## 5.2. FORTRAN Program

The FORTRAN IV program used for the calculations is given in Appendix III. This program is set up specifically for the problem of a constant driving pressure and a semi-infinite slab of material so it does not treat an unloading rarefaction problem nor the reflection of a shock wave.

The heart of the program, insofar as we are concerned, is in the calculation of $\alpha$, p and T, following that of v and q (Eqs. (5.10) through (5.13) above); therefore we consider it in detail.

When the material of cell j is in the region of phase 1, as determined by a test on p, the numerical computation proceeds to Eqs. (5.12) and (5.13) from Eq. (5.8). When the pressure in cell j reaches the transition value $p_M$ and overshoots it, temperature and the relative specific volume of phase 1 must be readjusted by use of Eqs. (5.11) and (5.12). At this time the special program parameter NSA(J) is set equal to 2 for the cell j and kept at that value until the material is all converted to phase 2. Calculation of pressure is accomplished by substituting $v_1$ and T from Eqs. (5.11) and (5.12) into (5.13). Once the given cell becomes pure phase 2, NSA(J) is set equal to 3, and the calculation again proceeds as for phase 1. However, as long as we use the relaxation relation (Eq. (3.26)), with the approximation ($v_2$-$v_1$ = constant), we always have:

$$\alpha < 1$$

$$v_1 = v - \alpha(v_2 - v_1). \qquad (5.14)$$

If we are reminded that pressure is essentially calculated from $v_1$, then from Eq. (5.14), regardless of whether we set $\alpha$ to unity when it is close to unity, the value of $v_1$ is practically the same. Therefore we can, for the present case, discard the case for NSA(J) = 3, which is enclosed by the dotted lines in the flow chart.

The expanded flow chart for this part of the program is given in Fig. 5.3.

## 5.3. Numerical Results

### 5.31 Transient Case

The particular concern here is with development of the double wave structure associated with the phase transition. A uniform pressure is applied at time t = 0 to the surface of a half space, x = 0, and maintained constant as the plane wavefront develops and propagates inward. For an applied pressure of 0.200 Mbar*, Figs 5.4 and 5.5 show pressure profiles of the developing wave at times measured from the first application of pressure. Fig. 5.4 illustrates the development and decay of the first wave caused by the $\alpha$ - $\varepsilon$ phase transition. After about ten relaxation times the profile has the clear double-wave structure shown in Fig. 5.5.

The thickness of the first wave front is determined by q and by the choice of space increment, $\Delta x$ (Fig. 5.1). The width of the second front is controlled by the relaxation time of the phase transition. When it is well separated from the first wave,

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*1 Megabar = $10^{12}$ dynes/cm$^2$