D+00	0.607552D+00
1.1e+0	0.420949D+00	0.354910D+00	0.590497D+00
1.2e+0	0.305951D+00	0.257851D+00	0.550840D+00
1.3e+0	0.241344D+00	0.203468D+00	0.527982D+00

1.4e+0	0.230482D+00	0.194366D+00	0.523904D+00
1.5e+0	0.230123D+00	0.194406D+00	0.524689D+00
1.6e+0	0.228179D+00	0.189602D+00	0.514608D+00
1.7e+0	0.146923D+00	0.264222D-01	0.196031D+00
1.8e+0	0.124988D+00	-0.805142D-05	0.149986D+00
1.9e+0	0.125000D+00	-0.481348D-11	0.150000D+00
2e+0	0.125000D+00	0.115374D-11	0.150000D+00

4.3. Reaction Diffusion Equations (Hyman, 1976)

A system of autocatalytic chemical reactions, described by Robertson, can be written in the form,

The differential equations describing the kinetics of this system are very stiff, and Robertson's model has become a standard test problem for stiff ODE methods. We modify the equations to include spatial variations and passive diffusion. The corresponding system of PDEs for these reactions is,

$$\begin{aligned} \frac{\partial u}{\partial t} &= -k_1 u + k_2 v w + d \frac{\partial^2 u}{\partial x^2} \\ \frac{\partial v}{\partial t} &= k_1 u - k_2 v w - k_3 v^2 + d \frac{\partial^2 v}{\partial x^2} \\ \frac{\partial w}{\partial t} &= k_3 v^2 + d \frac{\partial^2 w}{\partial x^2} \end{aligned}$$

where the independent variable x lies between 0 and 1, the diffusion coefficient $d = 0.1$ and $u = [A]$, $v = [B]$, and $w = [C]$ denote the concentrations of the chemical components.

Initial Conditions : $v = w = 0$ and $u = 1.5$ (for $x \geq 0.50$) and $u = 0.5$ (for $x < 0.5$).

Boundary Conditions : At both boundaries ($x = 0$ and $x = 1$), we have

$$\frac{\partial u}{\partial x} = \frac{\partial v}{\partial x} = \frac{\partial w}{\partial x} = 0$$

File 'user.for' :

```
program user
  integer npde,nx,ny,nz,nr,meth,idim
  include 'inc.for'
  double precision u(npde,nx,ny,nz,nr),tol,dx,dy,dz,dr,du,x,y,z,r
  common /c1/ tol,dx,dy,dz,dr,du
```

```

common /c6/ x(nx),y(ny),z(nz),r(nr)
common /c7/ idim,meth(npde,12)
double precision tout(5),tint,tlast,rtol,atol
integer nout,mf,itol
external bdat
tint=0.d0
  tout(1)=2.d2
  tout(2)=4.d2
  tout(3)=6.d2
  tout(4)=8.d2
  tout(5)=1.d3
tlast=1.d3
nout=5
itol=1
rtol=1.d-7
atol=1.d-9
mf=22
  meth(1,11)=2
  meth(2,11)=2
  meth(3,11)=2
dx=1.d0/dbl(nx-1)
do 10 i=1,nx
  x(i)=(i-1)*dx
10 continue
do 50 j=1,nx
  if ((5.d-1-x(j)).gt.tol) then
    u(1,j,1,1,1)=5.D-1
  else
    u(1,j,1,1,1)=1.5d0
  endif
  u(2,j,1,1,1)=0.D0
  u(3,j,1,1,1)=0.D0
50 continue
call face(u,rtol,atol,tint,tlast,tout,nout,mf,itol)
stop
end

```



```

subroutine eqn(ut,u,ux,uy,uz,ur,uxx,uyy,uzz,urr,fx,fy,fz,fr,t,x,y
&      ,z,r,ix)
integer ix,npde
include 'inc.for'
double precision ut(npde),u(npde),ux(npde),uy(npde),uz(npde),ur
&      (npde),uxx(npde),uyy(npde),uzz(npde),urr(npde),
&      fx(npde),fy(npde),fz(npde),fr(npde),t,x,y,z,r
ut(1) = -4.d-2*u(1)+1.d4*u(2)*u(3)+1.d-1*uxx(1)
ut(2) = 4.d-2*u(1)-1.d4*u(2)*u(3)-3.d7*u(2)*u(2)+1.d-1*uxx(2)
ut(3) = 3.d7*u(2)*u(2)+1.d-1*uxx(3)
return
end

