HYDRA-3D : A MODEL FOR STUDYING HYDROGEN TRANSPORT IN CONTAINMENTS

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ABSTRACT

The development of a 3D computer code "HYDRA-3D" for studying hydrogen transport in containment systems is described in this paper. The time-dependent conservation equations for mixture mass, mixture momentum, mixture energy and species mass are solved using finite difference technique. Effects of molecular diffusion and turbulence have been taken into account. Sample calculations involving steam injection in a cubical compartment show reasonable trends in pressure and species concentrations throughout the computation domain.

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1.0 INTRODUCTION

In the case of Loss-Of-Coolant-Accident (LOCA) coincident with functional failure of Emergency-Core-Cooling-System (ECCS), the overheating of fuel cladding could lead to a rapid generation of hydrogen due to metal water reaction. In addition, radiolysis of water due to radiations from fission/decay products gradually adds hydrogen in the containment atmosphere. Beyond certain concentration limits, this hydrogen could form flammable or even explosive mixture with the containment air, leading to high pressure loads on the containment, which could jeopardize its integrity. Apart from ensuring that the global concentration of hydrogen in containment does not exceed safe limits, the possibility of high hydrogen concentration build-up in certain local pockets is also to be considered. This calls for thorough investigation of hydrogen transport phenomena.

The dynamics of hydrogen distribution depends not only on the geometry of the containment, but also on the prevailing thermodynamic conditions, which in turn are influenced by

various engineered systems. HYDRA-3D (Hydrogen Dispersion Transient Analysis in 3 Dimension) is a 3D finite-difference computer code for analysing the details of hydrogen transport throughout the containment and to evaluate the effectiveness of hydrogen management systems. This state-of-the-art computer program considers history of steam and hydrogen releases, effect of suppression pool, sub-compartmentalization, inter-compartment communication, availability of cooling and mixing devices, heat transfer to/from structures, condensation and evaporation, etc. This program uses finite-difference fluid dynamic model for solving three-dimensional time-dependent Navier-Stokes equations (i.e. conservation equations for mixture mass, momentum and energy) with species mass conservation and transport in cartesian co-ordinates. The effect of molecular diffusion and turbulence are also taken into account. The program incorporates a flexible semi-automatic noding scheme allowing three dimensional analysis of containment system. For defining flux quantities at cell boundaries, staggered grid with donor celling approach has been adopted. Each computational cell is considered to be comprised of a mixture of Steam, Hydrogen, Oxygen and Nitrogen. Mass balances are solved for each of these species providing individual mass fractions in the mixture. The governing set of non-linear finite-difference equations are solved iteratively using semi-implicit computational technique to obtain the pressure, temperature and species concentration fields throughout the computation domain.

In this paper, the mathematical model, numerical solution scheme, code structure, and the results from sample calculations are presented.

2.0 MATHEMATICAL MODEL

2.1 Nomenclature:

D_{IJ}	Binary diffusion coefficient between Species I and J
$\bar{D}$	Wall/structural drag/frictional force vector
e	Specific internal energy of gas mixture
$\bar{g}$	Body force vector
h_I	Specific enthalpy of species I
k	Apparent or total thermal conductivity of gas mixture
L	Length scale
p	Pressure
Q_t	Decay of turbulent energy to thermal energy, per unit volume and time
Q_s	Energy exchange with internal structure, per unit volume and time
Q_w	Energy exchange with walls, per unit volume and time
q_t	Turbulent kinetic energy per unit mass
$\bar{q}$	Heat flux vector
$\bar{S}$	Source term vector in governing equations
S_{en}	Energy source per unit volume and time
S_{mass}	Mass source per unit volume and time
$\bar{S}_{mom}$	Source momentum vector in governing equations
S_I =	Species mass source per unit volume and time for Ith component
T	Temperature

t	Time
$\bar{V}$	Mass average velocity of gas mixture
$\bar{U}_I$	Velocity of Species I
Y_I	Mass fraction of Species I
X_I	Mole fraction of Species I
x	X co-ordinate
$\bar{\tau}$	Nine - component viscous stress tensor
ρ_m	Density of gas mixture
μ_{eff}	Apparent or total viscosity of the gas mixture

Subscripts

I, J	Species component
i, j, k	Staggered cell index
m	mixture

Superscript

n	Time level

2.2 Conservation Equations:

The partial differential equations that express the principles of conservation of mass, momentum and energy in a Cartesian (x, y, z) co-ordinate system are presented below:

2.2.1 Mixture Mass Equation:

$$\frac{\delta \rho_m}{\delta t} + \nabla\cdot(\rho_m \bar{V}) = S_{mass,m} \qquad (1)$$

2.2.2 Mixture Momentum Equation:

$$\frac{\delta \bar{V}}{\delta t} + \bar{V}\cdot\nabla\bar{V} = -\frac{1}{\rho_m}(\nabla p) - \frac{1}{\rho_m}\nabla\cdot\bar{\tau} - \frac{\bar{D}}{\rho_m} + \bar{g} + \frac{\bar{S}_{mom}}{\rho_m} \qquad (2)$$

2.2.3 Mixture Energy Equation:

$$\frac{\delta(\rho_m e)}{\delta t} + \nabla\cdot(\rho_m \bar{V} e) = - \nabla\bar{q} - p(\nabla\cdot\bar{V}) + \rho_m(\bar{V}\cdot\bar{g}) + Q_t - Q_s - Q_w + S_{en} \quad (3)$$

2.2.4 Species Conservation Equations:

The conservation equations for the four constituents of the gas mixture, i.e., oxygen, steam, hydrogen and nitrogen, are expressed as follows :

For I = 1 to 3

$$\frac{\delta Y_I}{\delta t} + \bar{V}\cdot\nabla Y_I = \frac{S_I}{\rho_m} - \frac{1}{\rho_m}\left[\nabla\cdot(\rho_m Y_I \bar{U}_I)\right] \quad (4)$$

and, for I = 4

$$Y_I = 1 - \sum_{J=1}^{3} Y_J \quad (5)$$

2.3 Turbulence Model:

The turbulence model used here is a subgrid scale transport model as developed for the KIVA code [1,2] and utilized in the HMS-BURN Code [3]. The transport equation for the product ρ qt is given as

$$\frac{\delta(\rho_m qt)}{\delta t} + \nabla\cdot(\rho_m qt \bar{V}) = - \frac{2}{3}\rho_m qt (\nabla\cdot\bar{V}) + \bar{\tau}:\nabla\bar{V} + \nabla\cdot(\mu_{eff}\nabla qt) - \rho_m qt^{3/2} / L \quad (6)$$

To determine the species velocity, U_I, from the multi-component molecular diffusion flux, the well-known Stefan - Maxwell equation for dilute gases is utilized [4, 5] :

$$\nabla X_I = \sum_{J=1}^{3} (X_I X_J / D_{IJ})\cdot(\bar{U}_J - \bar{U}_I) \quad (7)$$

3.0 NUMERICAL SCHEME

The governing partial differential equations as described above are written in a semi-implicit finite difference form with staggered cell concept. Donor-cell or upwinding technique is invoked to express the convective terms in the staggered cell centre or face position. The non-linear terms in governing equations are linearized with Taylor series approximation and by neglecting the higher order derivatives. Flow properties in the staggered cell concept are defined at the cell faces, whereas, other intrinsic properties like pressure, temperature, species concentrations, etc. are defined at the cell centre.

