

VULCAN: A One-Dimensional Simulation of  
Explosive Heat Transfer I.

by

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ABSTRACT

This paper describes the development of VULCAN up to the point where a working code is available. The analysis of the problem, the working fluids, the program construction and testing are all described and finally some applications of the code are suggested.

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## I. INTRODUCTION

It has been known for some time that the sudden contact of a hot liquid and a cold vapourisable liquid can, under certain conditions, lead to an explosive transfer of heat into kinetic energy. This phenomenon has been observed in foundary accidents when molten metal falls on to water<sup>1</sup>, spills of water on to liquid butane<sup>2</sup>, and in the American Spert reactor accident<sup>3</sup> where the hot liquid was aluminium and the cold liquid was water. Simple estimates show that the rapid transfer-rate of energy can only occur if the contact area increases sufficiently rapidly; however, this process is not yet understood. In spite of this, if the increase in contact area is allowed for in some sensible fashion, useful information such as pressure contours, kinetic energy, etc., as functions of time and initial conditions may be obtained from computer simulation of the dynamics. A comprehensive two-dimensional code is already available<sup>4</sup>, however, this code is not equipped to handle phase changes. VULCAN is an attempt at a one-dimensional simulation of the explosion in which phase changes, temperature dependant thermal conductivities, specific heats and realistic equations of state are used. The cold fluid is compressible whilst the hot one is incompressible although the latter restriction could be removed easily. At present the working fluids are aluminium and water but it is hoped to produce a version with sodium and uranium dioxide as working fluids.

In paragraph II we derive the differential equations describing the phenomenon and display by the relevant difference equations while in paragraph III the working fluids are specified. Paragraph IV describes the program construction and in paragraph V the results of



the code's ability to reproduce heat conduction, sound waves, shock waves and phase changes are displayed. Paragraph VI describes some possible applications and future developments.

## II. THE PHYSICAL MODEL

### A. Differential Equations.

Consider a column of liquid with constant cross-sectional area  $A$ . In Lagrangian co-ordinates the equations of motion and energy are

$$\rho_0 \frac{\partial u}{\partial t} = -\rho_0 g - \frac{\partial P}{\partial z} \quad (1)$$

$$\rho c \frac{\partial T}{\partial t} + \left[ T \left( \frac{\partial P}{\partial T} \right)_v - P \right] \rho \frac{\partial v}{\partial t} = \frac{\partial}{\partial z} \left( k \frac{\partial T}{\partial z} \right) - P \rho \frac{\partial v}{\partial t} \quad (2)$$

The second equation is obtained via the thermodynamic relationship for the internal energy

$$\begin{aligned} dE &= \left( \frac{\partial E}{\partial T} \right)_v dT + \left( \frac{\partial E}{\partial v} \right)_T dv \\ &= C_v dT + \left[ T \left( \frac{\partial P}{\partial T} \right)_v - P \right] dv \end{aligned}$$

In addition, since

$$\left( \frac{\partial P}{\partial T} \right)_v = - \left( \frac{\partial v}{\partial T} \right)_p \left( \frac{\partial P}{\partial v} \right)_T$$

we have

$$\left( \frac{\partial P}{\partial T} \right)_v = \gamma / K$$





where  $\gamma$  is the coefficient of cubical expansion and  $K$  is the isothermal compressibility. In equations (1) and (2)  $u$  is the velocity,  $\rho_0$  the initial density,  $g$  the acceleration due to gravity,  $z_0$  the initial position,  $c$  the specific heat at constant volume,  $k$  the thermal conductivity,  $v$  the specific volume, and  $T$  and  $P$  the temperature and pressure respectively.

The pressure is given by the equation of state

$$P = P(\rho, T) \quad (3)$$

Equation 2 must be modified in regions of mixed phase where phase transitions may take place. Consider a Lagrangian cell of mass  $M$  and volume  $V$  such that it is composed of vapour of mass  $m_v$  and liquid of mass  $m_l$ . If  $v_v$  and  $v_l$  are the specific volumes of vapour and liquid respectively then

$$V = m_v v_v + m_l v_l$$

Defining the fraction of vapour,  $\alpha$ , to be

$$\alpha = m_v / M \quad (0 \leq \alpha \leq 1)$$

then

$$\alpha = \frac{V/M - v_l}{v_v - v_l}$$

The internal energy is

$$E = \alpha E_v + (1-\alpha) E_l$$

where  $E_v$  and  $E_l$  are the internal energies of vapour and liquid respectively. Hence

$$dE = \alpha dE_v + (1-\alpha) dE_l + (E_v - E_l) d\alpha$$



From the definition of enthalpy we have

$$E_v - E_\ell = L - p (v_v - v_\ell)$$

where  $L$  is the latent heat of vapourisation. Consequently in a mixed phase region the energy equation becomes

$$\begin{aligned} \rho \bar{c} \frac{\partial T}{\partial t} + \left\{ T \left[ \alpha \left( \frac{\partial P}{\partial T} \right)_{\text{vapour}} + (1-\alpha) \left( \frac{\partial P}{\partial T} \right)_{\text{liquid}} \right] - P \right\} \rho \frac{\partial v}{\partial t} + \\ + \rho \left[ L - P (v_v - v_\ell) \right] \frac{\partial \alpha}{\partial t} = \frac{\partial}{\partial z} \left( \bar{k} \frac{\partial T}{\partial z} \right) - P \rho \frac{\partial v}{\partial t} \end{aligned} \quad (4)$$

$\bar{c}$  is the specific heat at constant volume of the mixture and is given by

$$\bar{c} = \alpha C_v + (1-\alpha) C_\ell$$

where  $C_v$  and  $C_\ell$  are the vapour and liquid specific heats respectively.

$\bar{k}$  is the thermal conductivity of the mixture and is taken to be determined by

$$\frac{1}{\bar{k}} = \frac{\alpha}{k_v} + \frac{(1-\alpha)}{k_\ell}$$

where  $k_v$  and  $k_\ell$  are the vapour and liquid thermal conductivities respectively. The pressure is given by the vapour pressure law

$$P_v = P_v(T) \quad (5)$$

Since the hot fluid is assumed incompressible there are no difficulties in including phase changes in this region. All that is required is the melting temperature and the latent heat of fusion.

At the interface between the two fluids we have the boundary conditions  $T$  and  $\frac{\partial T}{\partial z}$  continuous. The bottom of the column is assumed



rigid and thermally insulating while the top surface can be chosen to be either rigid or free depending on the particular situation that is under investigation. A variety of initial conditions are of interest - a typical example would be the fluids at rest with the hot fluid at constant temperature  $T_H$  and the cold one at constant temperature  $T_C$ .

The increase in effective contact area may be allowed for in an artificial manner either by increasing the area  $A$  in the neighbourhood of the interface or else by decreasing all distances normal to the interface thus increasing temperature gradients. Part of the purpose of the code is to investigate whether either of these mechanisms will produce an explosive heat transfer.

#### B. Difference Equations.

We divide the column into a Lagrangian mesh and denote the positions and velocities of the boundaries of the cells by  $Z_i$  and  $U_i$  respectively. All other quantities are associated with the mid-points of the cells. The equation of motion is differenced as

$$\frac{U_i^{n+\frac{1}{2}} - U_i^{n-\frac{1}{2}}}{\Delta t} = - \frac{(P_{i+\frac{1}{2}}^n - P_{i-\frac{1}{2}}^n)}{M_i} - g \quad (6)$$

$$M_i = (M_{i+\frac{1}{2}} + M_{i-\frac{1}{2}})/2$$

where  $M_{i+\frac{1}{2}}$  is the mass of the  $(i + \frac{1}{2})^{\text{th}}$  cell and is equal to

$\rho_0 \tilde{\Delta Z}_i$ ,  $\tilde{\Delta Z}_i$  being the initial mesh spacing at this cell. The cell



boundaries may then be advanced by the equation

$$\frac{Z_i^{n+1} - Z_i^n}{\Delta t} = U_i^{n+\frac{1}{2}} \quad (7)$$

The energy equation is differenced as

$$\begin{aligned} M_{i+\frac{1}{2}} C_{i+\frac{1}{2}}^n \frac{(T_{i+\frac{1}{2}}^{n+1} - T_{i+\frac{1}{2}}^n)}{\Delta t} + T_{i+\frac{1}{2}}^n \left[ (\partial P / \partial T)_V \right]_{i+\frac{1}{2}}^n \times \\ \times (U_{i+\frac{1}{2}}^{n+\frac{1}{2}} - U_i^{n+\frac{1}{2}}) = 2k (T_{i+1}^n) \frac{(T_{i+3/2}^n - T_{i+\frac{1}{2}}^n)}{Z_{i+2}^{n+1} - Z_i^{n+1}} \cdot \\ - 2k (T_i^n) \frac{(T_{i+\frac{1}{2}}^n - T_{i-\frac{1}{2}}^n)}{Z_{i+1}^{n+1} - Z_{i-1}^{n+1}} \cdot \end{aligned} \quad (8)$$

Equation 8 requires expressions for  $T_i$  and  $T_{i+1}$  and these temperatures are calculated as follows. Since  $T$  and  $\partial T / \partial z$  are continuous we have

$$\frac{k (T_{i-\frac{1}{4}}) (T_i - T_{i-\frac{1}{2}})}{Z_i - Z_{i-1}} = \frac{k (T_{i+\frac{1}{4}}) (T_{i+\frac{1}{2}} - T_i)}{Z_{i+1} - Z_i}$$

hence 
$$T_i = \frac{T_{i+\frac{1}{2}} + \beta T_{i-\frac{1}{2}}}{1 + \beta} \quad (9)$$

where 
$$\beta = \frac{k (T_{i-\frac{1}{4}}) (Z_{i+1} - Z_i)}{k (T_{i+\frac{1}{4}}) (Z_i - Z_{i-1})} \quad (10)$$

Of course,  $T_{i \pm \frac{1}{4}}$  are also unknown, consequently  $\beta$  and thus  $T_i$  must be calculated iteratively using  $k (T_{i-\frac{1}{2}})$  and  $k (T_{i+\frac{1}{2}})$  as starting values.