```

```

subroutine func(xf,yf,zf,rf,u,ux,uy,uz,ur,uxx,uyy,uzz,urr,t,x,y,z
&      ,r,ix,npde)
double precision xf(npde),yf(npde),zf(npde),rf(npde),u(npde),ux
&      (npde),uy(npde),uz(npde),ur(npde),uxx(npde),uyy
&      (npde),uzz(npde),urr(npde),t,x,y,z,r
integer ix,npde
return
end

```

```

subroutine bound(u,b,x,y,z,r,t)
integer npde
include 'inc.for'
double precision u(npde),b(npde,24),x,y,z,r,t
c at x=0,
b(1,1)=0.d0
b(1,2)=1.d0
b(1,3)=0.d0
b(2,1)=0.d0
b(2,2)=1.d0
b(2,3)=0.d0
b(3,1)=0.d0
b(3,2)=1.d0

```

```

      b(3,3)=0.d0
c at x=1,
      b(1,4)=0.d0
      b(1,5)=0.d0
      b(1,6)=0.d0
      b(2,4)=0.d0
      b(2,5)=0.d0
      b(2,6)=0.d0
      b(3,4)=0.d0
      b(3,5)=0.d0
      b(3,6)=0.d0
      return
      end

```

```

block data bdat
  integer npde,nx,ny,nz,nr,meth,idim,mff
  include 'inc.for'
  include 'dims.h'
  data meth/36*0/
end

```

Include file 'inc.for' : parameter(npde=3, nx=8, ny=1, nz=1, nr=1)

Sample Output :

TIME = 200.00000000000000

X	U(1)	U(2)	U(3)
0e+0	0.872896D+00	0.542694D-05	0.627099D+00
1.43e-1	0.872899D+00	0.542699D-05	0.627096D+00
2.86e-1	0.872910D+00	0.542714D-05	0.627085D+00
4.29e-1	0.872927D+00	0.542739D-05	0.627068D+00
5.71e-1	0.872951D+00	0.542774D-05	0.627043D+00
7.14e-1	0.872983D+00	0.542819D-05	0.627012D+00
8.57e-1	0.873021D+00	0.542874D-05	0.626973D+00
1e+0	0.873067D+00	0.542938D-05	0.626928D+00

4.4. Elliptic Equation (Melgaard & Sincovec, 1981)

This example is an elliptic PDE that represents a parallel plate heated by a nearly oblong object. The PDE is,

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} - 6xy e^x e^y (xy + x + y - 3)$$

on the grid $0 \leq x \leq 1, 0 \leq y \leq 1$

Boundary and Initial Conditions : $u = 0$.

For this problem the steady-state solution is $3 e^x e^y (x - x^2) (y - y^2)$, which can be approximated by integrating the original problem until the time derivative is nearly zero. We choose a uniformly spaced 10×10 mesh and relative and absolute error tolerances of 10^{-6} and 10^{-8} respectively. Another run with a 20×20 mesh reduced the error by approximately 1/4th, indicating that the errors were mainly due to the spatial discretization as expected.

File 'user.for' :

```
program user
  integer npde,nx,ny,nz,nr,meth,idim
  include 'inc.for'
  double precision u(npde,nx,ny,nz,nr),tol,dx,dy,dz,dr,du,x,y,z,r
  common /c1/ tol,dx,dy,dz,dr,du
  common /c6/ x(nx),y(ny),z(nz),r(nr)
  common /c7/ idim,meth(npde,12)
  double precision tout(1),tint,tlast,rtol,atol
  integer nout,mf,itol
  external bdat
  tint=0.d0
  tout(1)=2.d0
  tlast=2.d0
  nout=1
  itol=1
  rtol=1.d-6
  atol=1.d-8
```

```

mf=22
  meth(1,8)=2
  meth(1,11)=2
dx=1.d0/dbl(nx-1)
dy=1.d0/dbl(ny-1)
do 10 i=1,nx
  x(i)=(i-1)*dx
10 continue
do 20 i=1,ny
  y(i)=(i-1)*dy
20 continue
do 50 k=1,ny
do 50 j=1,nx
  u(1,j,k,1)=0.D0
50 continue
  call face(u,rtol,atol,tint,tlast,tout,nout,mf,itol)
stop
end