With reference to Figure 1, the mixture momentum equation in the semi-implicit finite difference form at the $(i+\frac{1}{2},j,k)$ staggered cell face can be expressed as

$$(V_x)^{n+1}_{i+\frac{1}{2}} = \left[- \frac{\Delta t}{(\rho_m)^{n}_{i+\frac{1}{2}} (\Delta x)_i} \right] \cdot \left[(p)^{n+1}_{i+1} - (p)^{n+1}_{i} \right]$$

$$- (\Delta t) \cdot [V_x \cdot (\Delta V_x/\Delta x) + V_y \cdot (\Delta V_x/\Delta y) + V_z \cdot (\Delta V_x/\Delta z)]^{n}_{i+\frac{1}{2}}$$

$$- (\Delta t) \cdot (STRS)^{n}_{i+\frac{1}{2}} - (\Delta t) \cdot (D_x/\rho_m)^{n}_{i+\frac{1}{2}} + (\Delta t) \cdot (g_x)_{i+\frac{1}{2}}$$

$$+ (\Delta t) \cdot (Smom_x/\rho_m)^{n}_{i+\frac{1}{2}} + (V_x)^{n}_{i+\frac{1}{2}} \qquad (8)$$

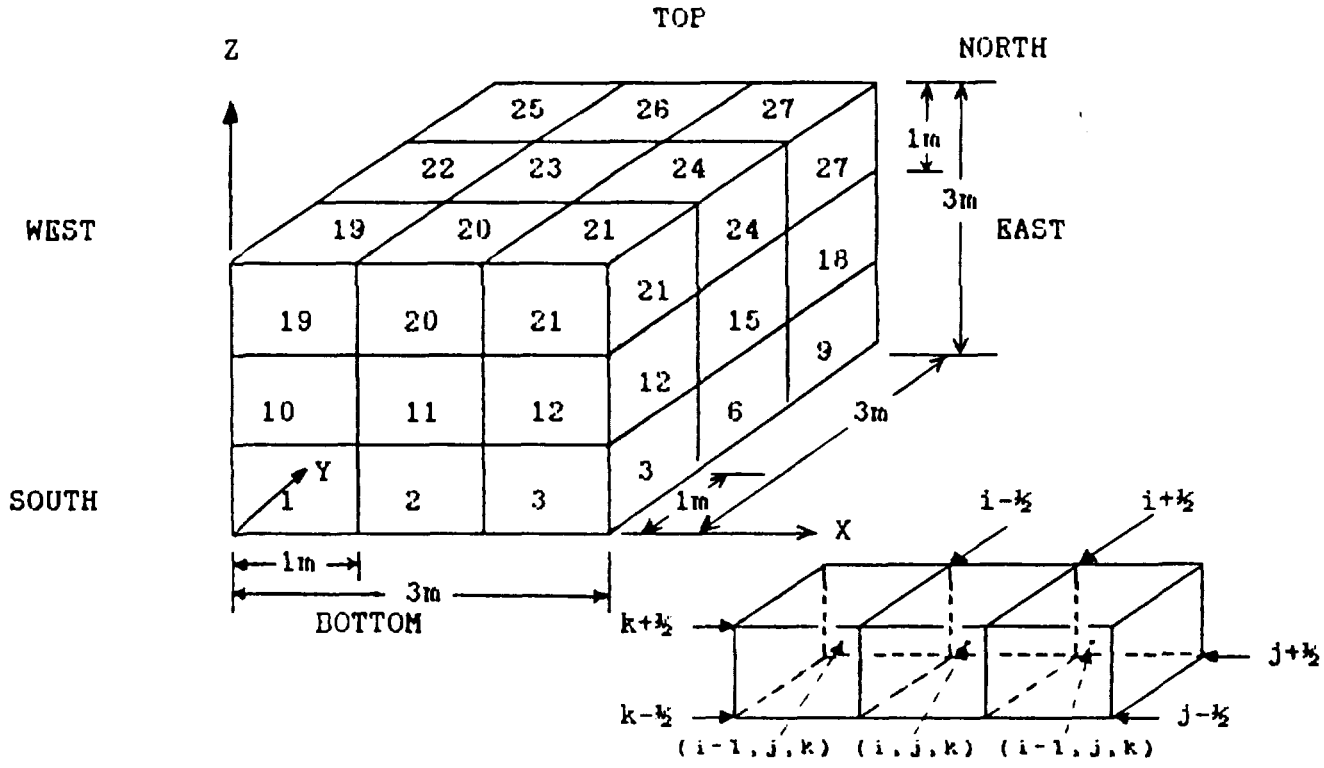

Figure 1 : Computational volume with dimensions, cell numbers, and indexing system

In other words, the above equation for velocity can be expressed as

$$(V_x)^{n+1}_{i+\frac{1}{2}} = C_1 \left[(p)^{n+1}_{i+\frac{1}{2}} - (p)^{n+1}_{i} \right] + C_2 \qquad (9)$$

The mass average velocities at other staggered cell faces are expressed in a manner similar to that described above.