This allows us to calculate  $T_i$  and then by putting

$T_{i+\frac{1}{2}} = \frac{1}{2} (T_i + T_{i+\frac{1}{2}})$  the procedure may be repeated.  $T_{i+1}$  is calculated in a like manner. However, this procedure is unduly time consuming and so in regions where the temperature gradient is small we approximate  $T_i$  by

$$T_i = (T_{i+\frac{1}{2}} + T_{i-\frac{1}{2}})/2 \quad (11)$$

The exception to this method is the interface region where equations 9 and 10 are always used.

Equation 4 is differenced in the same manner as equation 2, the extra term being differenced as

$$M_{i+\frac{1}{2}} \left[ L - P_{i+\frac{1}{2}}^n (v_v(T_{i+\frac{1}{2}}^n) - v_l(T_{i+\frac{1}{2}}^n)) \right] \frac{(\alpha_{i+\frac{1}{2}}^{n+1} - \alpha_{i+\frac{1}{2}}^n)}{\Delta t}$$

Since  $v_v$  is a rapidly varying function of temperature we have to iterate to find consistent new values of  $T$  and  $\alpha$ .

The interface between the two fluids requires special treatment<sup>5</sup>.

At any interface  $\frac{P_{i+\frac{1}{2}}^n - P_{i-\frac{1}{2}}^n}{M_i}$  of equation 6 is replaced by

$$\left\{ 3 (P_{i+\frac{1}{2}}^n - P_{i-\frac{1}{2}}^n) - \frac{1}{3} (P_{i+3/2}^n - P_{i-3/2}^n) \right\} / (M_1 + M_2)$$

where  $M_1$  and  $M_2$  are the masses of the cells on each side of the interface.

The pressure is advanced via the equation of state

$$P_{i+\frac{1}{2}}^{n+1} = P(T_{i+\frac{1}{2}}^{n+1}, \rho_{i+\frac{1}{2}}^{n+1}) \quad (12)$$



One final point that requires discussion is the introduction of a pseudo-viscosity term. Since we are attempting to simulate an explosive interaction the final code must be capable of propagating shock waves. It is known, however, that if no viscosity is present numerical ringing occurs behind the shock. This ringing may be damped out by introducing an artificial viscosity,  $q$ , as follows<sup>6</sup>.

$$q_{i+\frac{1}{2}}^n = \begin{cases} \frac{2a^2}{v_{i+\frac{1}{2}}^n + v_{i+\frac{1}{2}}^{n-1}} \left[ (\delta u)_{i+\frac{1}{2}}^n \right]^2 & ; \text{ if } (\delta u)_{i+\frac{1}{2}}^u < 0 \\ 0 & ; \text{ otherwise} \end{cases} \quad (13)$$

$a$  is a constant chosen to suit each specific problem and  $(\delta u)_{i+\frac{1}{2}}^n = U_{i+1}^n - U_i^n$ .  $q$  is included in the physical equations by replacing  $p$  by  $(p + q)$  whenever the former occurs. It may turn out that the damping effected by the thermal conductivity is sufficient to eliminate ringing in which case the pseudo-viscosity can be switched off by setting  $a = 0$ .

The stability of the complete scheme is still under investigation. If the hydrodynamic and heat flow equations were uncoupled the respective stability criteria would be

$$C\Delta t/\Delta X < 1$$

$$\sigma\Delta t/(\Delta X)^2 < \frac{1}{2} \quad \sigma = k/\rho c$$

where  $C$  is the adiabatic sound speed. Normally the first condition is much more restrictive. Richtmyer and Morton<sup>7</sup> have considered a scheme similar to ours and postulate that the former condition is appropriate. In our case, however, the situation is complicated by



the possible presence of an effective contact area  $A$ . We postulate that under these conditions  $\sigma$  is given by  $\sigma = kA/\rho c$ . With this modified  $\sigma$  we have used both conditions in choosing  $\Delta t$ . In addition, the pseudo-viscosity may alter the former condition in the presence of strong shocks<sup>8</sup> and we have also allowed for this possibility.

### III. THE WORKING FLUIDS

At present the working fluids are aluminium and water. In this section we list the physical properties of these fluids that are used in the code.

#### A. Equation of State.

Since only the cold fluid, ie water, is taken to be compressible we only have to discuss the equation of state for water. The  $p$ - $V$  plane may be divided into three regions. (see Fig. 1).

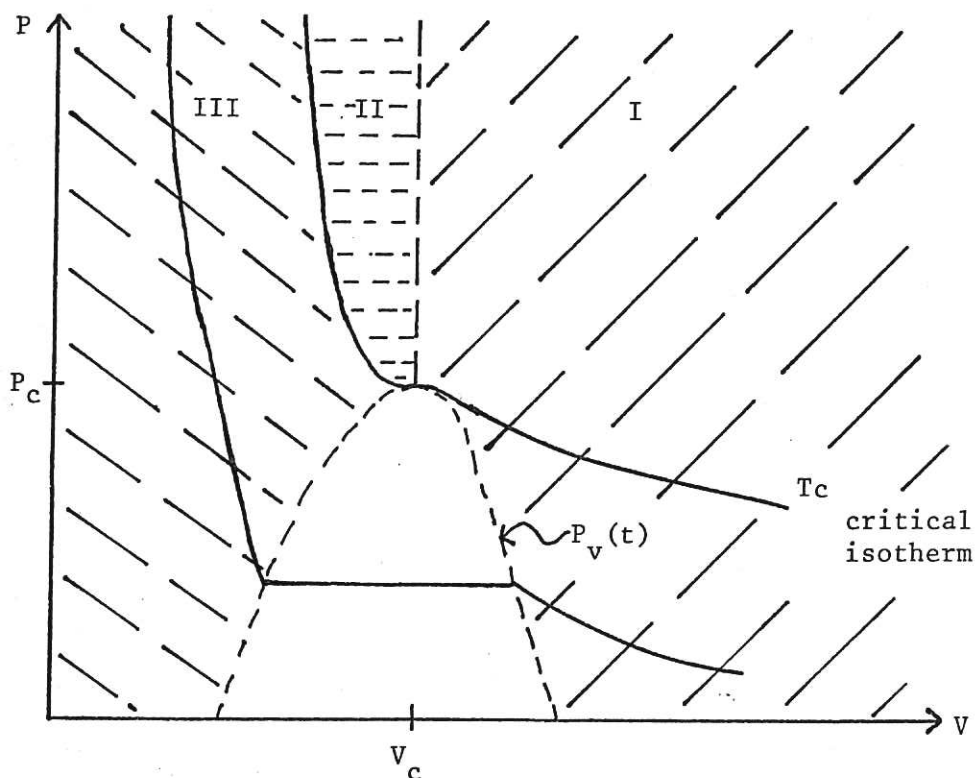


Fig. 1  $p$ - $V$  plane in the region of gas-liquid transition.



