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TOIL

(A Two-material Version of the OIL Code)

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July 7, 1967

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The TOIL computer code is described herein as it existed on July 7, 1967. The code has been in continuous development for one year and in its presented form has been applied successfully by General Atomic to the kind of problems discussed later in this report. However, the development and improvement of the code are being continued, so that duplication of results (or even close agreement) between problems run with the code as published and the code as it existed either before or after this time is not necessarily to be expected.

General Atomic has exercised due care in preparation, but does not warrant the merchantability, accuracy, and completeness of the code or of its description contained herein. The complexity of this kind of program precludes any guarantee to that effect. Therefore, any user must make his own determination of the suitability of the code for any specific use, and of the validity of the information produced by use of the code.

— A modification of the OIL code, to treat two different materials (two equations of state) has been formulated.

One of the advantages that a Lagrangian formulation has over an Eulerian formulation is the ability and ease at which material interfaces can be represented and propagated. Several approaches are possible for following a material interface in an Eulerian formulation. Several investigators are following interfaces (material) as they move through the fixed Eulerian grid. Others have combined Eulerian with Lagrangian formulation.

This scheme to be reported requires very little modification to the OIL⁽¹⁾ code. Familiarity with the OIL code is assumed.

There are four (4) regions or steps in the OIL code that require modification for treating two different materials:

- (1) Maintaining an interface between materials which is accomplished by a mixed cell, in other words, the interface lies somewhere in our mixed cell.
- (2) Calculating the pressure in a mixed cell.
- (3) The manner in which the change in specific internal energy due to pressure forces only (PH1) is to be distributed to a cell containing both materials.
- (4) The scheme in PH2 (the calculation of the transport terms) of distributing the specific internal energy (the total less the kinetic) for the cells containing both materials.

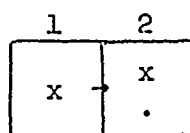
Item 1. requires modification of the subroutine (PH2). The discussion will be concerned with the radial direction of mass transport, the mass transport in the axial direction being similar. Calculation of the masses that cross the fixed Eulerian boundaries are performed as in OIL, however the density ρ in $\Delta M = \bar{\rho} \bar{u} A \Delta t$ (\bar{u} is the weighted velocity, A the area and Δt is the time step) is calculated on the basis of the total mass in the

cell. Thus, up to this point, we have calculated the mass fluxes, now we must determine (for a mixed cell) how much of each material to move. Three possible situations concerned with two materials arise.

1. Material moving from a non-mixed cell to a mixed cell.

This presents no difficulty or modification.

Example (non-mixed to mixed)



Mass flow is from cell 1 to cell 2.

$$\Delta M = \rho^1 \bar{U} A \Delta t$$

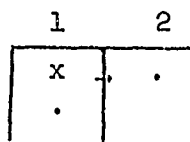
$$\Delta M_x = \Delta M$$

$$\Delta M_{\cdot} = 0$$

where ρ^1 = density of x material in cell 1.

2. Material moving from a mixed cell to a non-mixed cell is calculated as follows: The acceptor material from the donor cell is moved to the acceptor cell. If the flux is such that this will more than empty the acceptor material from the donor cell, the excess is removed by assigning it to the other material.

Example (mixed to non-mixed)



Mass flow is from cell 1 to cell 2.

$\Delta M = \rho^1 \bar{U} A \Delta t$ where ρ^1 is the total density of both materials in cell 1 if $\Delta M > M_{\cdot}^1$

$$\Delta M_{\cdot} = M_{\cdot}^1$$

and

$$\Delta M_x = \Delta M - M_x^1$$

if $\Delta M \leq M_x^1$

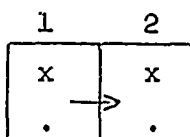
$$\Delta M_x = \Delta M$$

and

$$\Delta M_x = 0$$

3. Material moving from a mixed cell to a mixed cell requires some modification in order to keep the material interface defined in a single mixed cell. The prescription or recipe if you like, is that each material flux is weighted by the fraction of its mass to total in the acceptor cell, rather than the donor cell.

Example (mixed to mixed)



Mass flow is from cell 1 to cell 2.

$\Delta M = \rho^1 \bar{U} A \Delta t$, where ρ^1 is the total density of both materials in cell 1. Then

$$\Delta M_x = \frac{M_x^2}{M_x^2 + M^2} \Delta M$$

and

$$\Delta M^1 = \frac{M^2}{M_x^2 + M^2} \Delta M$$

Note: the superscripts refer to zone number and the subscript to material number.

Item 2 is the calculation of the pressure in a mixed cell. The present scheme is to iterate on the volume occupied by each material until the two pressures calculated are the same. The partial volumes of each material are saved for use in (PHL).

Item 3 concerns the change in specific internal energy for a mixed cell due to pressure forces only in (PHL). The change in internal energy for the entire cell is

$$\Delta Q = \Delta t (\text{Vol}) P \left[\frac{\partial v}{\partial z} + \frac{1}{r} \frac{\partial ru}{\partial r} \right] .$$

The change in specific internal energy for each material is proportional to the density of each material, or

$$\Delta I_x = \frac{\Delta Q}{f} \frac{1}{\frac{M_x}{f} + \frac{M}{1-f}}$$

and

$$\Delta I_{\cdot} = \frac{\Delta Q}{1-f} \frac{1}{\frac{M_x}{f} + \frac{M}{1-f}}$$

where (x) and (·) refer to the two different materials and f is the factor to multiply times the volume of the total cell to calculate the volume occupied by (x) material.

Item 4 deals with the specific internal energy due to the transport terms. The specific internal energy for each material is proportional to the specific total energy of that material (the total specific energy of the cell plus that which is transported in less the amount transported out).

$$\Delta E_x = \Sigma M_x \left[\tilde{I}_x + \frac{\tilde{U}^2 + \tilde{V}^2}{2} \right]$$

$$\Delta E_{\cdot} = \Sigma M_{\cdot} \left[\tilde{I}_{\cdot} + \frac{\tilde{U}^2 + \tilde{V}^2}{2} \right]$$

Where the (·) tilda refers to the velocities and specific internal energy after (PHL).

$M_X^{n+1} = \Delta M_X$ = total mass of cell plus that which is transported in less the amount transported out for the x material.

$M_\cdot^{n+1} = \Delta M_\cdot$ = similar term for the dot material.

Then the new internal energy for the mixed cell is

$$Q = \Delta E_\cdot + \Delta E_X - \frac{1}{2} \left(U_{n+1}^2 + V_{n+1}^2 \right) (\Delta M_X + \Delta M_\cdot) .$$

Thus each material then has the following specific internal energy

$$I_X^{n+1} = \frac{\Delta E_X}{\Delta M_X} \frac{Q}{\Delta E_X + \Delta E_\cdot}$$

$$I_\cdot^{n+1} = \frac{\Delta E_\cdot}{\Delta M_\cdot} \frac{Q}{\Delta E_X + \Delta E_\cdot} .$$

TEST PROBLEMS

The first test problem was a comparison with SHELL (a two-material particle-in-cell code). A right circular cylindrical projectile of density three times that of the target impacted at a velocity of 1×10^6 cm/sec into a semi-infinite target. A separate equation of state was used for each material.