The velocities so derived are than substituted in the mixture mass, mixture energy, species conservation and turbulence model equations. On linearizing the appropriate terms, the solution matrix for each computational staggered cell appears as shown below:

$$
\underset{A}{\begin{bmatrix} x & x & x & x & x & x \\ x & x & x & x & x & x \\ x & x & x & x & x & x \\ x & x & x & x & x & x \\ x & x & x & x & x & x \\ x & x & x & x & x & x \end{bmatrix}}
\begin{bmatrix} (p)^{n+1} \\ (T)^{n+1} \\ (Y_1)^{n+1} \\ (Y_2)^{n+1} \\ (Y_3)^{n+1} \\ (q_t)^{n+1} \end{bmatrix}
+ \underset{LX}{\begin{bmatrix} x \\ x \\ x \\ x \\ x \\ x \end{bmatrix}} (p)^{n+1}_{i-1}
+ \underset{LY}{\begin{bmatrix} x \\ x \\ x \\ x \\ x \\ x \end{bmatrix}} (p)^{n+1}_{j-1}
+ \underset{LZ}{\begin{bmatrix} x \\ x \\ x \\ x \\ x \\ x \end{bmatrix}} (p)^{n+1}_{k-1}
$$

$$
+ \underset{RX}{\begin{bmatrix} x \\ x \\ x \\ x \\ x \\ x \end{bmatrix}} (p)^{n+1}_{i+1}
+ \underset{RY}{\begin{bmatrix} x \\ x \\ x \\ x \\ x \\ x \end{bmatrix}} (p)^{n+1}_{j+1}
+ \underset{RZ}{\begin{bmatrix} x \\ x \\ x \\ x \\ x \\ x \end{bmatrix}} (p)^{n+1}_{k+1}
= \underset{B}{\begin{bmatrix} x \\ x \\ x \\ -x \\ x \\ x \end{bmatrix}} \qquad (10)
$$

The entire pressure matrix for the computational cells are constructed as per Equation (10) and solved by an iterative method. The pressures at new time level (n+1) are then substituted in respective balance equations to obtain other parameters such as temperature, mass fraction, turbulent kinetic energy, etc.

4.0 SOURCE CODE MODULES FOR HYDRA-3D

The source code for HYDRA-3D consists of nearly one dozen compilation units, henceforth referred to as 'modules'. Each module is, in turn, a collection of subroutines and functions, such that the routines related to each other for some specific task are kept together in a single module. The major tasks of these twelve modules are as follows:

a) Main control unit controls the entire sequence and flow of operations. Also handles computation and storage of momentum and error terms at the cell level.

b) Constructs and solves system equations at cell level. Constructs pressure matrix at grid level, solves for new parameters (pressure, temperature, mass fractions).

c) Constructs and solves species equations at cell level.

d) A sort of Memory Manager. Contains memory mapper routines between global storage of 'parameters for all cells' and global 'scratch pad' for parameters of a 'single cell'

e) Contains various routines for computation of various properties at cell level.

f) Averaging schemes for properties.

g) Schemes to compute terms which involve various derivatives.

h) Schemes to compute heat transfer terms between cells and walls.

i) Schemes to compute drag related terms in fluids.

j) Routines for dump and restart and routines for on-line display of selected parameters at cell level.

k) Schemes for semi-automatic generation of grid of cells and initialization of system parameters at cell level.

l) Schemes to read user input, such as geometrical and other data for grid generation, in a very flexible and user friendly format. An in-built lexical analyzer has been incorporated for this purpose.

5.0 SAMPLE PROBLEM

The computational domain for this test case was taken to be a cubic compartment of side 3m each. The compartment was divided into 27 cells, each of size 1m x 1m x 1m. Figure 1 shows a

schematic of the compartment geometry with relevant dimensions, and the identification number of each cell.

Steam injection into the central cell (i.e., cell No.14) was considered. It was assumed that steady state conditions prevail for the first 100 time steps (i.e., for 100 milliseconds). Steam was then injected for 400 milliseconds, from Time Step 101 to Time Step 500. Details of steam injection are as follows :

Location of injection	: Cell 14
Gas injected	: Steam
Rate of steam injection	: 1.0 kg/m^3-sec
Steady State	: Time t = 0 to t = 100 ms
Steam injection	: Time t = 100 ms to t = 500 ms
Time Step size	: 1 ms
Total time of computations	: Time t = 0 Sec to t = 1.7 sec

Relative humidity of 5% was assumed uniformly throughout the entire volume as an initial condition. Turbulence and frictional effects have not been included in this particular calculation.

Results of computation are shown in Figures 2, 3 and 4. These figures depict, respectively, the variations of pressure, temperature, and mass fraction of steam with time. Variations for these parameters are shown for Cell 14 (i.e., cell into which steam was injected), and the six surrounding Cells, i.e., Cell Nos. 5, 23, 13, 15, 11 and 17.

Variation of the pressure in Cell No.14, shown in Figure 2 (along with the pressure variations in other cells) shows that the pressure increases significantly between t = 0.1 sec and t = 0.5 sec. This is in keeping with the fact that steam was injected into this cell during this period. Between t = 0.5 and t = 0.6

sec, the increase in pressure is much less. Beyond t = 0.6 sec, the increase in pressure is negligible, and the system is seen to be moving toward equilibrium. The pressures in cells on the same horizontal level as Cell 14 equilibrate with the pressure in Cell 14 rapidly. This indicates that pressure equalization is driven by bulk movement of gases, i.e., it is controlled by convective effects.

Figure 3 shows the variation of temperature in some of the cells in which pressure variation was shown (in Figure 2). The temperature in Cell 14 is seen to rise by about 11 to 12°K for every 0.1 sec between t = 0.1 sec & t = 0.5 sec. Thereafter, the rate of increase slows down, because steam injection stops at 0.5 sec. The temperature of Cell 23 continues rising (though at a much slower rate than in Cell 14) because steam is lighter than air, and hence rises upward. Temperature in Cells 11, 13, 15 and 17 are nearly equal, because they all are situated at the same horizontal plane, and are equidistant from Cell 14.

Finally, the mass fraction of steam (refer Figure 4) increases significantly between t = 0.1 and t = 0.5 sec, and then starts decreasing. The value of the mass fraction of steam should be the same in cells at the same horizontal level when equilibrium is reached, i.e., in cells 11, 13, 14, 15 and 17. We notice that with the passage of time, the concentration of steam in Cell 23 increases, because of the upward migration of steam. Values of the concentration of steam are seen to be approaching equilibrium values in Cells 11, 13, 15 and 17. Judging by the rate of decrease of Y_{H2O} in Cell 14, it will be several seconds beyond the computed 1.7 seconds before the system reaches equilibrium.

Calculated flow circulation patterns are shown in Figures 5 and 6. The overall pattern is shown in Figure 5. For better visualization, the compartment volume has been broken up into three layers, and the flow patterns are shown in further detail in Figure 6. The flow is upward through the central cells (e.g., Cell 5 and 14), and downward through the cells on the periphery (e.g., Cells 10, 12, 16, 18). In each layer (Figure 6), there is horizontal motion between cells as indicated by the arrows. These patterns seem physically reasonable.