Region I Low density gas -  $\rho^* \leq 1, t^* \geq 1$

Region II High density gas -  $\rho^* > 1, t^* \geq 1$

Region III Liquid -  $\rho^* > 1, t^* < 1$

The reduced pressure, density and temperature are defined by

$$p^* = P/P_c$$

$$\rho^* = v_c/v$$

$$t^* = T/T_c$$

where the critical pressure, specific volume and temperature are given by

$$P_c = 221.2 \text{ bar}$$

$$v_c = 3.17 \times 10^{-3} \text{ m}^3/\text{kg}$$

$$T_c = 647.3 \text{ }^\circ\text{K}$$

Hirschfelder et al<sup>9</sup> have described a generalised equation of state for gases and liquids; thus the three regions are described as follows:

Region I

$$P_I^*/t^* = -W_1(t^*)\rho^{*2} - W_2(t^*)\rho^{*3} + g(\rho^*)$$

$$W_1(t^*) = k_0 t^{*-1} + (\beta' - k_0) t^{*-2} \quad (14)$$

$$W_2(t^*) = \frac{1}{2} (1 - k_0 - \alpha' + 2\beta') (1 - t^{*-2})$$

$$g(\rho^*) = \frac{(1 + \beta')^3 \rho^*}{\beta' (3\beta' - 1) - (3\beta'^2 - 6\beta' - 1) \rho^* + \beta' (\beta' - 3) \rho^{*2}}$$





Region II

$$\begin{aligned}
 P_{II}^*/t^* &= -W_1(t^*) \rho^{*2} - W_2(t^*) \rho^{*3} + 1 + \beta' \rho^{*2} + \\
 &+ S(\rho^* - 1)^5/\rho^* + D(\rho^*, t^*) \\
 D(\rho^*, t^*) &= (\rho^* - 1)^3 (t^* - 1) \left\{ \rho^{*-1} (h_0 t^{*-1} + h_1) + \right. \\
 &\left. + h_2 t^{*-1} + h_3 \right\}
 \end{aligned} \tag{15}$$

Region III

$$P_{III}^* = P_{II}^*(\rho^*, t^*) - P_{II} \left[ \rho_{\ell}^*(t^*), t^* \right] + P_V^*(t^*) \tag{16}$$

$P_V^*(t^*)$  is the reduced vapour pressure and  $\rho_{\ell}^*$  is the reduced density of the saturated liquid. We have used Hirschfelder's equations in regions I and II with the following values for the constants:

$$\begin{aligned}
 \alpha' &= 7.858 & \beta' &= 8.962 & k_0 &= 4.71 & S &= 2.734 \\
 h_0 &= 88.5 - 3.12 \beta' \\
 h_1 &= -44.4 + 5.22 \beta' \\
 h_2 &= -47.8 + 4.06 \beta' \\
 h_3 &= 23.7 - 3.26 \beta'
 \end{aligned}$$

In region III we have not used Hirschfelder's equations since a small error in  $\rho^*$  leads to an enormous error in  $P_{III}^*$ . Instead we have used the relationship

$$\begin{aligned}
 \delta p &= \left( \frac{\partial P}{\partial V} \right)_T \delta V + \left( \frac{\partial P}{\partial T} \right)_V \delta T \\
 &= \frac{1}{K} \left( -\frac{\delta V}{V} + \gamma \delta T \right)
 \end{aligned} \tag{17}$$

where  $K$  and  $\gamma$  are the isothermal bulk modulus and coefficient of cubical expansion respectively.



Their values are taken to be<sup>10</sup>

$$K = 4.45 \times 10^{-10} \text{ n/m}^2$$

$$\gamma = 7.30 \times 10^{-5} + 7.81 \times 10^{-6} (T - 273.15) \text{ deg}^{-1}.$$

Finally for the vapour pressure equation we have used the equation cited in Steam Tables<sup>11</sup>, viz.

$$P_v^* (t^*) = \exp \left\{ \frac{\frac{1}{t^*} \sum_1^5 k_v (1-t^*)^v}{1 + k_6(1-t^*) + k_7 (1-t^*)^2} - \frac{1-t^*}{k_8 (1-t^*)^2 + k_9} \right\} \quad (18)$$

The constants are given by

$$k_1 = 7.691234$$

$$k_2 = - 2.608024 \times 10$$

$$k_3 = - 1.681707 \times 10^2$$

$$k_4 = 6.423286 \times 10$$

$$k_5 = - 1.189646 \times 10^2$$

$$k_6 = 4.167117$$

$$k_7 = 2.097507 \times 10$$

$$k_8 = 10^9$$

$$k_9 = 6$$

#### B. Specific Heats.

In the case of aluminium the specific heat is given by<sup>10</sup>

$$\text{liquid } C = 1085 \text{ j/kg/}^\circ\text{K}$$

$$\text{solid } C = (763 + 0.458T) \text{ j/kg/}^\circ\text{K}$$

(19)

(T in  $^\circ\text{K}$ ). We assume that the latter expression is valid at all temperatures below the melting point. The melting temperature and



latent heat are

$$T_{\text{melt}} = 933 \text{ } ^\circ\text{K}$$

$$L = 3.9767 \text{ j/kg}$$

For water we have used the tabulated values given in Steam Tables<sup>11</sup> using interpolation to obtain intermediate values. These tables are valid within the ranges  $0 \leq T \leq 800^\circ\text{C}$ ,  $0 \leq P \leq 1000 \text{ bar}$ . Although it is  $C_p$ , the specific heat at constant pressure, that it is tabulated, nevertheless we have used these values to estimate  $C_v$  via the thermodynamic relationship.

$$C_p - C_v = TV\gamma^2/K$$

$$= R \text{ (for an ideal gas)}$$

In addition, tables of the specific volume of vapour and liquid along the saturated vapour pressure line and also latent heat were obtained from ref. 10. Three point Lagrange interpolation is used on the latter tables as required.

### C. Thermal Conductivities.

For aluminium the thermal conductivity is given by<sup>10</sup>

$$\begin{aligned} \text{liquid } k &= 79.7143 + 1.7143 \times 10^{-2} T \text{ W/m}^\circ\text{K} \\ \text{solid } k &= 289.2 - 8.5 \times 10^{-2} T \text{ W/m}^\circ\text{K} \end{aligned} \quad (20)$$

In the case of water the following equations were used<sup>11</sup>

vapour

$$k \times 10^3 = k_1 \times 10^3 + (a' + b' \theta + c' \theta^2) \frac{1}{v} + \frac{d'}{(\theta - e')^{4.2}} \frac{1}{v^2} \quad (21)$$

$$k_1 \times 10^3 = a + b\theta + c\theta^2 + d\theta^3$$



where  $\theta$  is the temperature in  $^{\circ}\text{C}$ ,  $v$  is the specific volume in  $\text{cm}^3/\text{g}$   
and

$$\begin{aligned} a &= 17.6, \quad b = 5.87 \times 10^{-2}, \quad c = 1.04 \times 10^{-4}, \\ d &= -4.51 \times 10^{-8}, \quad a' = 103.51, \quad b' = 0.4198 \\ c' &= 2.771 \times 10^{-5}, \quad d' = 2.1482 \times 10^{14}, \quad e' = 0 \end{aligned}$$

liquid

$$\begin{aligned} k \times 10^3 &= a_0 + a_1 \left(\frac{T}{T_0}\right) + a_2 \left(\frac{T}{T_0}\right)^2 + a_3 \left(\frac{T}{T_0}\right)^3 + a_4 \left(\frac{T}{T_0}\right)^4 + \\ &+ (P-P_s) \left[ b_0 + b_1 \left(\frac{T}{T_0}\right) + b_2 \left(\frac{T}{T_0}\right)^2 + b_3 \left(\frac{T}{T_0}\right)^3 \right] + \\ &+ (P-P_s)^2 \left[ c_0 + c_1 \left(\frac{T}{T_0}\right) + c_2 \left(\frac{T}{T_0}\right)^2 + c_3 \left(\frac{T}{T_0}\right)^3 \right] \quad (22) \end{aligned}$$

where  $T$  is the temperature in  $^{\circ}\text{K}$ ,  $P$  and  $P_s$  the pressure and saturated vapour pressure in bars and

$$\begin{aligned} T_0 &= 273.15, \quad a_0 = -922.47, \quad a_1 = 2839.5, \\ a_2 &= -1800.7, \quad a_3 = 525.77, \quad a_4 = -73.440, \\ b_0 &= -0.94730, \quad b_1 = 2.5186, \quad b_2 = -2.0012, \\ b_3 &= 0.51536, \quad c_0 = 1.6563 \times 10^{-3}, \quad c_1 = -3.8929 \times 10^{-3}, \\ c_2 &= 2.9323 \times 10^{-3}, \quad c_3 = -7.1693 \times 10^{-4}. \end{aligned}$$

These expressions are valid within the ranges

$$\left. \begin{aligned} t_s &\leq T \leq 700^{\circ}\text{C} \\ 0 &\leq P \leq 500 \text{ bar} \end{aligned} \right\} \text{ vapour}$$

( $t_s$  = saturation temperature)

$$\left. \begin{aligned} 0 &\leq T \leq 350^{\circ}\text{C} \\ 0 &\leq P \leq 500 \text{ bar} \end{aligned} \right\} \text{ liquid}$$

Outside these limits we have used the limiting value closest to the required case.





#### IV. PROGRAM DESIGN

The program has been written and developed using the CRONUS package<sup>12</sup> which is a standardised method for the construction of FORTRAN programs to solve time - dependent problems. FORTRAN is the only language used and the program is not overlaid. Fig. 2 is an overall flow diagram showing the basic control. The positions and velocities of the cell boundaries are advanced in turn by simply applying equations 6 and 7.

Fig. 3 shows the overall method for advancing the temperature and pressure of each cell. First the specific heats and thermal conductivities of each cell are set. For a given cell these quantities are re-calculated only if the conditions in that cell have changed appreciably since they (the specific heat and thermal conductivity) were last calculated. The approximate saturated vapour pressure at each cell temperature is then calculated by linearly interpolating input tables. This approximate calculation is used to decide whether any vapour is present. If vapour is present then, of course, the saturated vapour pressure is calculated more exactly from equation 18. The temperatures of the cells of the hot fluid are updated by the normal methods of calorimetry. If the melting point is reached a change of phase occurs. The temperatures and pressure of the cells adjacent to the interface are advanced and then the remaining cells in the compressible fluid are dealt with.