Figure 1 displays the position of the projectile relative to the target. An (x) signifies that this cell was the original projectile, a (dot) signifies target material and an (M) signifies that the cell is mixed (contains both materials).

Figure 2 is a similar plot for the TOIL results. The position of the material interface, as indicated by the M's, is in good agreement between the two codes.

The total positive axial momentum in the grid as a function of time is displayed for the two codes in Fig. 3. The $\sim 6\%$ difference at late times is comparable to the differences calculated between SHELL and OIL.⁽²⁾

Figures 4 and 5 display pressure versus position along the axis into the target. The position of the shock front is in good agreement.

A comparison with the one-material Eulerian code (OIL) was made using TOIL for an aluminum right circular cylinder impacting at 2.6×10^6 cm/sec on a semi-infinite aluminum target. The same density and same equation of state was used for both the projectile (right circular cylinder) and the semi-infinite target. One would expect some differences due to the method of transporting mass from a mixed to a non-mixed cell.

Figures 6 and 7 display the position of the projectile relative to the target. Figure 8 displays the total positive axial momentum versus time for the comparison.

Figures 9 and 10 display pressures versus position along the axis for the two different times. The agreement is very good, considering the times are slightly different.

A spherical hot source problem was performed using two materials with the TOIL code and compared with a spherical version of the SPUTTER (a one-dimensional Lagrangian code).

Figure 11 indicates the original mixed interface between hot and cold material, and Figs. 12 and 13 display the material interface as a function of time. The sphericity of the material interface is indeed encouraging.

Figure 14 is the pressure versus position (radial or axial from TOIL) for the comparison between TOIL and SPUTTER. The near agreement, again, is very encouraging.

Additional test problems are being calculated. In addition, several calculations for DASA have been successfully performed using the TOIL code.