```

```

subroutine eqn(ut,u,ux,uy,uz,ur,uxx,uyy,uzz,urr,fx,fy,fz,fr,t,x,y
&      ,z,r,ix)
integer ix,npde
include 'inc.for'
double precision ut(npde),u(npde),ux(npde),uy(npde),uz(npde),ur
&      (npde),uxx(npde),uyy(npde),uzz(npde),urr(npde),
&      fx(npde),fy(npde),fz(npde),fr(npde),t,x,y,z,r
ut(1) = uxx(1)+uyy(1)-6.d0*x*y*exp(x)*exp(y)*(x*y+x+y-3.d0)
return
end

```

```

subroutine func(xf,yf,zf,rf,u,ux,uy,uz,ur,uxx,uyy,uzz,urr,t,x,y,z
&      ,r,ix,npde)
double precision xf(npde),yf(npde),zf(npde),rf(npde),u(npde),ux
&      (npde),uy(npde),uz(npde),ur(npde),uxx(npde),uyy
&      (npde),uzz(npde),urr(npde),t,x,y,z,r
integer ix,npde

```

```
return
end
```

```
subroutine bound(u,b,x,y,z,r,t)
integer npde
include 'inc.for'
double precision u(npde),b(npde,24),x,y,z,r,t
c at x=0,
  b(1,1)=1.d0
  b(1,2)=0.d0
  b(1,3)=0.d0
c at x=1,
  b(1,4)=1.d0
  b(1,5)=0.d0
  b(1,6)=0.d0
c at y=0,
  b(1,7)=1.d0
  b(1,8)=0.d0
  b(1,9)=0.d0
c at y=1,
  b(1,10)=1.d0
  b(1,11)=0.d0
  b(1,12)=0.d0
return
end
```

```
block data bdat
integer npde,nx,ny,nz,nr,meth,idim,mff
include 'inc.for'
include 'dims.h'
data meth/12*0/
end
```

Include file 'inc.for' : parameter(npde=1, nx=11, ny=11, nz=1, nr=1)

4.5. Burger's Equation (Melgaard & Sincovec, 1981)

The second two-dimensional test case is the familiar Burger's Equation,

$$\frac{\partial u}{\partial t} = -u \left(\frac{\partial u}{\partial x} + \frac{\partial u}{\partial y} \right) + 0.01 \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right)$$

Initial and Boundary Conditions : $u = (1.0 + e^{x+y-t})^{-1}$.

With these conditions the solution is a straight-line wave (u is constant along $x = -y$) moving in the direction $\theta = \pi/4$. Because of this straight-line nature of the solution, we may obtain the numerical solution of this problem by determining the solution over a rectangular strip. Therefore, we choose uniformly spaced rectangular meshes with $NX = 5$, $NY = 31$ and $NX = 10$, $NY = 61$ defined over $0 \leq y \leq 1$ and $0 \leq x \leq NX/(NY - 1)$ and relative and absolute error tolerances of 10^{-5} and 10^{-7} respectively. As before, the errors were mainly due to the spatial discretization.