Fig. 4 shows the detailed procedure for advancing the temperature and pressure of each cell of the cold fluid. First, the fraction of vapour present in the current cell is calculated and then the temperature of that cell is advanced by calculating the nett flow of



heat into the cell and hence the new temperature. If the cell contains vapour and liquid then the temperature and fraction of vapour present are calculated in a self consistent manner by iteration. Finally the pressure of the cell is updated using the equation of state. Since the difference equations are modified slightly at the interface this region is treated separately but the chain of flow is similar to that of Fig. 4.



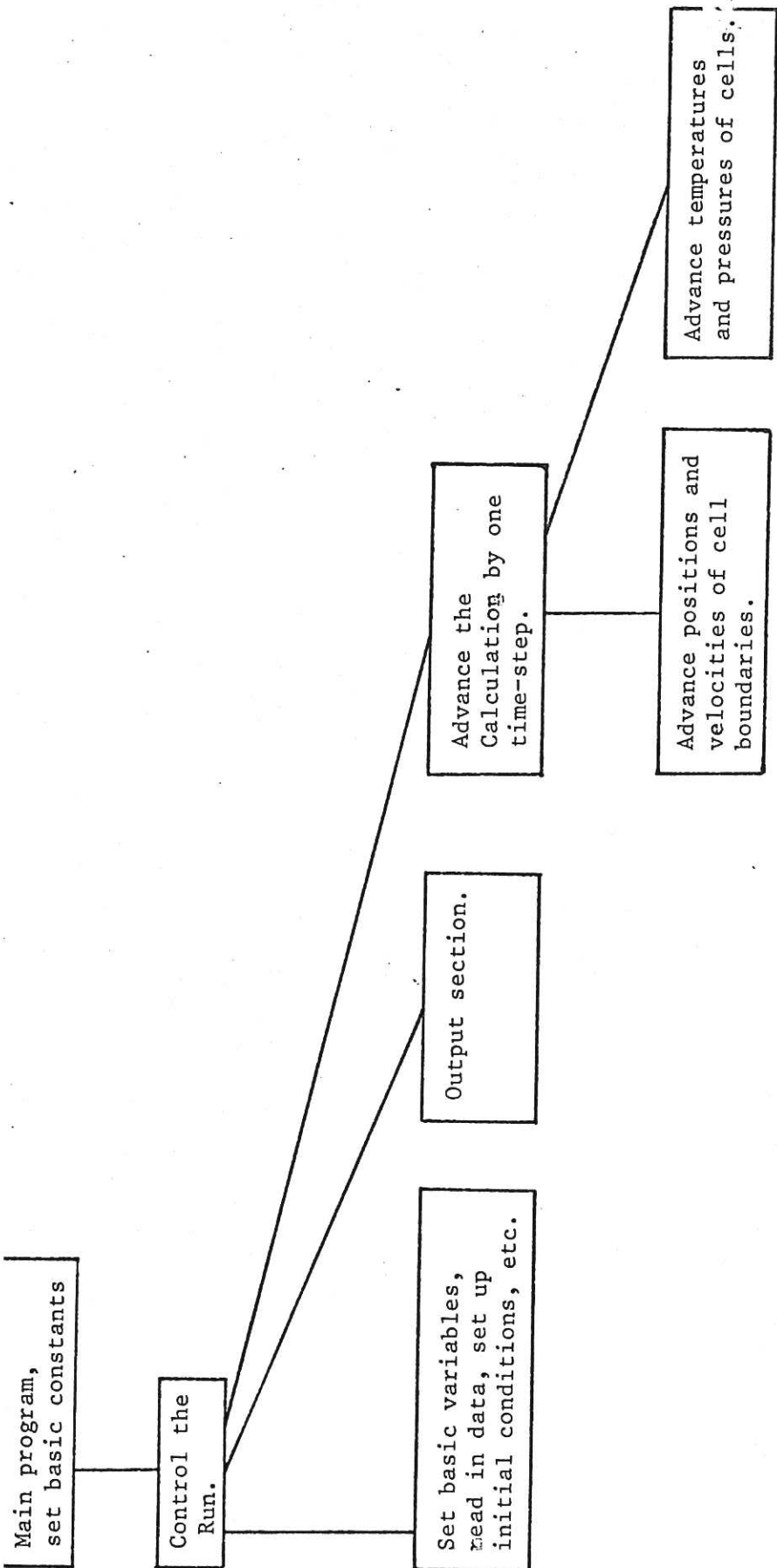


Fig. 2. Overall Structure of Calculation.



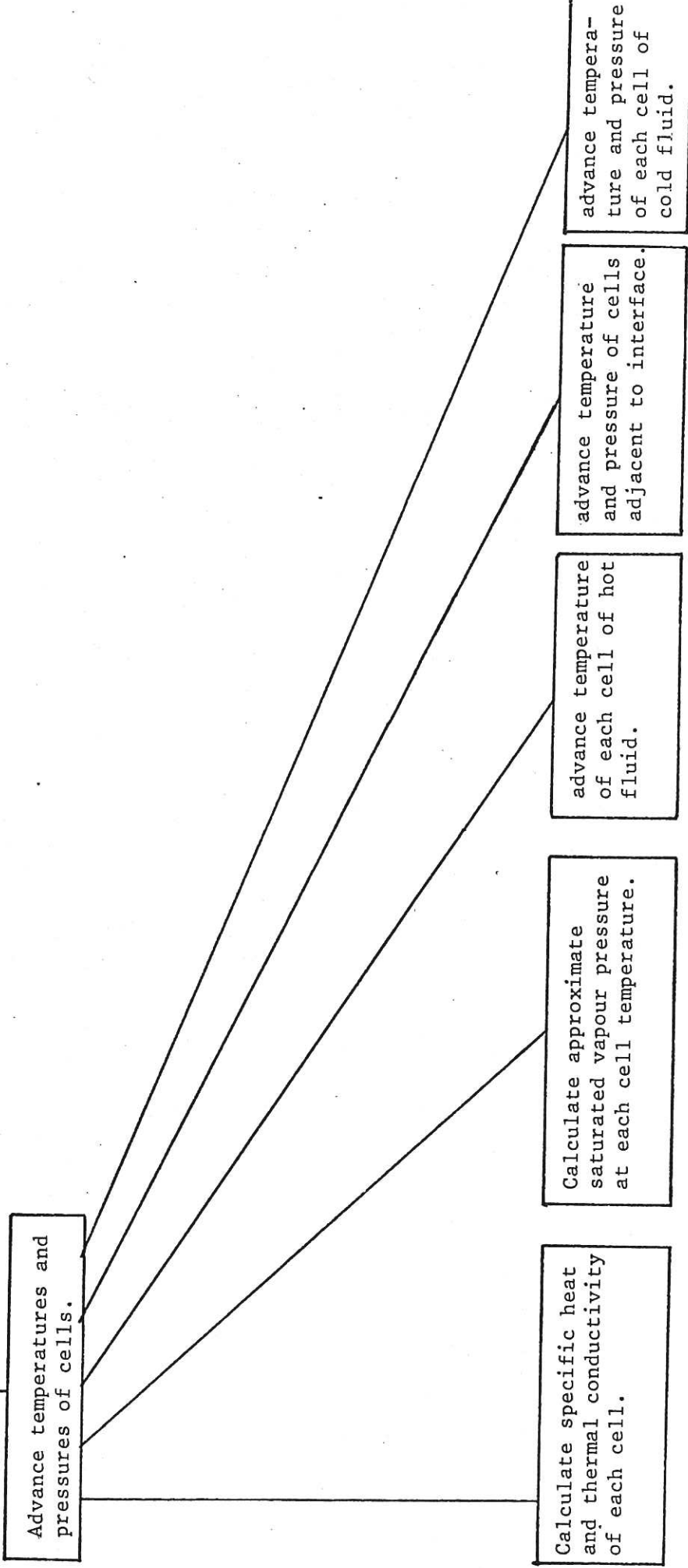


Fig. 3. The order of calculation for each cell with respect to temperature and pressure.