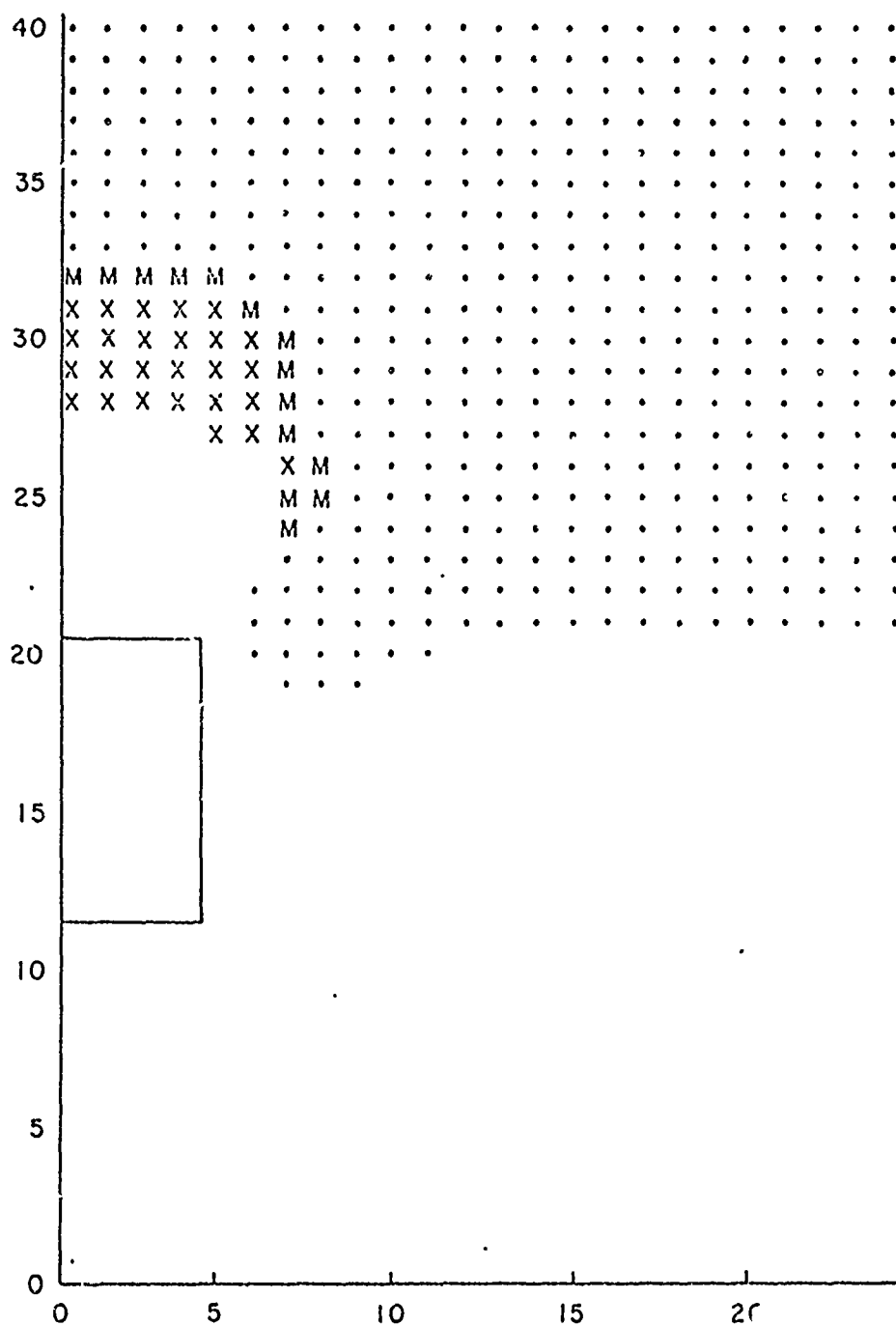


Fig. 1--Cell configuration for the SHELL code at a time of 17.4 μ sec

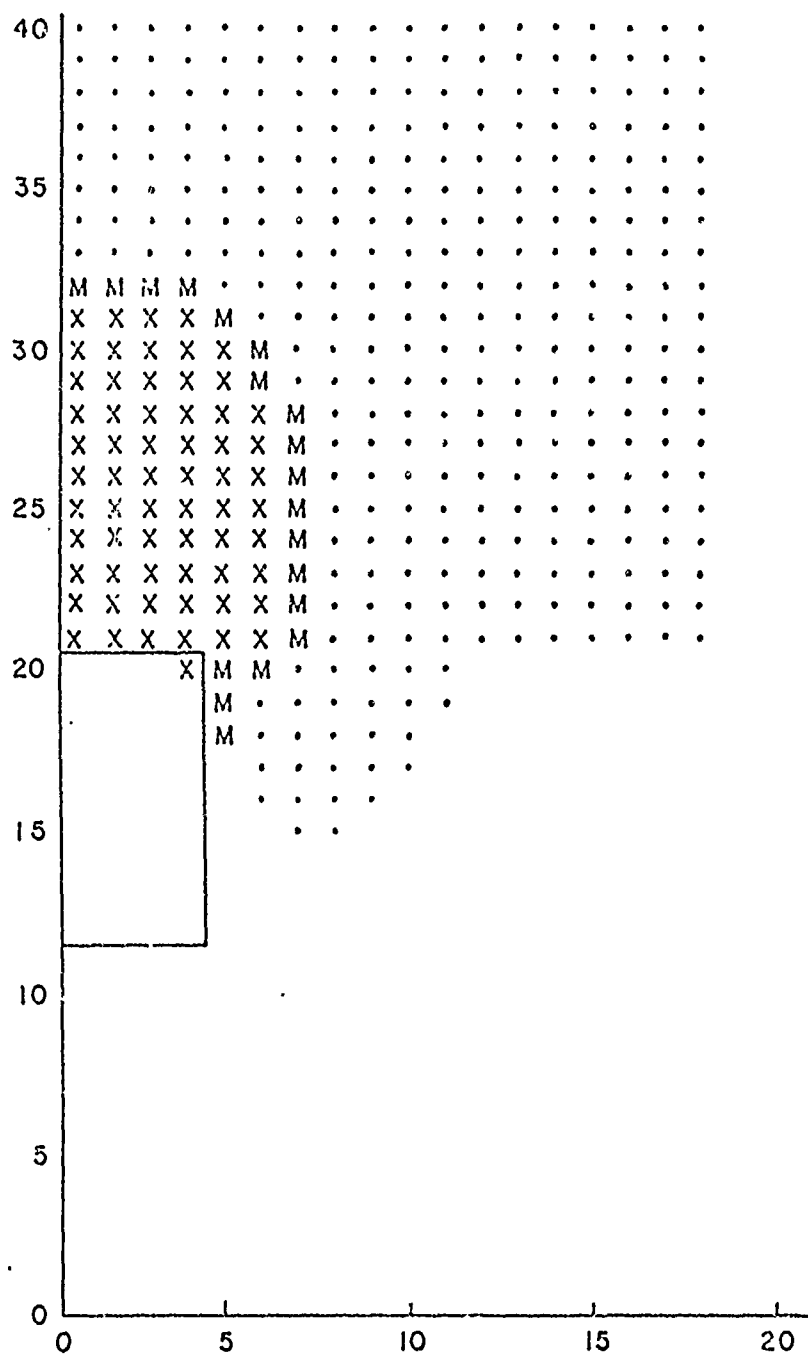


Fig. 2--Cell configuration for the TOIL code at a time of 16.1 μ sec