File 'user.for' :

```
program user
  integer npde,nx,ny,nz,nr,meth,idim
  include 'inc.for'
  double precision u(npde,nx,ny,nz,nr),tol,dx,dy,dz,dr,du,x,y,z,r
  common /c1/ tol,dx,dy,dz,dr,du
  common /c6/ x(nx),y(ny),z(nz),r(nr)
  common /c7/ idim,meth(npde,12)
  double precision tout(3),tint,tlast,rtol,atol
  integer nout,mf,itol
  external bdat
  tint=0.d0
  tout(1)=tint
  tout(i)=(i-1)*1.d-1
  tlast=5.d-1
  nout=6
  itol=1
  rtol=1.d-5
```

```

atol=1.d-7
mf=22
    meth(1,7)=2
    meth(1,8)=2
    meth(1,10)=2
    meth(1,11)=2
dx=dbl(nx/(ny-1))/dbl(nx-1)
dy=1.d0/dbl(ny-1)
    do 10 i=1,nx
        x(i)=(i-1)*dx
10 continue
    do 20 i=1,ny
        y(i)=(i-1)*dy
20 continue
    do 50 k=1,ny
        do 50 j=1,nx
            u(1,j,k,1,1)=1.d0/(1.d0+exp(x+y))
50 continue
    call face(u,rtol,atol,tint,tlast,tout,nout,mf,itol)
stop
end

subroutine eqn(ut,u,ux,uy,uz,ur,uxx,uyy,uzz,urr,fx,fy,fz,fr,t,x,y
& ,z,r,ix)
integer ix,npde
include 'inc.for'
double precision ut(npde),u(npde),ux(npde),uy(npde),uz(npde),ur
& (npde),uxx(npde),uyy(npde),uzz(npde),urr(npde),
& fx(npde),fy(npde),fz(npde),fr(npde),t,x,y,z,r
ut(1) = -u(1)*(ux(1)+uy(1))+1.d-2*(uxx(1)+uyy(1))
return
end

subroutine func(xf,yf,zf,rf,u,ux,uy,uz,ur,uxx,uyy,uzz,urr,t,x,y,z
& ,r,ix,npde)
double precision xf(npde),yf(npde),zf(npde),rf(npde),u(npde),ux

```



```

&      (npde),uy(npde),uz(npde),ur(npde),uxx(npde),uyy
&      (npde),uzz(npde),urr(npde),t,x,y,z,r
integer ix,npde
return
end

subroutine bound(u,b,x,y,z,r,t)
integer npde
include 'inc.for'
double precision u(npde),b(npde,24),x,y,z,r,t
c at x=0,
b(1,1)=1.d0
b(1,2)=0.d0
b(1,3)=1.d0/(1.d0+exp(x+y-t))
c at x=nx/(ny-1),
b(1,4)=1.d0
b(1,5)=0.d0
b(1,6)=1.d0/(1.d0+exp(x+y-t))
c at y=0,
b(1,7)=1.d0
b(1,8)=0.d0
b(1,9)=1.d0/(1.d0+exp(x+y-t))
c at y=1,
b(1,10)=1.d0
b(1,11)=0.d0
b(1,12)=1.d0/(1.d0+exp(x+y-t))
return
end

block data bdat
integer npde,nx,ny,nz,nr,meth,idim,mff
include 'inc.for'
include 'dims.h'
data meth/12*0/
end

```

Include file 'inc.for' : `parameter(npde=1, nx=10, ny=61, nz=1, nr=1)`

Sample Output :

$u = 0$ $u = 1$

4.6. Coupled System of PDEs (Melgaard & Sincovec, 1981)

The third two-dimensional case consists of two coupled, nonlinear PDEs with all three types of boundary conditions,

$$\begin{aligned}\frac{\partial u}{\partial t} &= v \left(\frac{\partial}{\partial y} \left(v \frac{\partial u}{\partial y} \right) + \frac{\partial}{\partial y} \left(u \frac{\partial v}{\partial y} \right) \right) - 3 v \frac{\partial v}{\partial x} + 4 \frac{\partial u}{\partial y} - \frac{\partial v}{\partial y} \\ \frac{\partial v}{\partial t} &= \frac{\partial}{\partial x} \left(v \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial x} \left(u \frac{\partial v}{\partial x} \right) - \frac{\partial v}{\partial y}\end{aligned}$$

on a uniform grid in the region, $0 \leq x \leq 1, 0 \leq y \leq 1$.

Initial Conditions : $u = x + y, v = 2x + 3y$.

Boundary Conditions :

At $x = 0$, $u = t + y, v = t + 3y$.