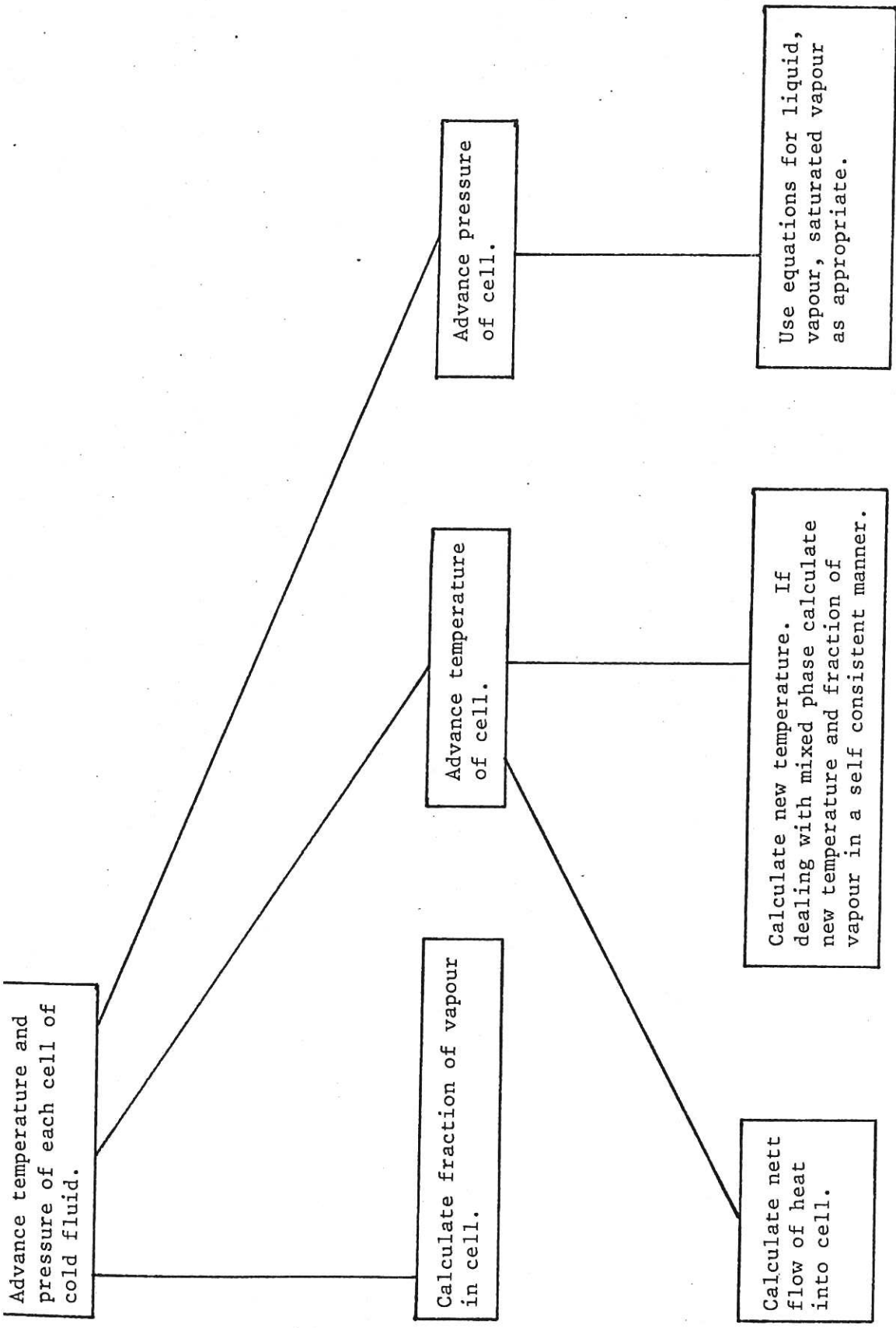


Fig. 4. Detailed Order of Calculation for Advancing the Temperature and Pressure of the Cold Fluid.



## V. PROGRAM TESTING

Apart from testing individual subprograms the program as a whole has been tested in four ways.

### A. Heat Conduction.

To test the code's ability to conduct heat we assume a uniform incompressible fluid throughout with a given initial temperature profile. Phase changes are also omitted. The subsequent temperature distribution is determined by the equation

$$\frac{\partial T}{\partial t} = \frac{1}{\rho c} \frac{\partial}{\partial z} \left( k \frac{\partial T}{\partial z} \right)$$

This equation may be solved analytically<sup>13</sup> for temperature dependent  $\rho$ ,  $c$  and  $k$  and so we may compare the numerical and analytic solutions and thus gauge the accuracy of the former. If we take

$$k = k_0 (1 + \alpha T)$$

$$C = C_0 (1 + \alpha T)$$

$$\rho = \text{constant}$$

then the solution of the heat conduction equation in the region

$[0, \ell]$  is given by

$$\begin{aligned} \Phi = & \frac{1}{\ell} \int_0^{\ell} \phi(x) dx + \frac{2}{\ell} \sum_{n=1}^{\infty} e^{-\sigma n^2 \pi^2 t / \ell^2} \\ & \cdot \cos \frac{n\pi x}{\ell} \int_0^{\ell} \phi(x) \cos \frac{n\pi x}{\ell} dx \end{aligned}$$

where

$$\Phi = \frac{1}{k_0} \int_0^T k dT = T + \frac{1}{2} \alpha T^2$$

$$\sigma = k/\rho c = k_0/\rho c_0$$

$\phi(x)$  is the initial value of  $\Phi$ .



If we take an initial temperature profile

$$T(x, 0) = \begin{cases} T_0 & ; 0 \leq x \leq l/2 \\ T_0/2 & ; l/2 < x \leq l \end{cases}$$

we find

$$\Phi = T_0 \left\{ \frac{3}{4} + \frac{5}{16} \alpha T_0 + \frac{1}{\pi} (1 + \frac{3}{4} \alpha T_0) \sum_{n=1}^{\infty} \frac{e^{-\sigma n^2 \pi^2 t / l^2}}{n} \left[ \sin \frac{n\pi}{2} \cos \frac{n\pi x}{l} \right] \right\}$$

The numerical and analytic solutions have been compared for  $\alpha = 0$  and  $\alpha = \frac{1}{4}$ . In both cases accuracy better than 1% is obtained, the former case being the more accurate.  $\alpha = \frac{1}{4}$  represents an extremely large correction to the thermal conductivity and so we conclude that the code is capable of conducting heat in a satisfactory manner.

#### B. Sound Waves.

To isolate sound wave propagation a uniform temperature is assumed throughout a uniform compressible fluid and phase changes again excluded. A sound wave is set up by displacing the initial positions of the cell boundaries about the mean positions by an amount

$$\epsilon = \epsilon_0 \sin \frac{(2i + 1)\pi x}{2l}$$

The excess pressure may then be calculated and the subsequent motion followed. From the resulting output the velocity of sound was measured and found to be 1584 m/s which compares favourably with 1509 m/s, the velocity derived from the equation of state.



### C. Shock Waves.

If the simulation is successful a shock wave should propagate through the cold fluid and hence it is necessary to investigate the behaviour of the code under these conditions. A uniform compressible fluid with constant temperature is assumed. This fluid is then given an initial velocity of 10 m/s in the direction of the rigid interface. The resulting shock wave is monitored for various values of the pseudo-viscosity constant  $\alpha$ . As expected numerical ringing is found to occur behind the shock with  $\alpha = 0$ , this effect being damped out increasingly as  $\alpha$  increases. In addition, the shock front becomes less well defined as  $\alpha$  increases. The speed of the shock is 1504 m/s and the pressure difference is 151 bar, these results being in excellent agreement with the predictions of weak shock theory. Figs. 5 - 9 display how various values of  $\alpha$  affect the shock.