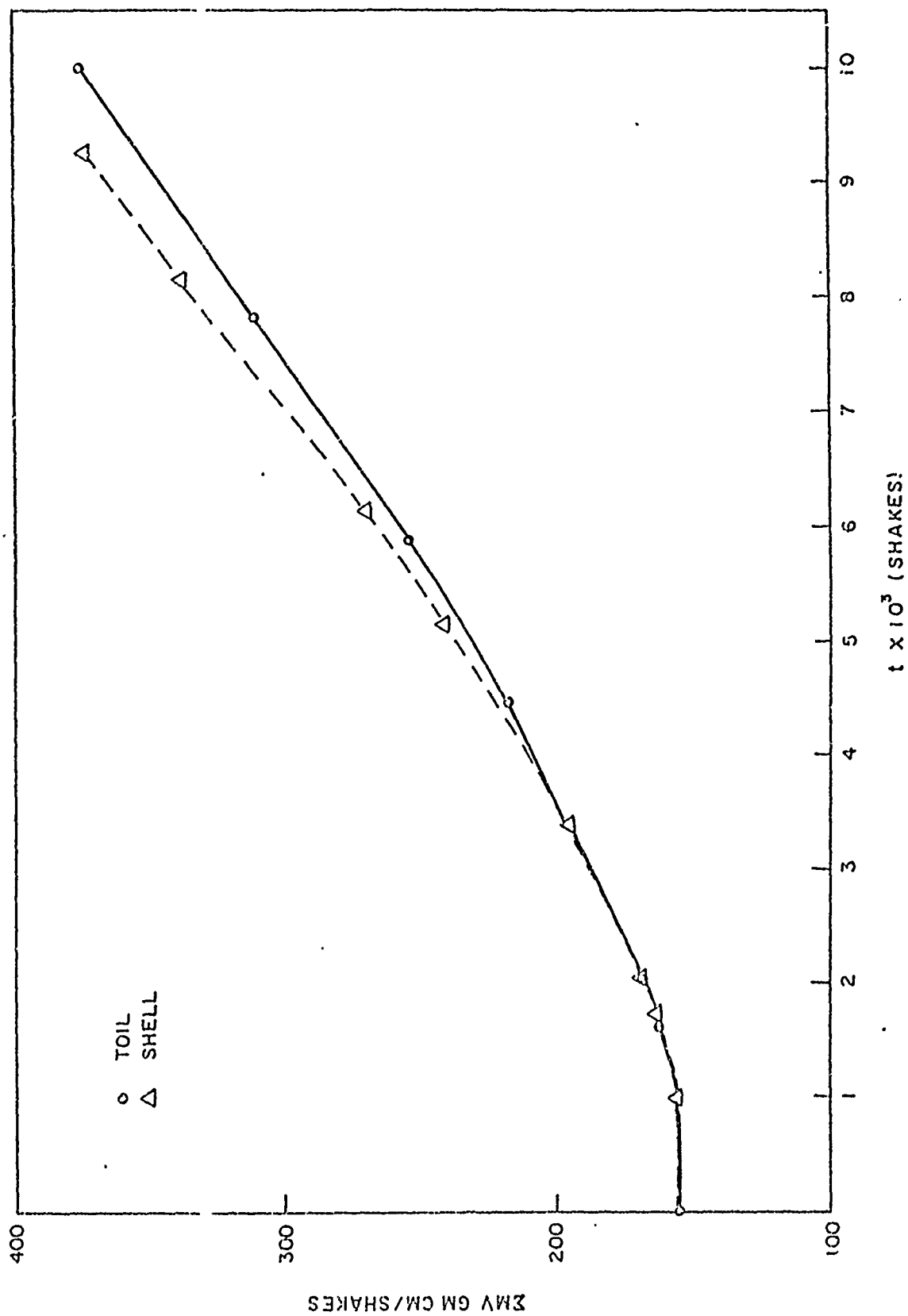


Fig. 3--Total positive axial momentum versus time

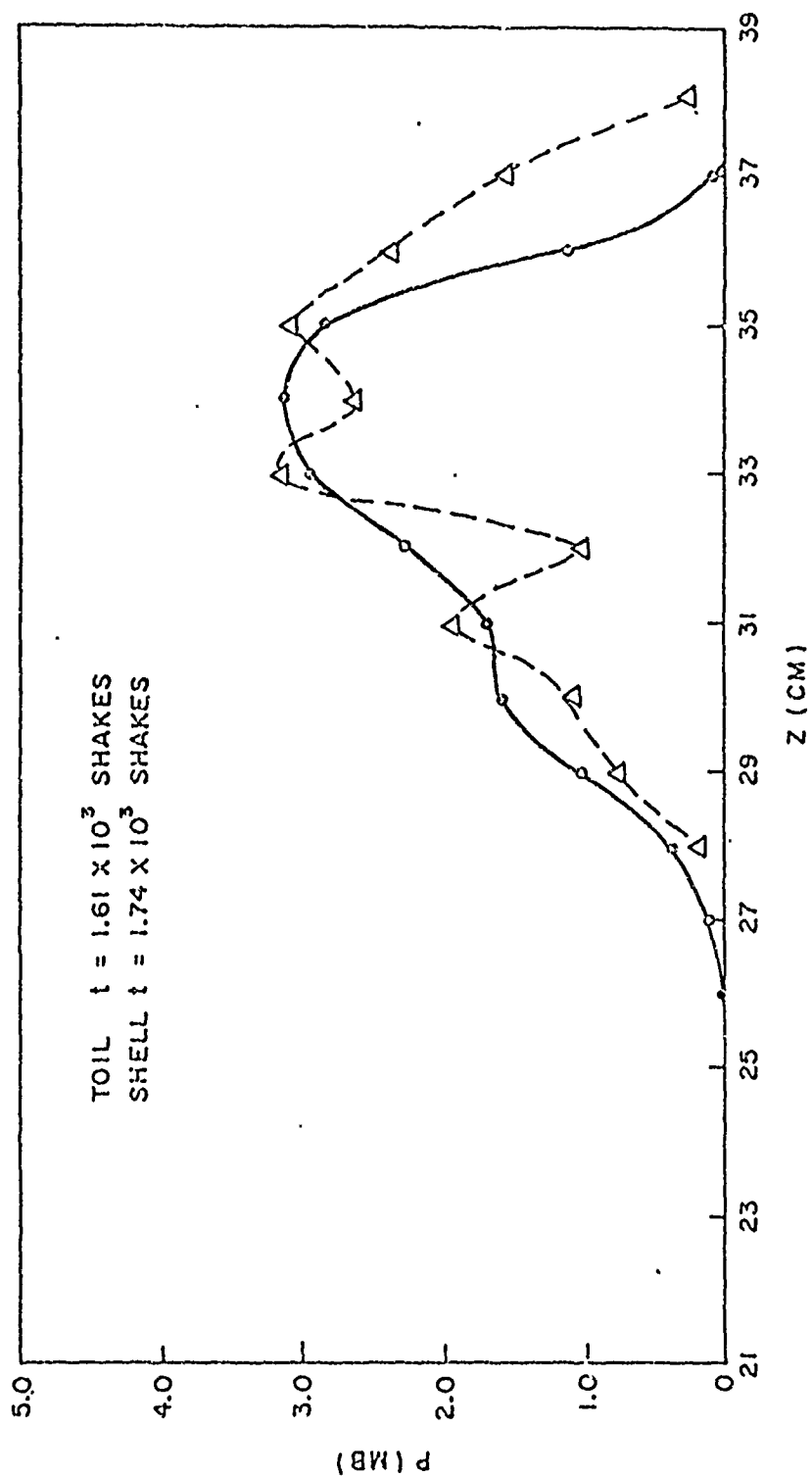


Fig. 4--Pressure distribution along the axis

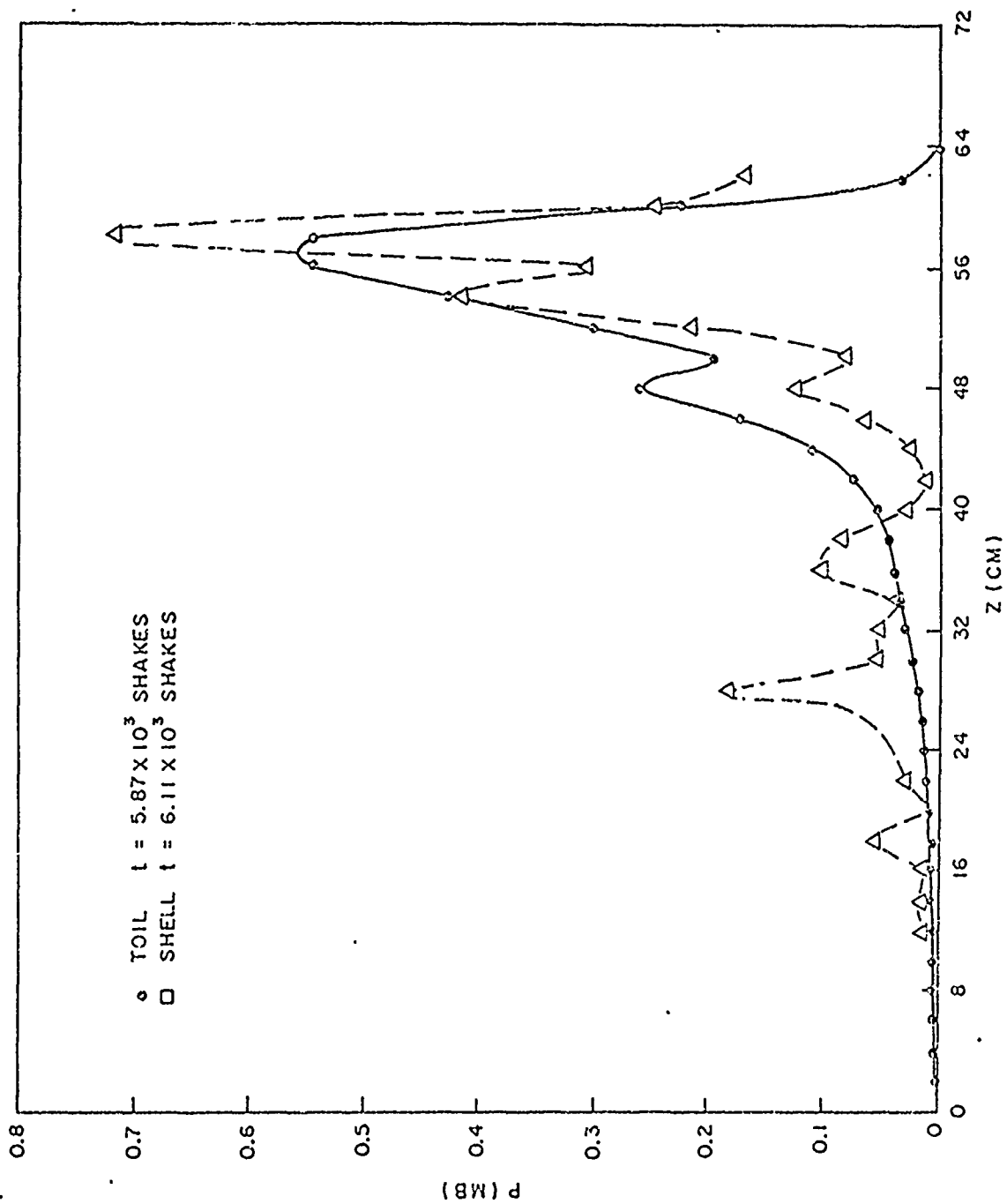