At $x = 1$, $u = t + y + 1, \partial v / \partial x = 2$.

At $y = 0$, $\partial u / \partial y = 1, v + \partial v / \partial y = t + 2x + 3$.

At $y = 1$, $u + \partial u / \partial y = t + x + 2, v = t + 2x + 3$.

Analytical Solution : $u = t + x + y, v = t + 2x + 3y$.

File user.for' :

```

program user
  integer npde,nx,ny,nz,nr,meth,idim
  include 'inc.for'
  double precision u(npde,nx,ny,nz,nr),tol,dx,dy,dz,dr,du,x,y,z,r
  common /c1/ tol,dx,dy,dz,dr,du
  common /c6/ x(nx),y(ny),z(nz),r(nr)
  common /c7/ idim,meth(npde,12)
  double precision tout(1),tint,tlast,rtol,atol
  integer nout,mf,itol
  external bdat
  tint=0.d0
  tout(1)=1.d0
  tlast=1.d0
  nout=1
  itol=1
  rtol=1.d-5
  atol=1.d-7

```

```

mf=22
  meth(1,7)=2
  meth(1,10)=2
  meth(1,11)=2
  meth(1,8)=2
  meth(2,7)=2
  meth(2,10)=2
  meth(2,11)=2
  meth(2,8)=2
dx=1.d0/dbl(nx-1)
dy=1.d0/dbl(ny-1)
do 10 i=1,nx
  x(i)=(i-1)*dx
10 continue
do 20 i=1,ny
  y(i)=(i-1)*dy
20 continue
do 50 k=1,ny
do 50 j=1,nx
  u(1,j,k,1)=x(j)+y(k)
  u(2,j,k,1)=2.d0*x(j)+3.d0*y(k)
50 continue
  call face(u,rtol,atol,tint,tlast,tout,nout,mf,itol)
stop
end

subroutine eqn(ut,u,ux,uy,uz,ur,uxx,uyy,uzz,urr,fx,fy,fz,fr,t,x,y
&      ,z,r,ix)
integer ix,npde
include 'inc.for'
double precision ut(npde),u(npde),ux(npde),uy(npde),uz(npde),ur
&      (npde),uxx(npde),uyy(npde),uzz(npde),urr(npde),
&      fx(npde),fy(npde),fz(npde),fr(npde),t,x,y,z,r
  ut(1) = u(2)*(u(1)*uyy(2)+u(2)*uyy(1)+2.d0*uy(1)*uy(2))-3.d0*u(2)*
&      ux(2)+4.d0*uy(1)-uy(2)
  ut(2) = u(1)*uxx(2)+u(2)*uxx(1)+2.d0*ux(1)*ux(2))-uy(2)

```

```

return
end

```

```

subroutine func(xf,yf,zf,rf,u,ux,uy,uz,ur,uxx,uyy,uzz,urr,t,x,y,z
&      ,ix,npde)
double precision xf(npde),yf(npde),zf(npde),rf(npde),u(npde),ux
&      (npde),uy(npde),uz(npde),ur(npde),uxx(npde),uyy
&      (npde),uzz(npde),urr(npde),t,x,y,z,r
integer ix,npde
return
end

```

```

subroutine bound(u,b,x,y,z,r,t)
integer npde
include 'inc.for'
double precision u(npde),b(npde,24),x,y,z,r,t
c at x=0,
b(1,1)=1.d0
b(1,2)=0.d0
b(1,3)=t+y
b(2,1)=1.d0
b(2,2)=0.d0
b(2,3)=t+3.d0*y
c at x=1,
b(1,4)=1.d0
b(1,5)=0.d0
b(1,6)=t+y+1.d0
b(2,4)=0.d0
b(2,5)=1.d0
b(2,6)=2.d0
c at y=0,
b(1,7)=0.d0
b(1,8)=1.d0
b(1,9)=1.d0
b(2,7)=1.d0
b(2,8)=1.d0

```

```

      b(2,9)=t+2.d0*x+3.d0
c at y=1,
      b(1,10)=1.d0
      b(1,11)=1.d0
      b(1,12)=t+x+2.d0
      b(2,10)=1.d0
      b(2,11)=0.d0
      b(2,12)=t+2.d0*x+3.d0
      return
end

```

```

block data bdat
  integer npde,nx,ny,nz,nr,meth,idim,mff
  include 'inc.for'
  include 'dims.h'
  data meth/24*0/
end

```

Include file 'inc.for' : parameter(npde=1, nx=11, ny=11, nz=1, nr=1)

Results obtained were consistent with the analytical solution.