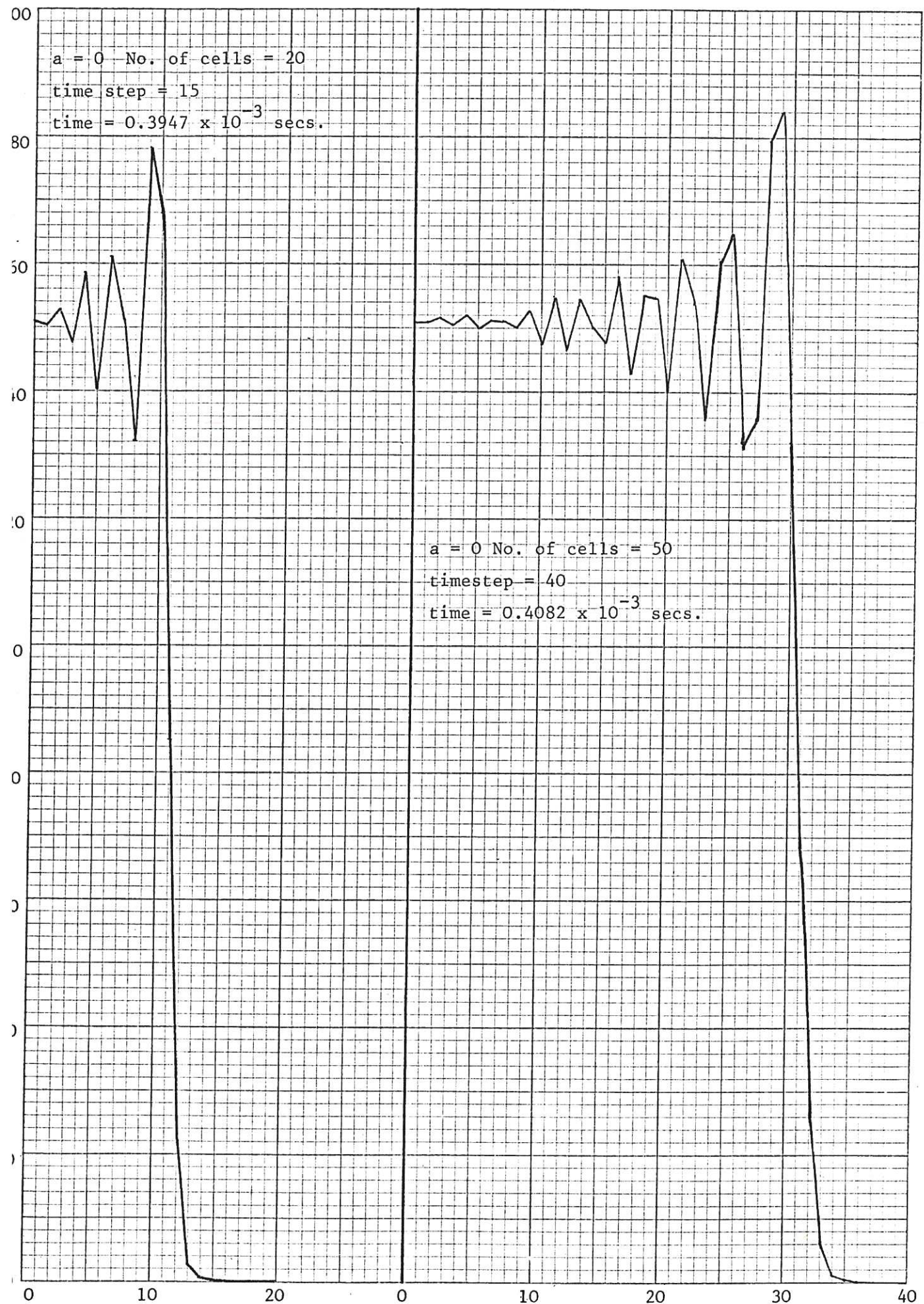


Fig. 5. Shock Test - Pressure (bars) as a function of cell number.



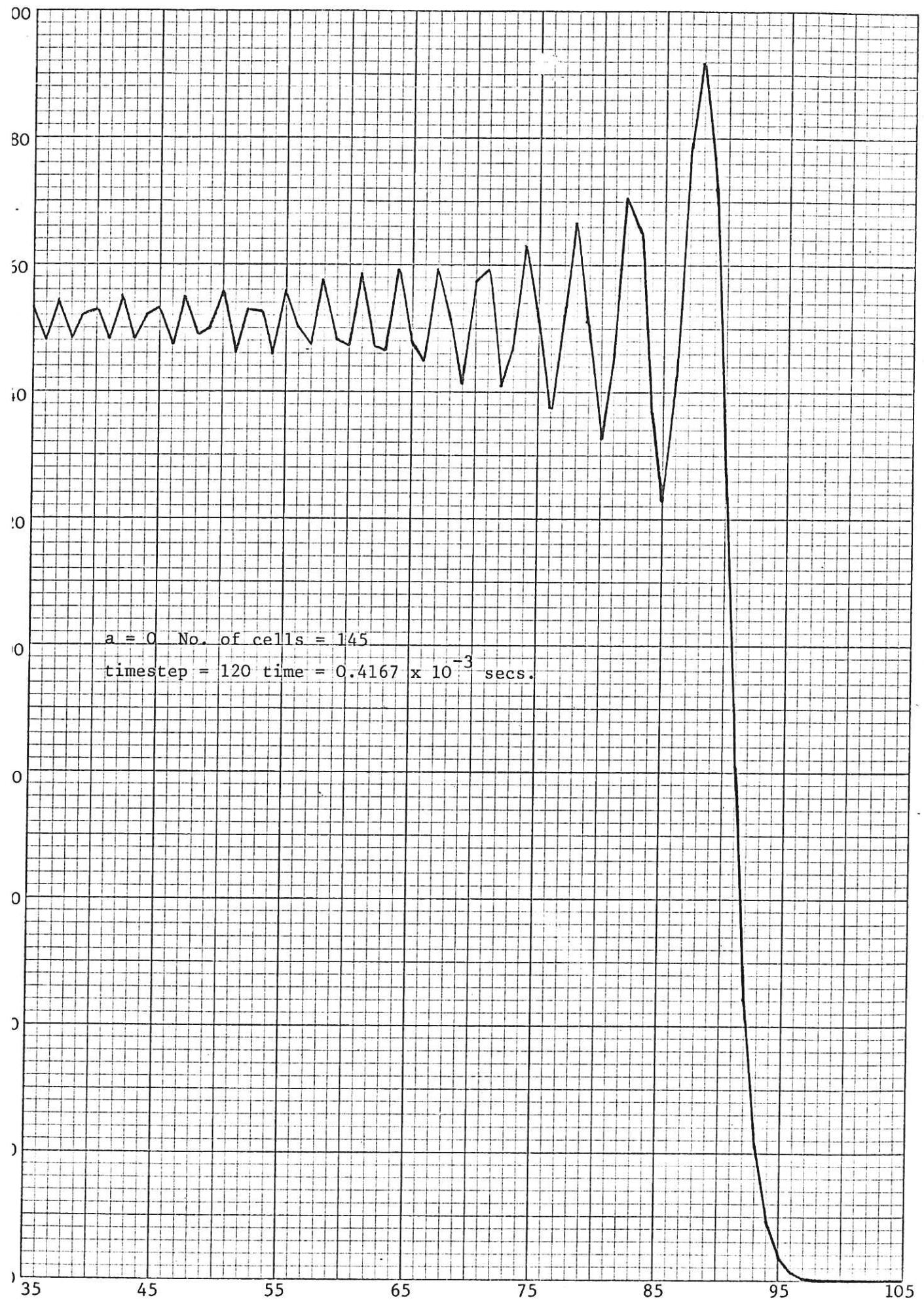


Fig. 6. Shock Test Pressure (bars) as a function of cell number.



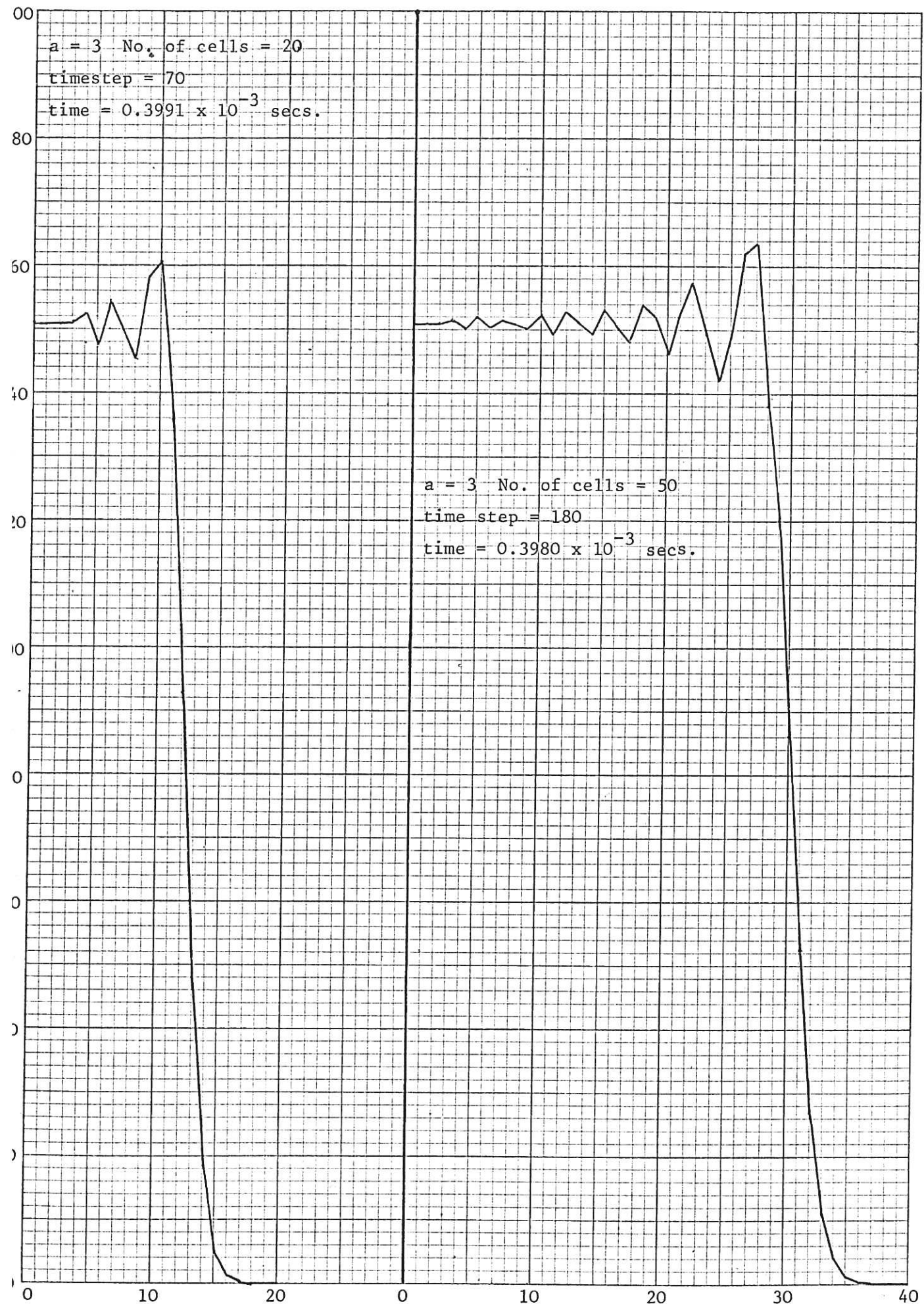


Fig. 7. Shock Test - Pressure (bars) as a function of cell number.