Fig. 5--Pressure distribution along the axis

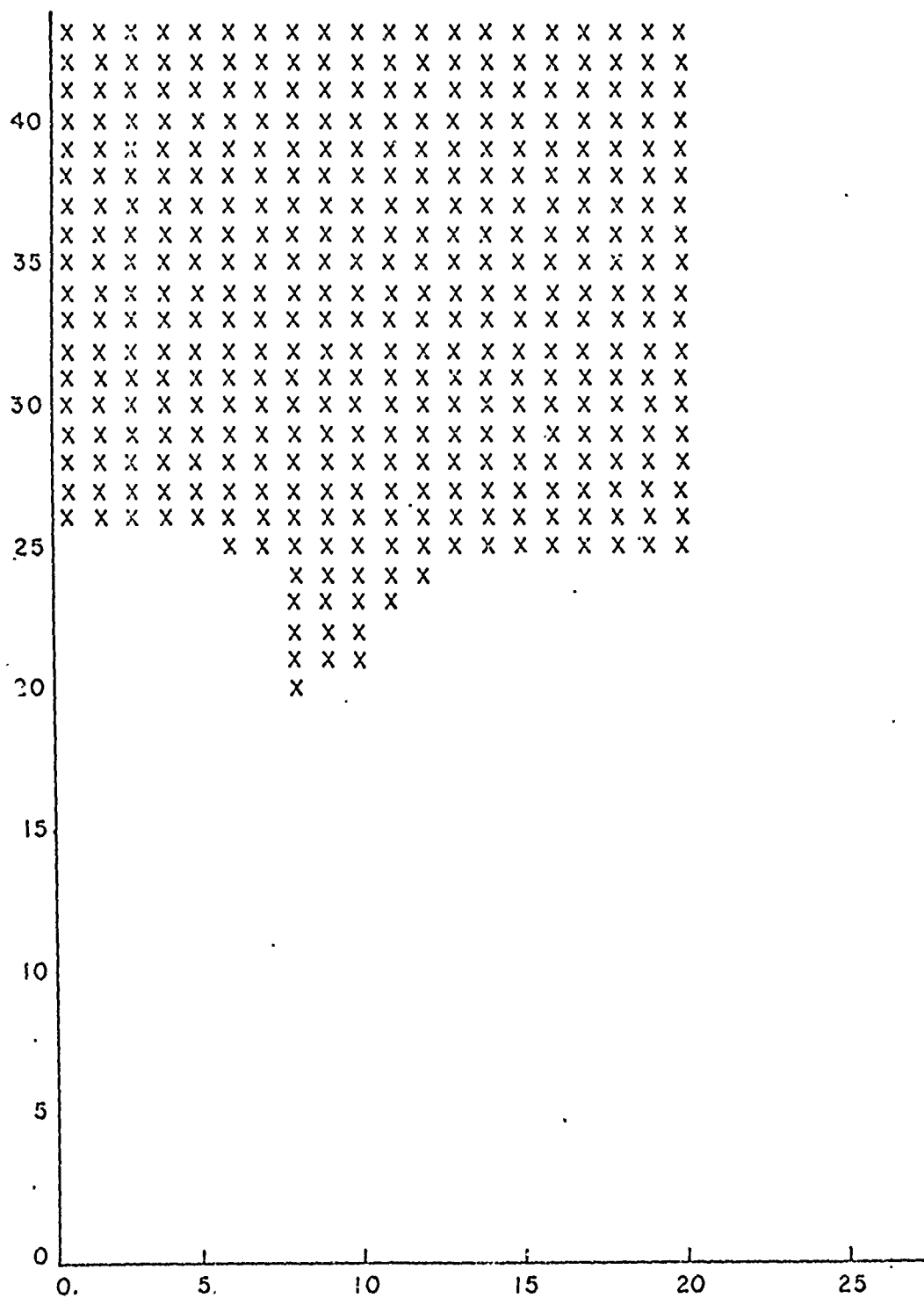


Fig. 6--Cell configuration for the OIL code (Note, no distinction made between the projectile and target material) at $t = 6.19 \mu\text{sec}$