6.0 SUMMARY AND CONCLUSIONS

A three-dimensional code (HYDRA-3D) has been developed to study the transport of hydrogen and other gases in containment systems. The conservation equations for mixture mass, mixture momentum, mixture energy, and species mass, are discretized in a Cartesian coordinate framework. A semi-implicit finite difference scheme is used for the discretization and solution of the governing equations. Molecular diffusion and turbulence effects have been incorporated in the mathematical model. Provision has been made for four species, e.g., hydrogen, oxygen, nitrogen and steam. The code comprises of about a dozen modules, and an in-built lexical analyzer makes input file formats very flexible and user-friendly.

The code has been tested for a sample cubic compartment simulation, with steam injection for 400 milliseconds in a central cell. Results indicate reasonable trends in time-dependent variations of pressure, temperature and mass fraction

of steam throughout the computation domain. The code is currently being applied to other test cases including a prototype containment with several inter-connected rooms.

7.0 REFERENCES

[1] Amsden A.A., Ramshaw J.D., O'Rourke P.J., Dukowics J.K., "KIVA: A Computer Program for Two and Three Dimensional Fluid Flows with Chemical Reactions and Fuel Sprays", Los Alamos National Laboratory Report LA-10245-MS (1985), U.S.A.

[2] Amsden A.A., et.al., "KIVA : A Comprehensive Model for 2D and 3D Engine Simulations", SAE International Congress and Exhibition, Feb.27 - Mar 2, 1985.

[3] Travis J.R., "HMS - BURN : A model for Hydrogen Distribution and Combustion in Nuclear Reactor Containments", Los Alamos National Laboratory.

[4] Cussler E.L., "Diffusion Mass Transfer in Fluid-Systems", pp 195 - 197, Cambridge University Press, New York, 1984.

[5] Bird R.B., Stewart W.E., Lightfoot E.N., "Transport Phenomena", pp 569-571, John Wiley & Sons Inc., New York, 1960.

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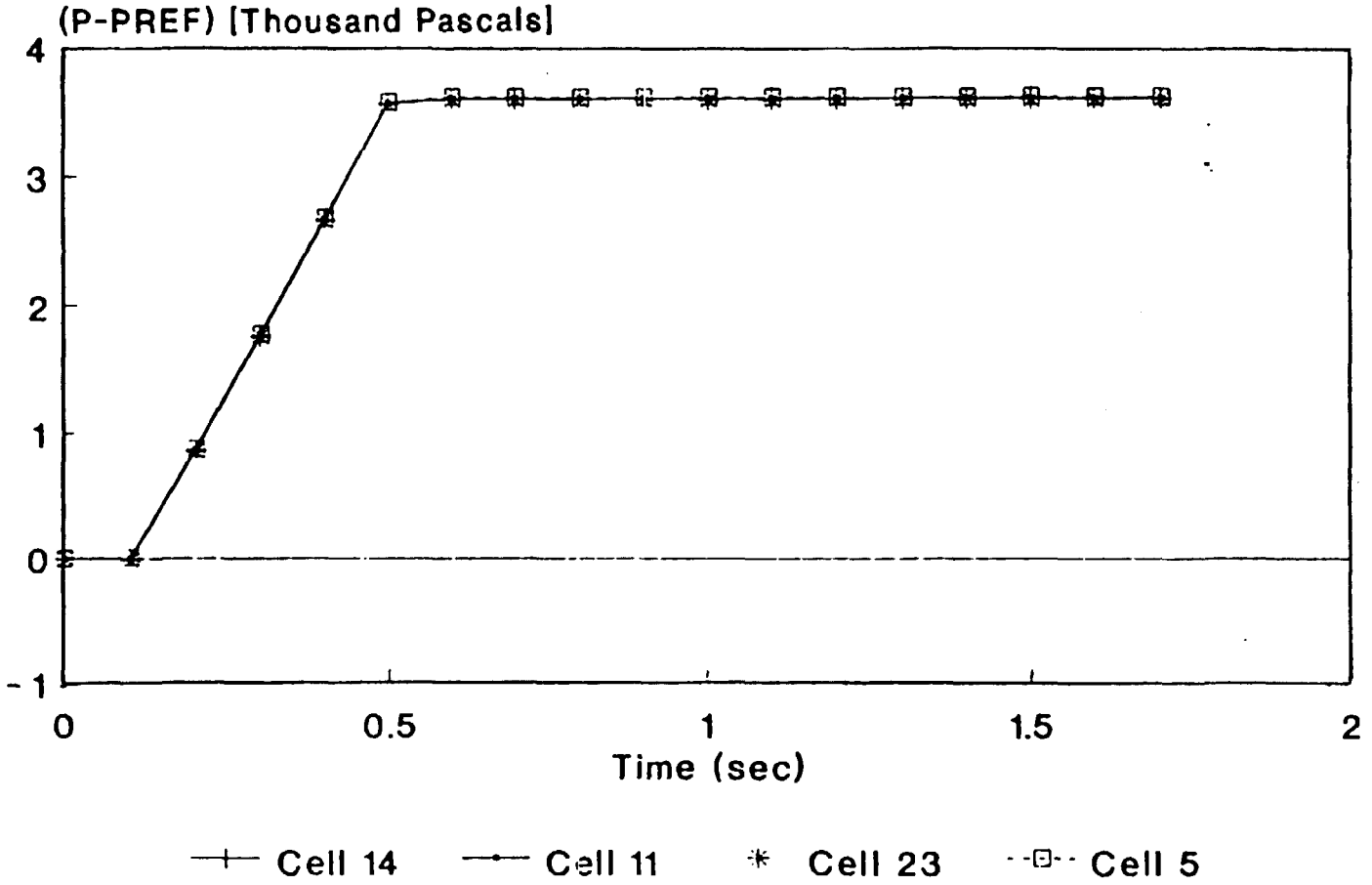