4.7. Anisotropic Diffusion

This problem is a simple three-dimensional anisotropic diffusion equation,

$$\frac{\partial u}{\partial t} = D_x \frac{\partial^2 u}{\partial x^2} + D_y \frac{\partial^2 u}{\partial y^2} + D_z \frac{\partial^2 u}{\partial z^2}$$

on a unit cube. The diffusion coefficients may be given different values and the profiles judged accordingly.

Initial Conditions : $u = 0$ except at the center where $u = 5$.

Boundary Conditions : Homogeneous Neumann boundary conditions are imposed. At all boundaries, the outward normal derivative is zero (impermeable walls).

File 'user.for' :

```
program user
  integer npde,nx,ny,nz,nr,meth,idim
  include 'inc.for'
  double precision u(npde,nx,ny,nz,nr),tol,dx,dy,dz,dr,du,x,y,z,r
  common /c1/ tol,dx,dy,dz,dr,du
  common /c6/ x(nx),y(ny),z(nz),r(nr)
  common /c7/ idim,meth(npde,12)
  double precision tout(1),tint,tlast,rtol,atol
  integer nout,mf,itol
  external bdat
  tint=0.d0
  tout(1)=5.d0
  tlast=5.d0
  nout=1
  itol=1
  rtol=1.d-5
  atol=1.d-7
  mf=22
  meth(1,11)=2
  meth(1,5)=2
  meth(1,8)=2
```

```

dx=1.d0/dbl(nx-1)
dy=1.d0/dbl(ny-1)
dz=1.d0/dbl(nz-1)
do 10 i=1,nx
  x(i)=(i-1)*dx
10 continue
do 20 i=1,ny
  y(i)=(i-1)*dy
20 continue
do 30 i=1,nz
  z(i)=(i-1)*dz
30 continue
do 50 l=1,nz
do 50 k=1,ny
do 50 j=1,nx
  u(1,j,k,l)=0.D0
50 continue
u(1,6,6,1)=5.d0
call face(u,rtol,atol,tint,tlast,tout,nout,mf,itol)
stop
end

```

```

subroutine eqn(ut,u,ux,uy,uz,ur,uxx,uyy,uzz,urr,fx,fy,fz,fr,t,x,y
&      ,z,r,ix)
integer ix,npde
include 'inc.for'
double precision ut(npde),u(npde),ux(npde),uy(npde),uz(npde),ur
&      (npde),uxx(npde),uyy(npde),uzz(npde),urr(npde),
&      fx(npde),fy(npde),fz(npde),fr(npde),t,x,y,z,r
ut(1) = 1.d-2*uxx(1)+1.d-2*uyy(1)+1.d-2*uzz(1)
return
end

```

```

subroutine func(xf,yf,zf,rf,u,ux,uy,uz,ur,uxx,uyy,uzz,urr,t,x,y,z
&      ,r,ix,npde)
double precision xf(npde),yf(npde),zf(npde),rf(npde),u(npde),ux

```



```

&      (npde),uy(npde),uz(npde),ur(npde),uxx(npde),uyy
&      (npde),uzz(npde),urr(npde),t,x,y,z,r
integer ix,npde
return
end