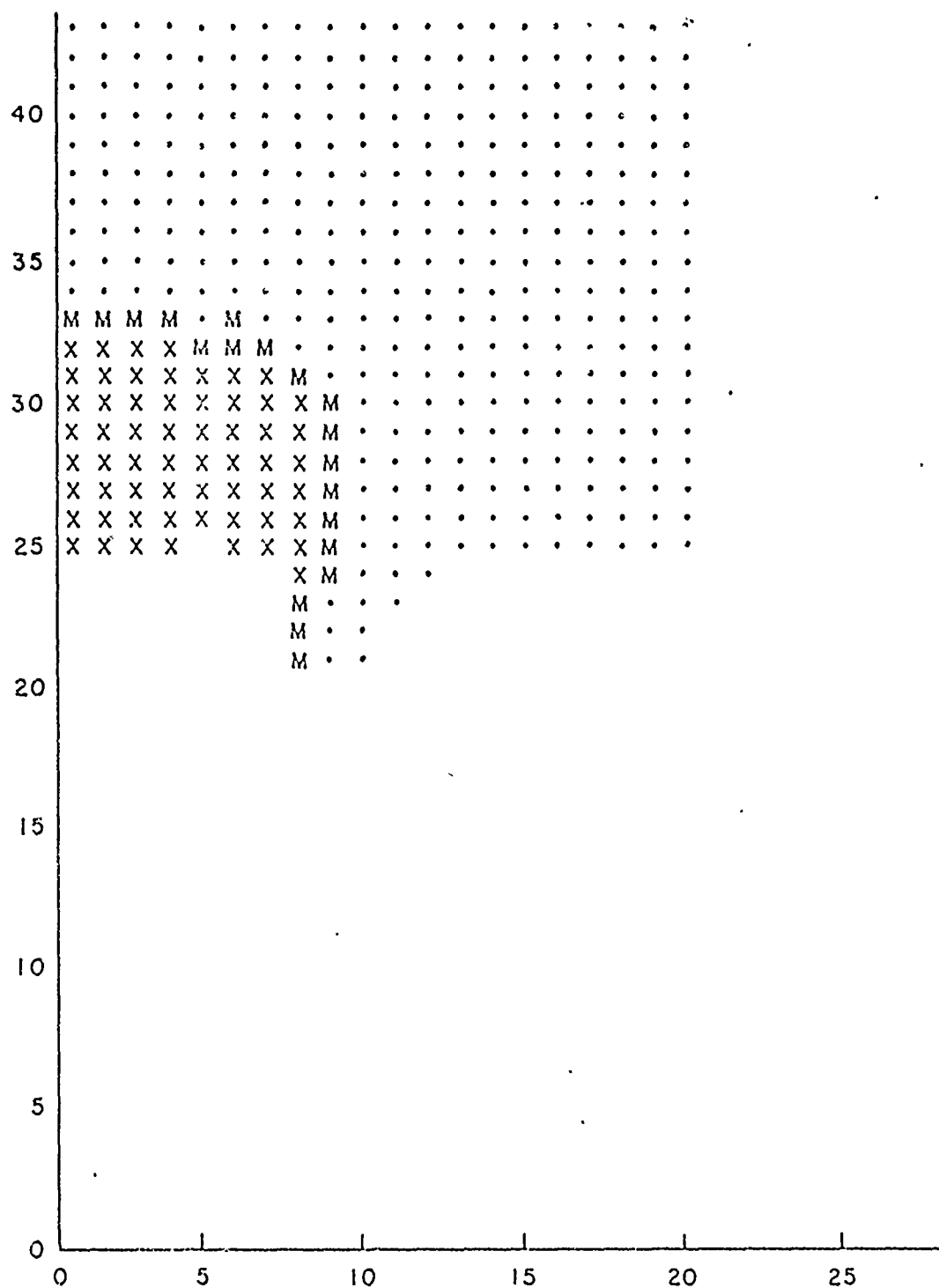


Fig. 7--Cell configuration for the TOIL code (Note, the distinction made between the projectile and target material) at $t = 6.19 \mu\text{sec}$