Figure 2a Pressure variation with time for Cells 14, 11, 23 and 5

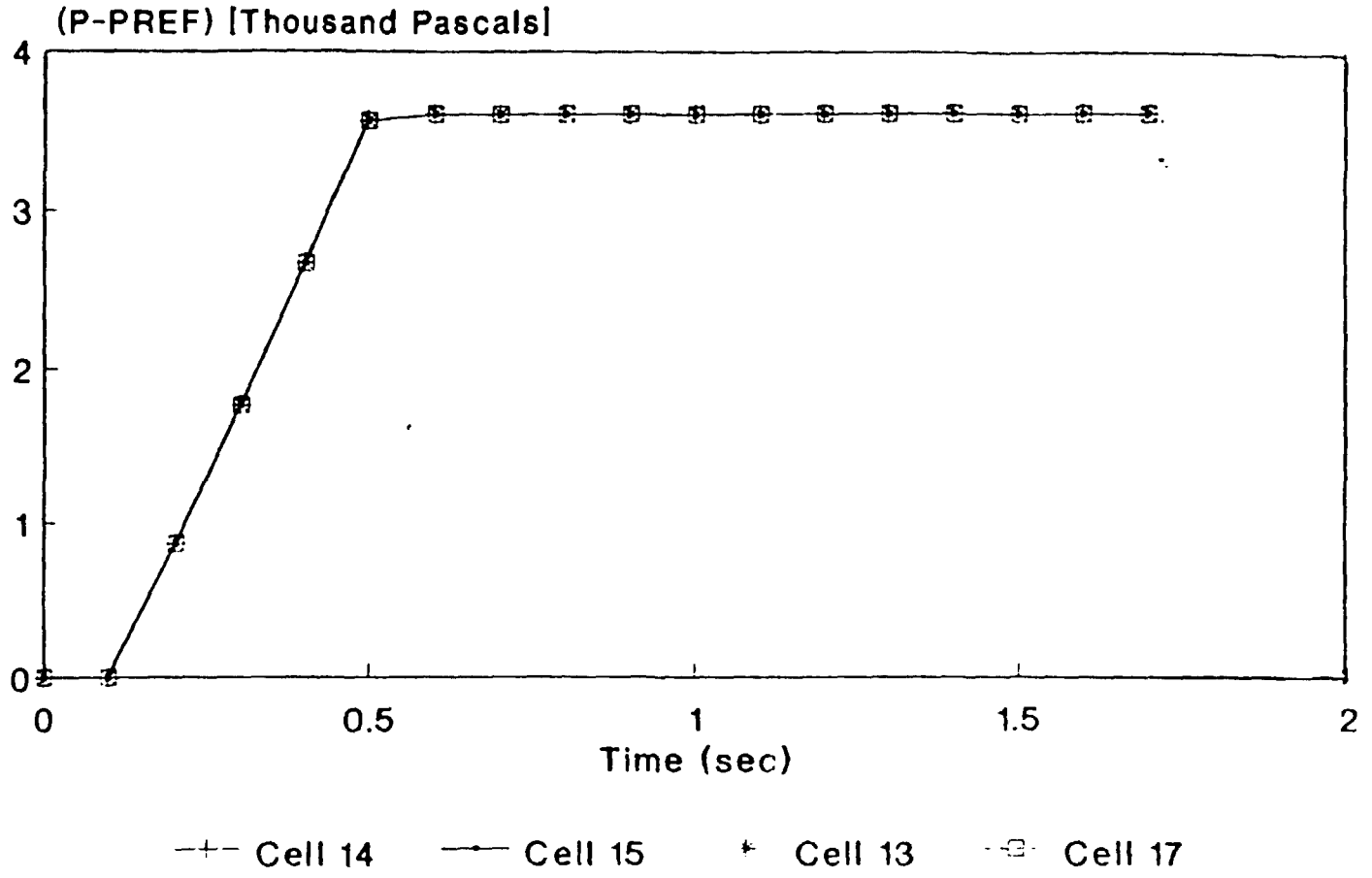

Figure 2b Pressure variation with time for Cells 14, 15, 13 and 17

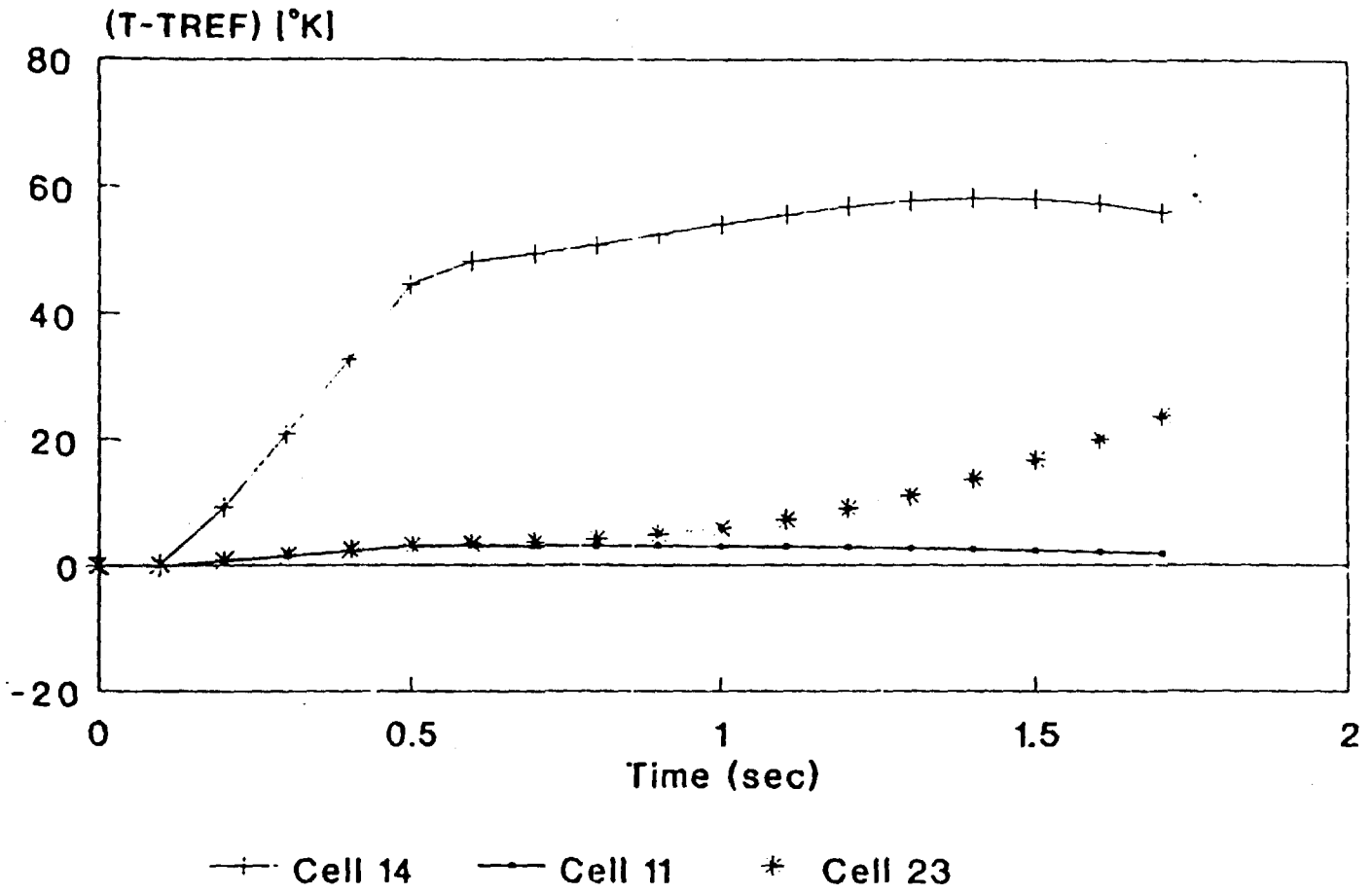