```

```

subroutine bound(u,b,x,y,z,r,t)
integer npde
include 'inc.for'
double precision u(npde),b(npde,24),x,y,z,r,t
c at x=0,
  b(1,1)=0.d0
  b(1,2)=1.d0
  b(1,3)=0.d0
c at x=1,
  b(1,4)=0.d0
  b(1,5)=1.d0
  b(1,6)=0.d0
c at y=0,
  b(1,7)=0.d0
  b(1,8)=1.d0
  b(1,9)=0.d0
c at y= 1 ,
  b(1,10)=0.d0
  b(1,11)=1.d0
  b(1,12)=0.d0
c at z=0,
  b(1,13)=0.d0
  b(1,14)=1.d0
  b(1,15)=0.d0
c at z=1,
  b(1,16)=0.d0
  b(1,17)=1.d0
  b(1,18)=0.d0
return
end

```

```
block data bdat  
  integer npde,nx,ny,nz,nr,method,ndim,mff  
  include 'inc.for'  
  include 'dims.h'  
  data method/12*0/  
end
```

Include file 'inc.for' : parameter(npde=1, nx=11, ny=11, nz=11, nr=1)

Results were consistent with what would be qualitatively expected.

4.8. Lotka - Volterra Model in 3-D (Brown & Hindmarsh, 1988)

This problem is based on a reaction-diffusion system arising from a Lotka-Volterra predator-prey model, with diffusion effects in three space dimensions. There are two species variables, c^1 and c^2 representing respectively the prey and predator species densities over a spatial habitat consisting of a unit cube, and time t ranging from 0 to 10 seconds. The equations are,

$$\frac{\partial c^i}{\partial t} = d_i \Delta c^i + f(c^1, c^2) \quad (i = 1, 2)$$

$$d_1 = 0.05, \quad d_2 = 1.0$$

$$f^1(c^1, c^2) = c^1 (b_1 - a_{11} c^1 - a_{12} c^2), \quad f^2(c^1, c^2) = c^2 (b_2 - a_{21} c^1 - a_{22} c^2),$$

$$a_{11} = 10^6, \quad a_{12} = 1, \quad a_{21} = 10^6 - 1, \quad a_{22} = 10^6,$$

$$b_1 = b_2 = (1 + \alpha x y z) (10^6 - 1 + 10^{-6}).$$

Initial Conditions : $c^1(x, y, z, 0) = 500 + 250 \cos(\pi x) \cos(3\pi y) \cos(10\pi z)$

$c^2(x, y, z, 0) = 200 + 150 \cos(10\pi x) \cos(\pi y) \cos(3\pi z).$

Boundary Conditions : Homogeneous Neumann boundary conditions at all boundaries. The outward normal derivatives are zero.

The coefficients have been chosen so that as $t \rightarrow \infty$, the solution of the system approaches a steady state which is (intentionally) not flat in space. This steady state is given roughly by the asymptotic solution of the problem without diffusion, namely:

$$c^1 = (1 - 10^6) (1 + \alpha x y z), \quad c^2 = 10^{-6} (1 + \alpha x y z).$$

The two PDEs are discretized on a regular J by K by L grid. We consider $\alpha = 0$ and $\alpha = 0.2$ and vary $J = K = L$ from 6 to 20. Tolerance parameters are taken to be $RTOL = 10^{-6}$ and $ATOL = 10^{-8}$. Results were consistent with the asymptotic solution but run-times were higher since Brown and Hindmarsh tested a problem-specific code.

File 'user.for' :

```
program user
  double precision pi
  (parameter pi=4.d0*atan(1.d0))
  integer npde,nx,ny,nz,nr,meth,idim
  include 'inc.for'
  double precision u(npde,nx,ny,nz,nr),tol,dx,dy,dz,dr,du,x,y,z,r
  common /c1/ tol,dx,dy,dz,dr,du
  common /c6/ x(nx),y(ny),z(nz),r(nr)
  common /c7/ idim,meth(npde,12)
  double precision tout(1),tint,tlast,rtol,atol
  integer nout,mf,itol
  external bdat
  tint=0.d0
  tout(1)=1.d1
  tlast=1.d1
  nout=1
  itol=1
  rtol=1.d-6
  atol=1.d-8
  mf=22
  meth(1,11)=2
  meth(1,5)=2
  meth(1,8)=2
  meth(2,11)=2
  meth(2,5)=2
  meth(2,8)=2
  dx=1.d0/dble(nx-1)
  dy=1.d0/dble(ny-1)
  dz=1.d0/dble(nz-1)
  do 10 i=1,nx
    x(i)=(i-1)*dx
  10 continue
  do 20 i=1,ny
    y(i)=(i-1)*dy
  20 continue
```

```

do 30 i=1,nz
  z(i)=(i-1)*dz
30 continue
do 50 l=1,nz
do 50 k=1,ny
do 50 j=1,nx
  u(1,j,k,l,1)=5.d2+2.5d2*cos(pi*x)*cos(3.d0*pi*y)*
&      cos(1.d1*pi*z)
  u(2,j,k,l,1)=2.d2+1.5d2*cos(1.d0*pi*x)*cos(pi*y)*
&      cos(3.d0*pi*z)
50 continue
  call face(u,rtol,atol,tint,tlast,tout,nout,mf,itol)
stop
end