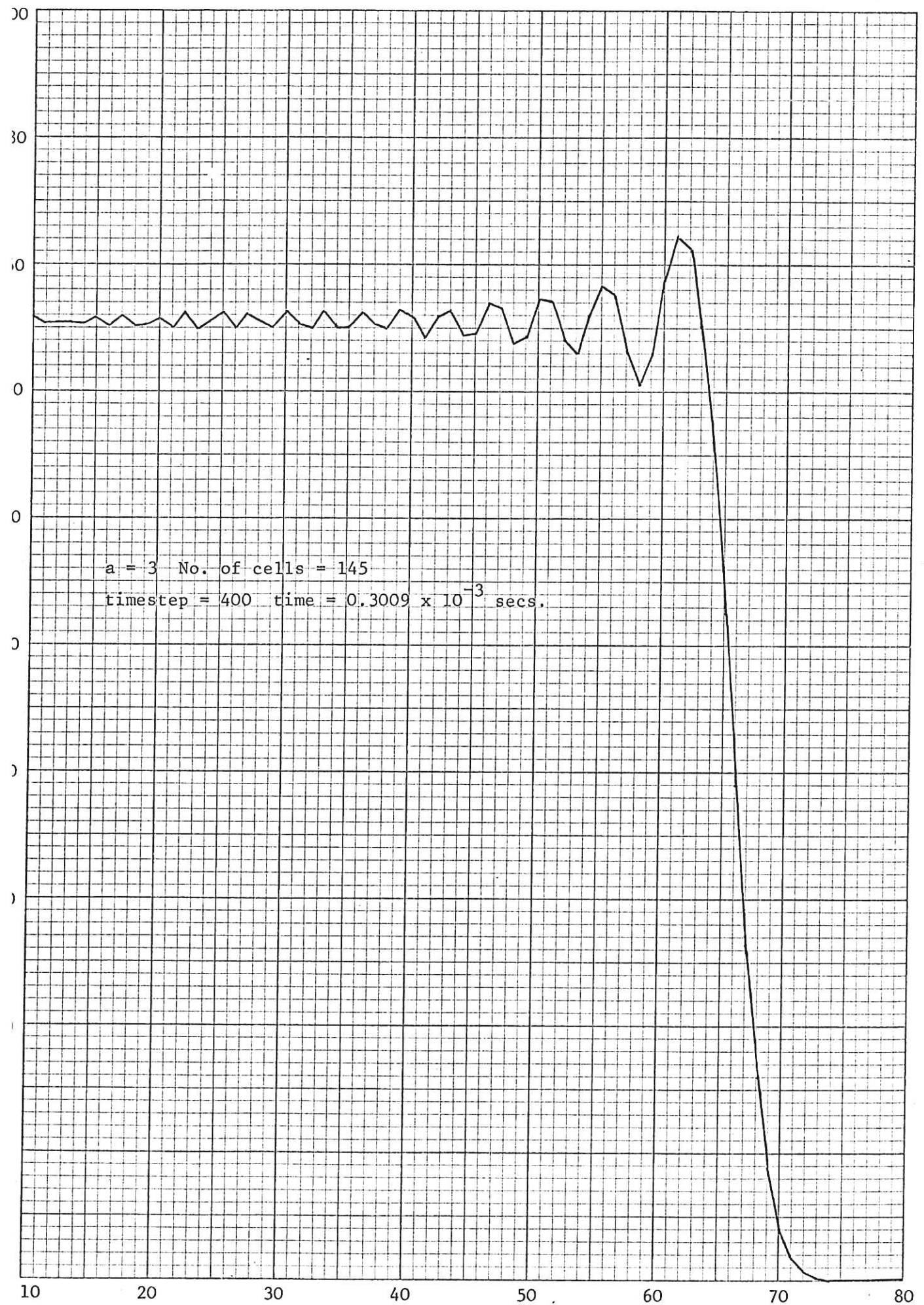


Fig. 8. Shock Test - Pressure (bars) as a function of cell number.





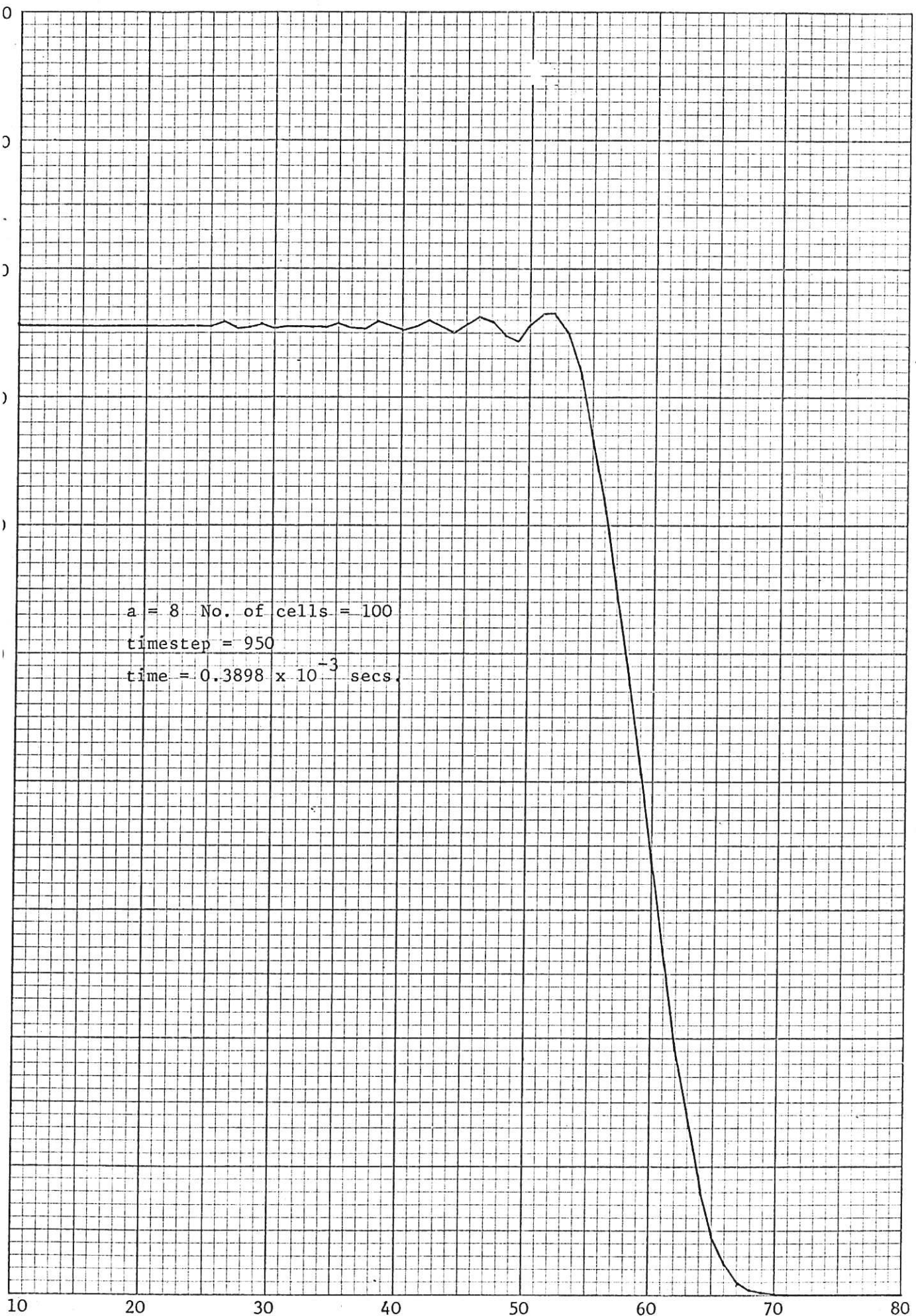


Fig. 9. Shock Test - Pressure (bars) as a function of cell number.



#### D. Phase Changes.

For this test initial conditions are such that a mixture of vapour and liquid is the appropriate equilibrium configuration. The computer prediction of  $\alpha$  may be compared with the value estimated via the definition.

$$\alpha = \frac{V/M - v_l}{v_v - v_l}$$

The results indicated that the code could indeed handle phase changes. For example, with  $V/M = 1/\rho = 2 \times 10^{-3} \text{ m}^3/\text{kg}$  at a temperature of  $473.15 \text{ }^\circ\text{K}$  the code predicted  $\alpha = 0.00634$  while the estimate via the definition of  $\alpha$  is  $0.00669$ . This estimate assumes that the temperature does not change but in fact the temperature must fall; if we use the final temperature predicted by the code to estimate  $\alpha$  via the definition the agreement with the computer prediction is much better.