Figure 3a Temperature variation with time for Cells 14, 11 and 23

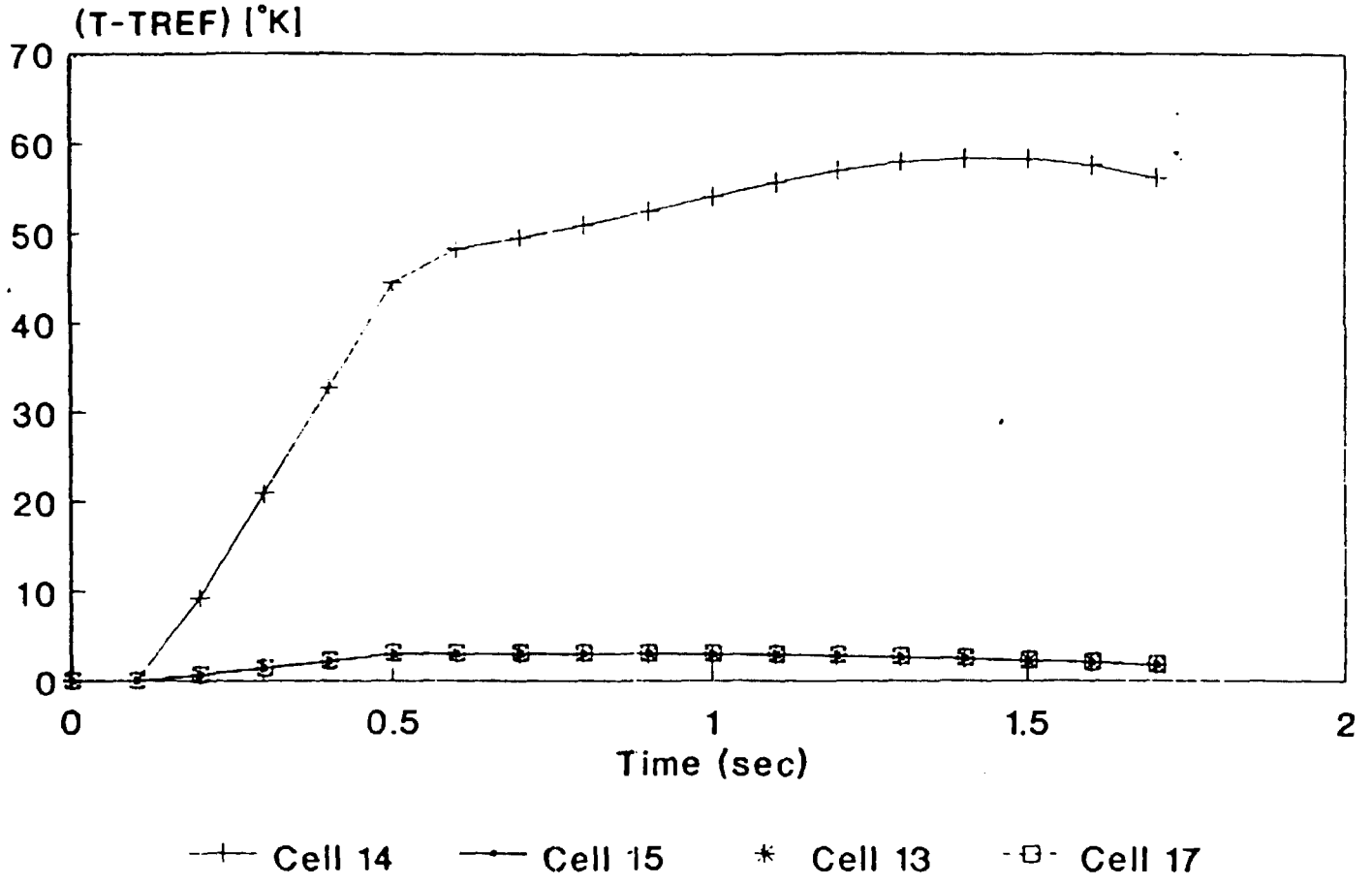

Figure 3b Temperature variation with time for Cells 14, 15 13 and 17

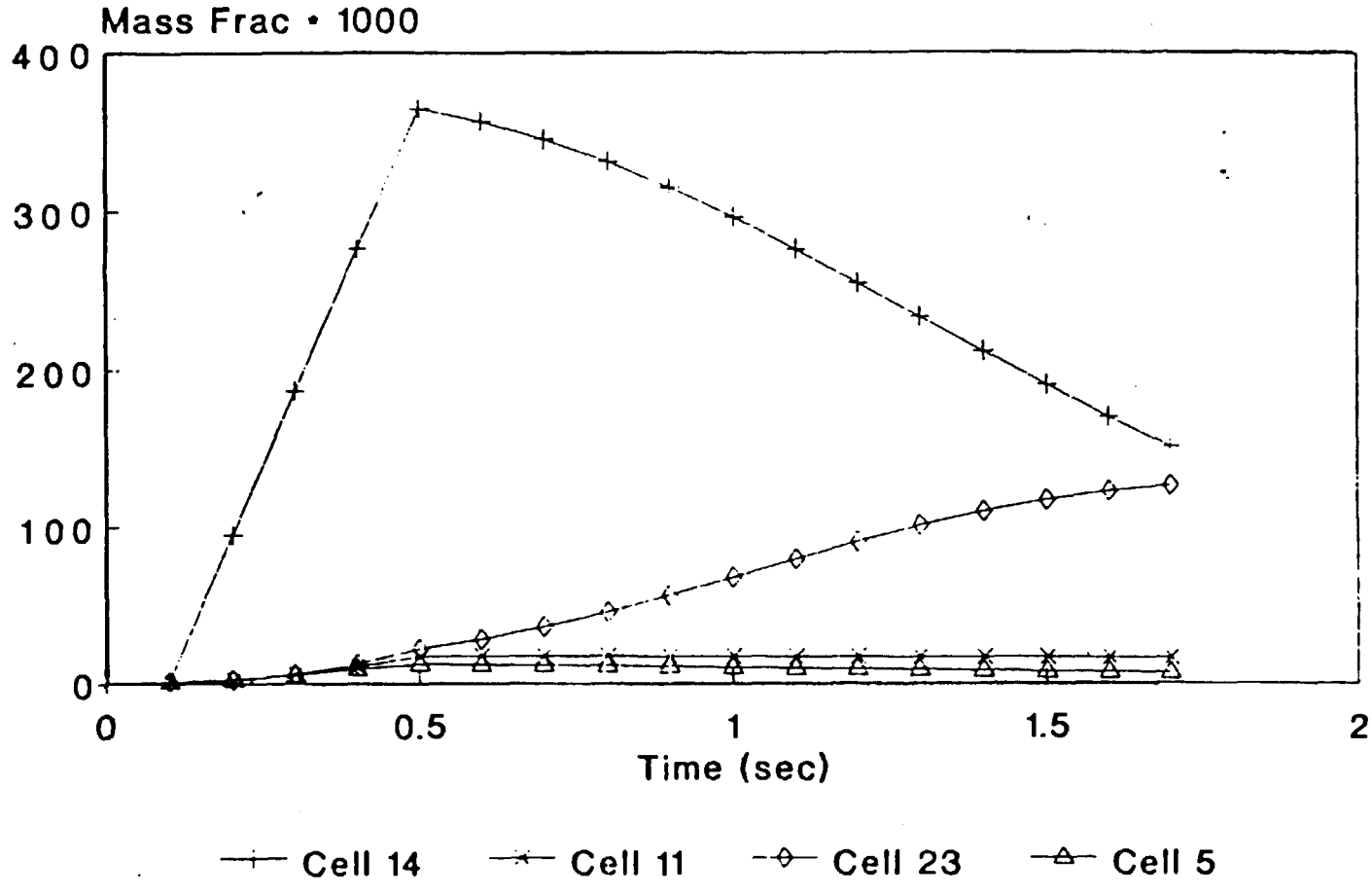