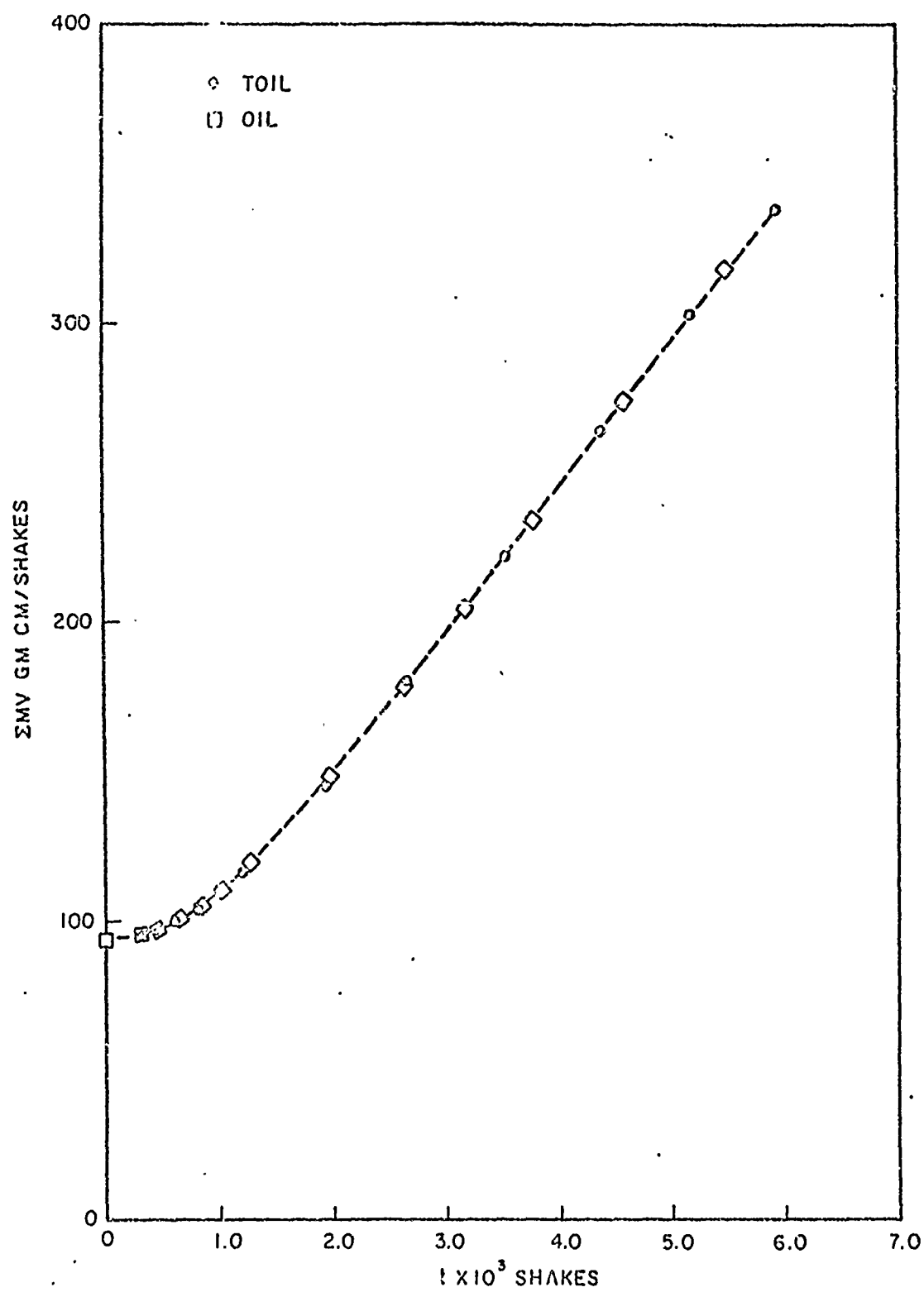


Fig. 8--Total positive axial momentum versus time for the TOIL-OIL comparison

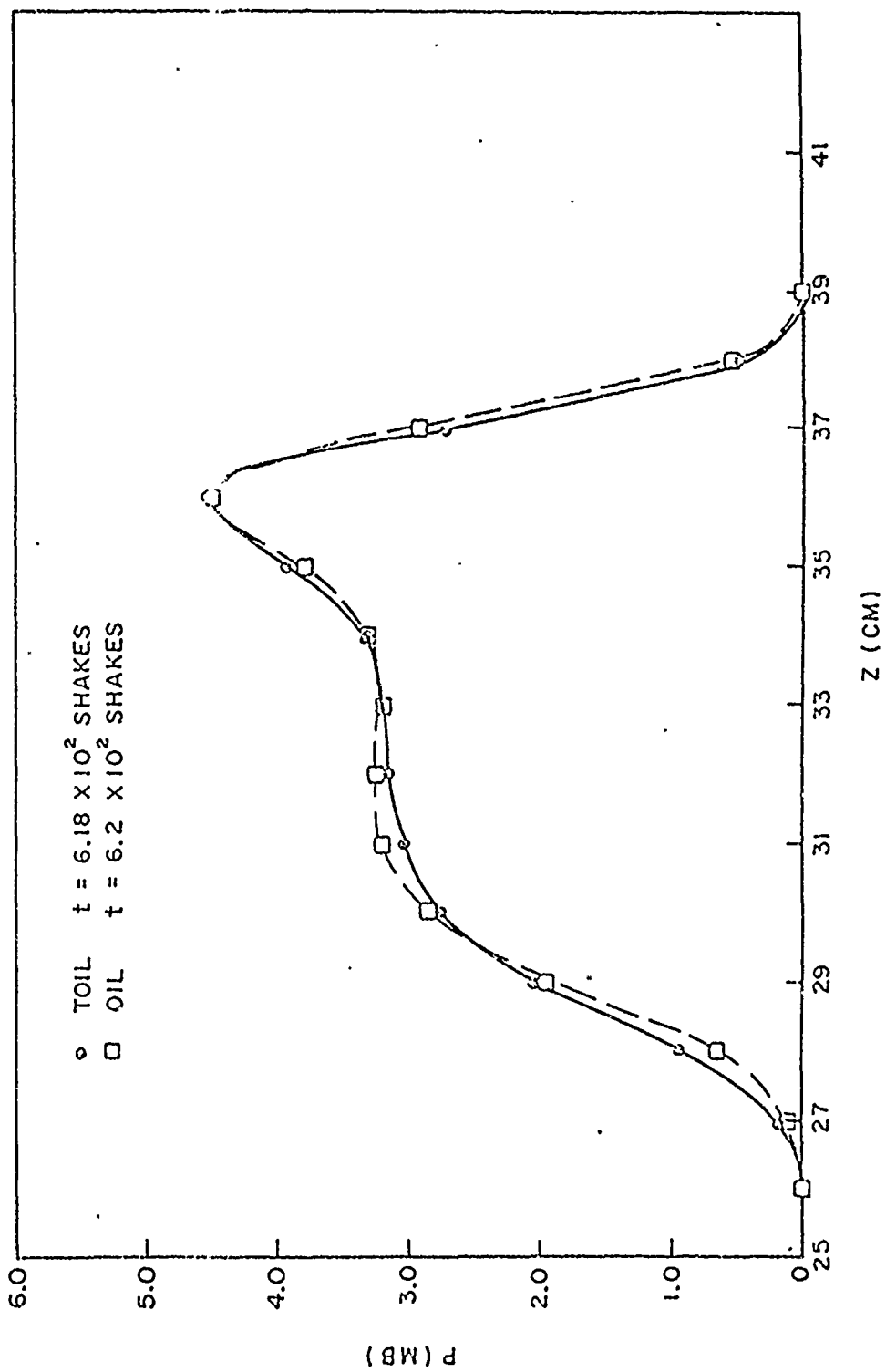


Fig. 9--Pressure distribution along the axis

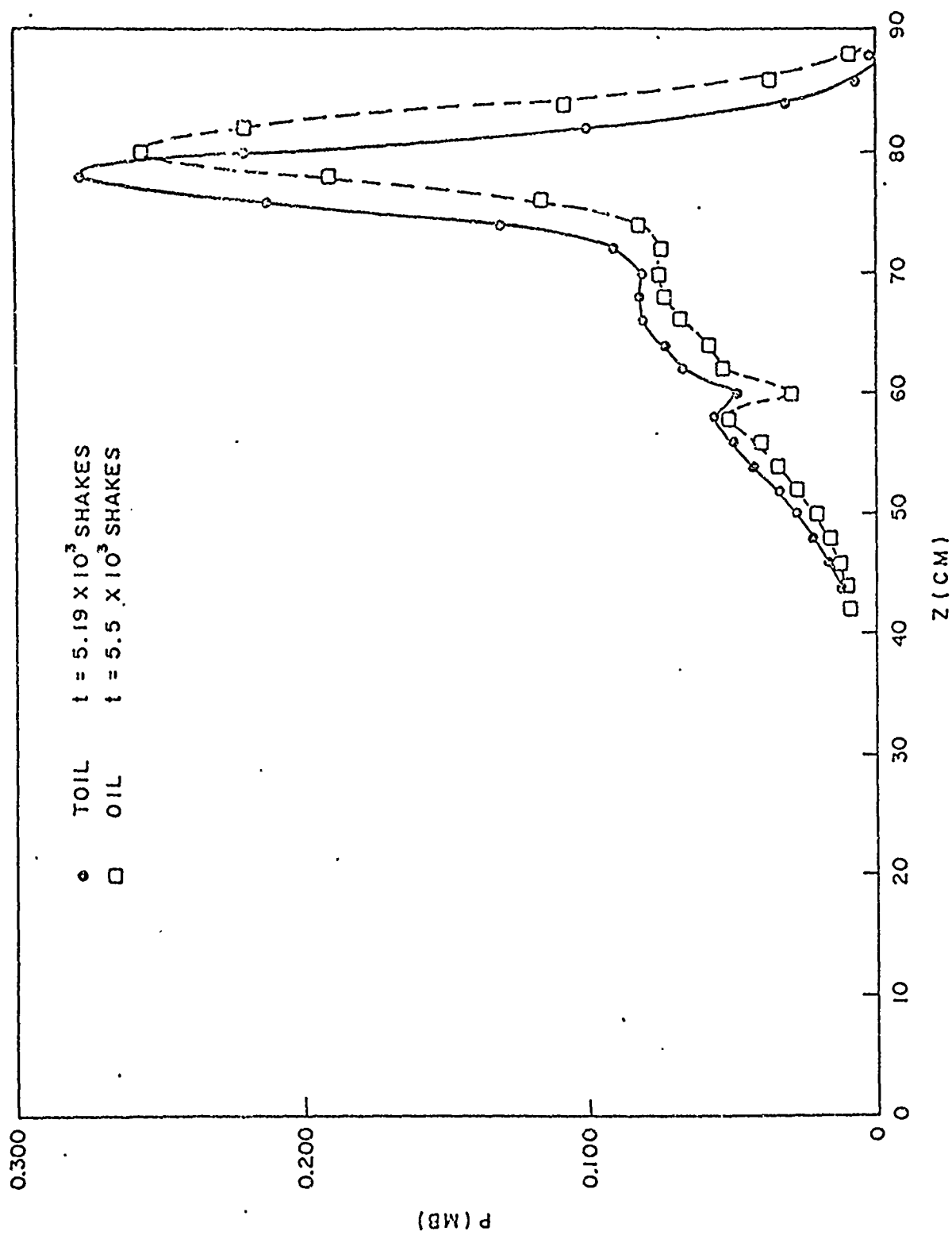


Fig. 10--Pressure distribution along the axis