```

```

subroutine eqn(ut,u,ux,uy,uz,ur,uxx,uyy,uzz,urr,fx,fy,fz,fr,t,x,y
&      ,z,r,ix)
integer ix,npde
include 'inc.for'
double precision ut(npde),u(npde),ux(npde),uy(npde),uz(npde),ur
&      (npde),uxx(npde),uyy(npde),uzz(npde),urr(npde),
&      fx(npde),fy(npde),fz(npde),fr(npde),t,x,y,z,r
double precision alpha,b
alpha = 0.d0
b = (1.d0+alpha*x*y*z)*(1.d6-1.d0+1.d-6)
ut(1) = 5.d-2*(uxx(1)+uyy(1)+uzz(1))+u(1)*(b-1.d6*u(1)-u(2))
ut(2) = uxx(1)+uyy(1)+uzz(1)+u(2)*(b-(1.d6-1.d0)*u(1)-1.d6*u(2))
return
end

```

```

subroutine func(xf,yf,zf,rf,u,ux,uy,uz,ur,uxx,uyy,uzz,urr,t,x,y,z
&      ,r,ix,npde)
double precision xf(npde),yf(npde),zf(npde),rf(npde),u(npde),ux
&      (npde),uy(npde),uz(npde),ur(npde),uxx(npde),uyy
&      (npde),uzz(npde),urr(npde),t,x,y,z,r
integer ix,npde

```

```
return  
end
```

```
subroutine bound(u,b,x,y,z,r,t)  
integer npde  
include 'inc.for'  
double precision u(npde),b(npde,24),x,y,z,r,t  
c at x=0,  
    b(1,1)=0.d0  
    b(1,2)=1.d0  
    b(1,3)=0.d0  
    b(2,1)=0.d0  
    b(2,2)=1.d0  
    b(2,3)=0.d0  
c at x=1,  
    b(1,4)=0.d0  
    b(1,5)=1.d0  
    b(1,6)=0.d0  
    b(2,4)=0.d0  
    b(2,5)=1.d0  
    b(2,6)=0.d0  
c at y=0,  
    b(1,7)=0.d0  
    b(1,8)=1.d0  
    b(1,9)=0.d0  
    b(2,7)=0.d0  
    b(2,8)=1.d0  
    b(2,9)=0.d0  
c at y= 1 ,  
    b(1,10)=0.d0  
    b(1,11)=1.d0  
    b(1,12)=0.d0  
    b(2,10)=0.d0  
    b(2,11)=1.d0  
    b(2,12)=0.d0  
c at z=0,
```

```

b(1,13)=0.d0
b(1,14)=1.d0
b(1,15)=0.d0
b(2,13)=0.d0
b(2,14)=1.d0
b(2,15)=0.d0

```

```

c at z=1,
  b(1,16)=0.d0
  b(1,17)=1.d0
  b(1,18)=0.d0
  b(2,16)=0.d0
  b(2,17)=1.d0
  b(2,18)=0.d0
  return
end

```

```

block data bdat
  integer npde,nx,ny,nz,nr,meth,idim,mff
  include 'inc.for'
  include 'dims.h'
  data meth/24*0/
end

```

Include file 'inc.for' : parameter(npde=1, nx=6, ny=6, nz=6, nr=1)

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