Figure 4a Variation of mass fraction of steam with time for Cells 14, 11, 23 and 5

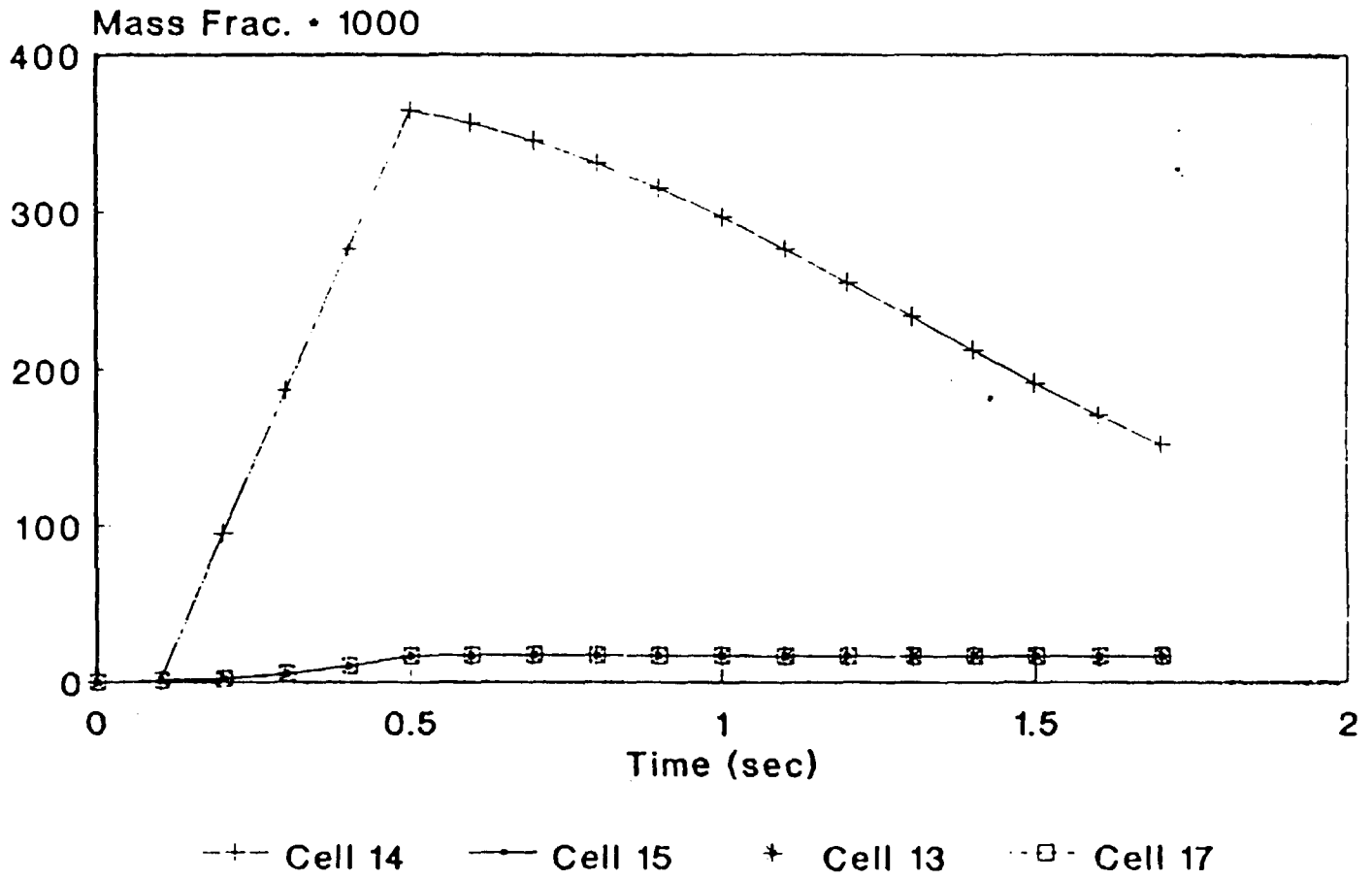

Figure 4b Variation of mass fraction of steam with time for Cells 14, 15, 13 and 17