As a final check a null run of the complete code is appropriate. ie uniform temperature throughout with the initial fluid stationary. Obviously, no changes should occur and this effect, or lack of it, is predicted by the complete code.

#### VI. APPLICATIONS

One of the most important points that must be investigated is, assuming a rapid heat transfer rate, what does the code predict? The crucial factor is, of course, obtaining a rapid heat transfer rate. Initially we may induce this effect by putting in a large contact area at the interface and this will then allow us to ascertain the code's possibilities. With a view to simulating the rapid heat transfer rate more realistically various other mechanisms will be



investigated. We have already mentioned the method by which temperature gradients may be increased; this may, however, introduce spurious pressure increases. Other possibilities are:

1. The contact area may be represented as an increasing function of time with a cut-off when the fluid solidifies.
2. A differential equation governing the increase in area may be proposed and then this equation solved simultaneously with the present equations.
3. Initial conditions can be set up such that bands of hot and cold fluid exist as in Fig. 10.

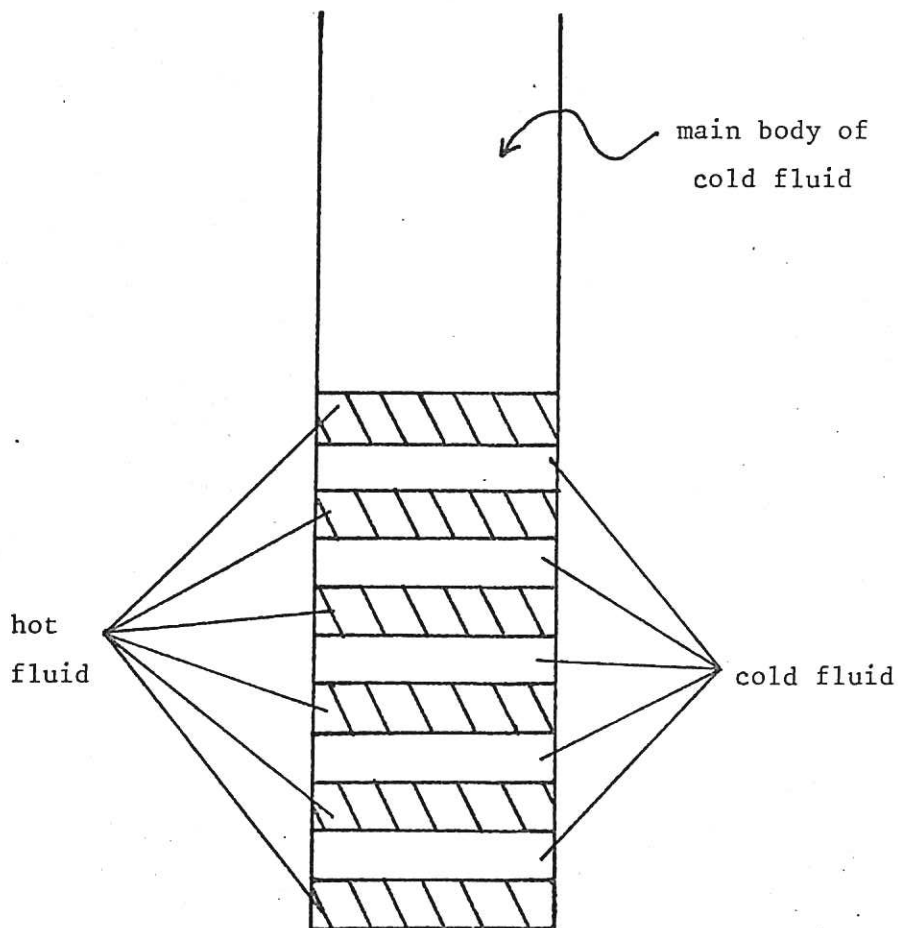


Fig. 10



When a suitably high heat transfer rate has been obtained experiments may be performed using various permutations of the following input conditions:

1. The lengths of the columns may be varied from small distances ( $\sim 1$  mm or less) to large distances ( $\sim 1$  m). ie the code can simulate the detailed behaviour in the region of the interface; alternatively, we may look at the effects far from the interface.
2. Various initial conditions may be imposed such as a variety of initial temperatures, external pressure, etc.
3. The top surface of the column may be either rigid or free corresponding to an open or closed system.
4. Gas layers may be inserted in various regions of the column.

Figures 11 - 14 indicate some typical experiments. (The hot fluid is the bottom layer).

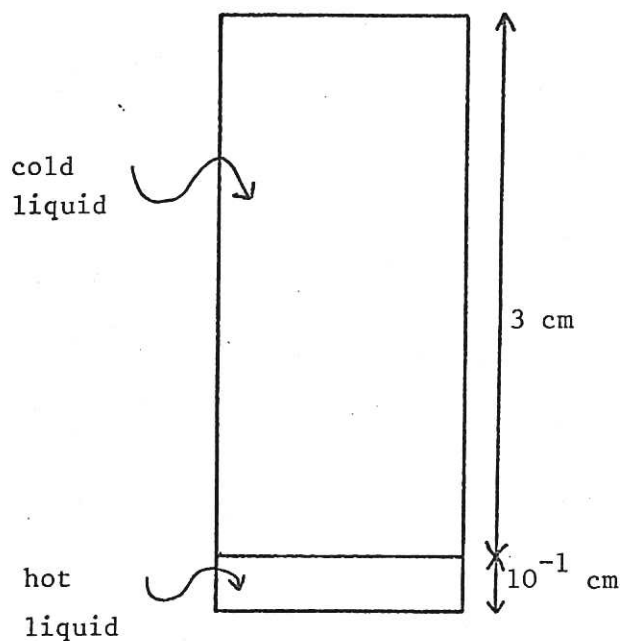


Fig. 11. Complete Simulation

The typical dimensions shown are determined by the shock transit time of water and the diffusivity of aluminium assuming that the total elapsed time is of the order of 1 ms.





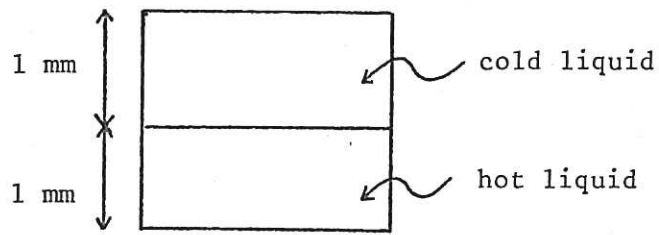


Fig. 12. Investigation of Vapour production.

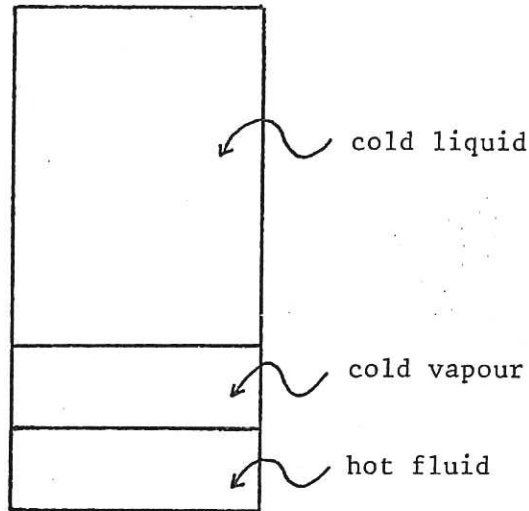


Fig. 13. Investigation of Propagation of Shock Wave after Vapour Layer is Formed.

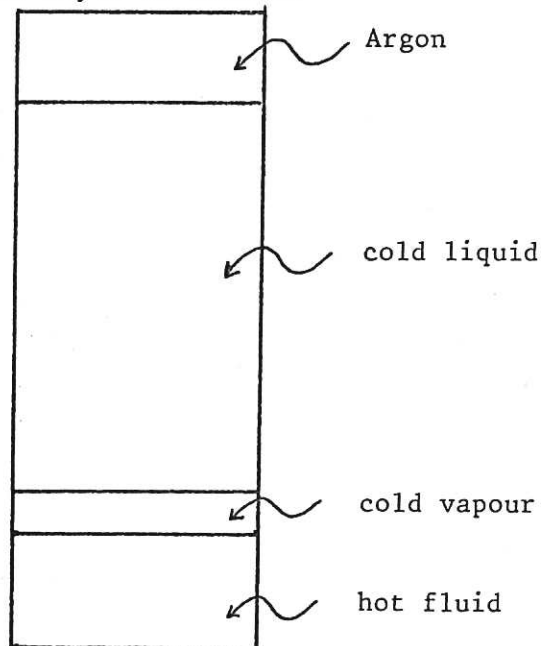


Fig. 14. Effect of Inert Gas Layers.



Two possible long term developments are:

1. To produce a version of the code with sodium and uranium dioxide as the working fluids.
2. To produce a version of the code which simulates three dimensional spherically symmetric problems. A typical problem that could then be dealt with is that of bubble growth.

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