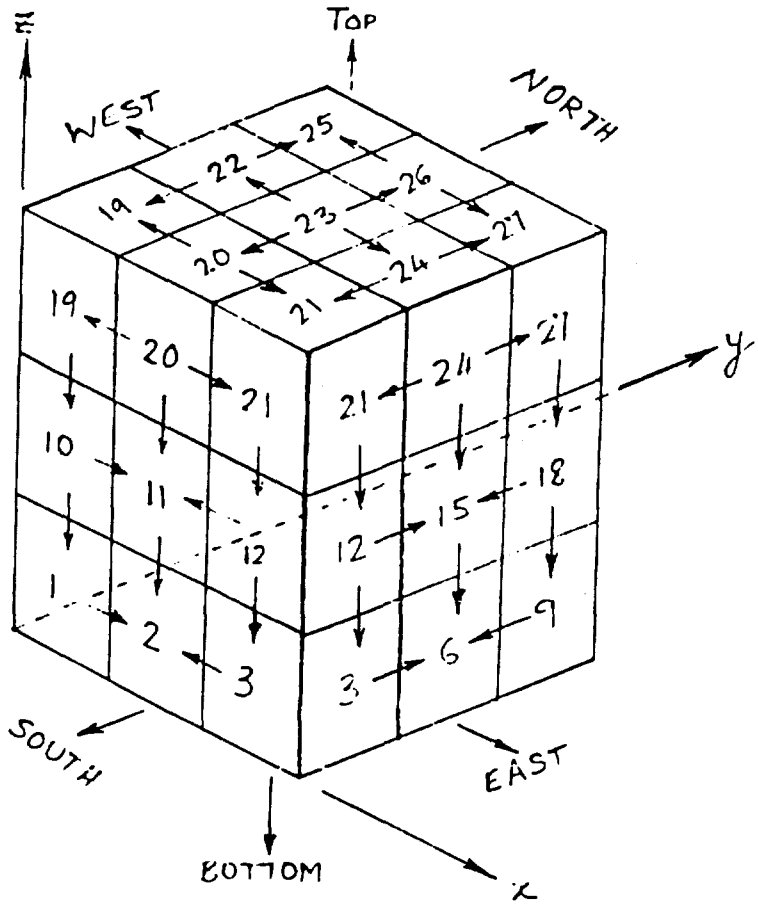

Figure 5 Overall flow patterns in the containment volume with 3 x 3 x 3 cell division scheme

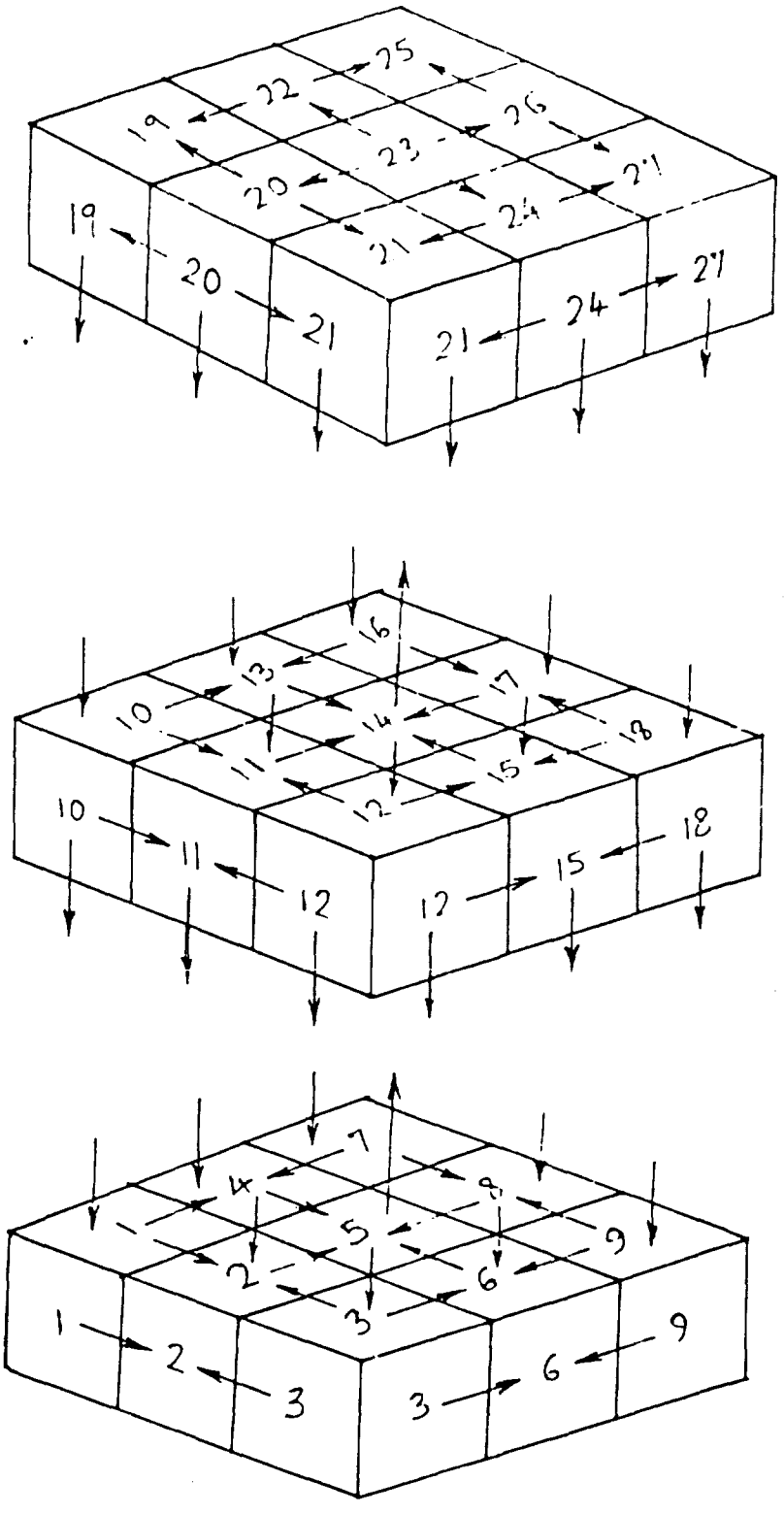

Figure 6 Containment volume of Figure 5 broken up into horizontal layers to show details of flow directions