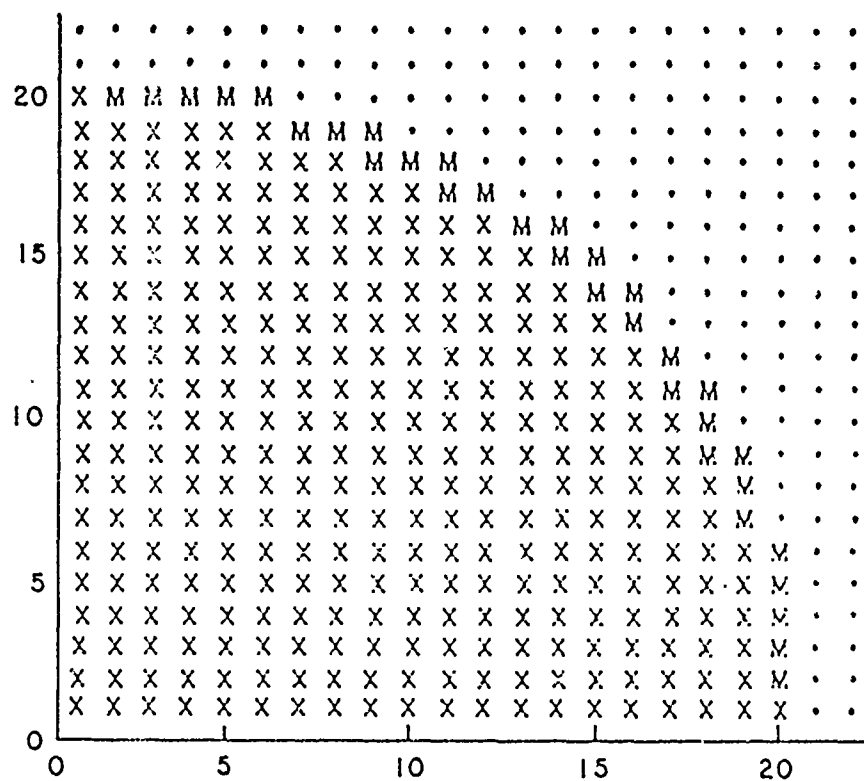


Fig. 11.--Cell configuration for the TOIL code (Note, x is for the hot material, dot for the cold material and M signifies both materials on the interface) at $t = 0$

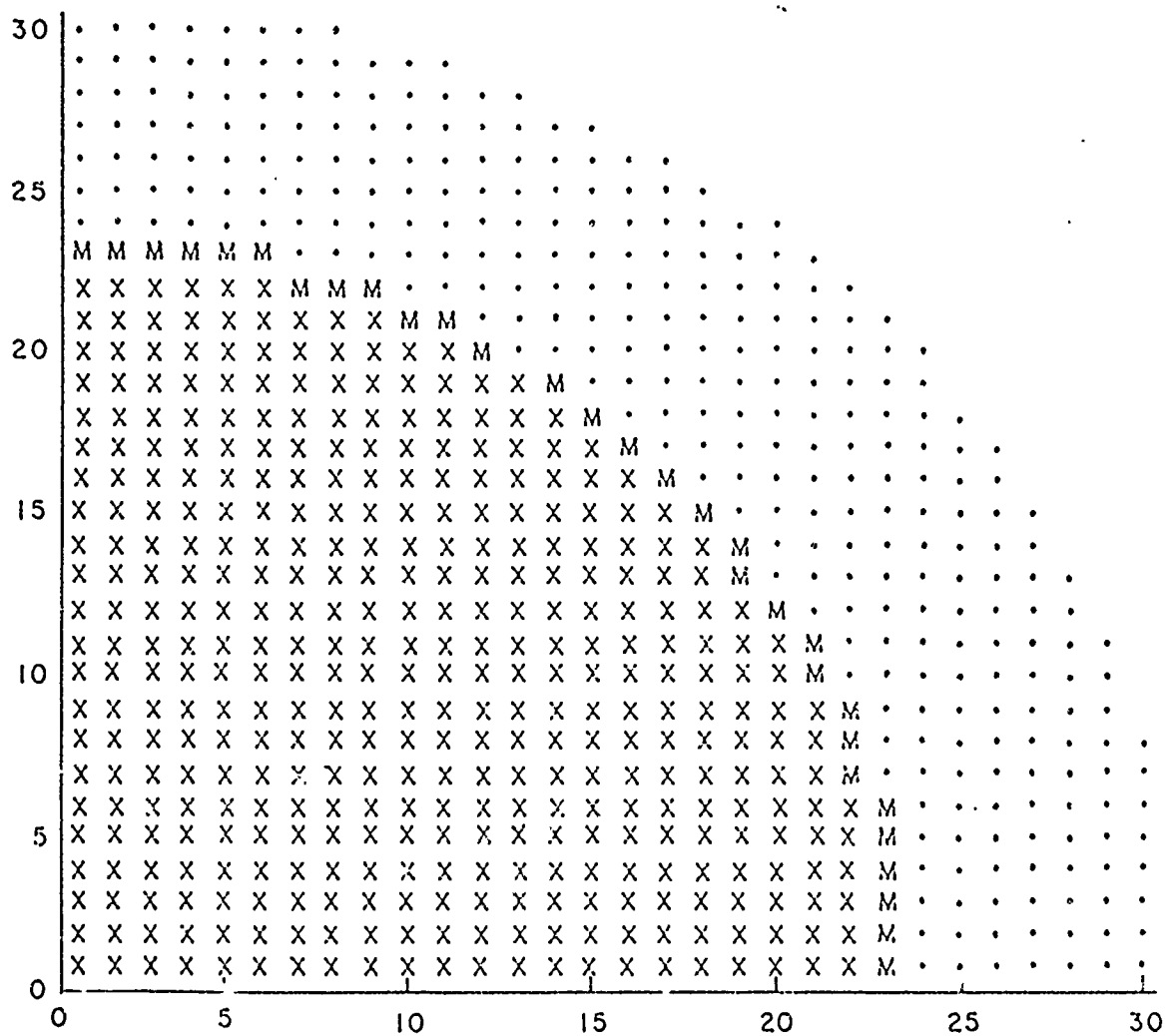


Fig. 12--Cell configuration for the TOIL code at $t = .96 \mu\text{sec}$

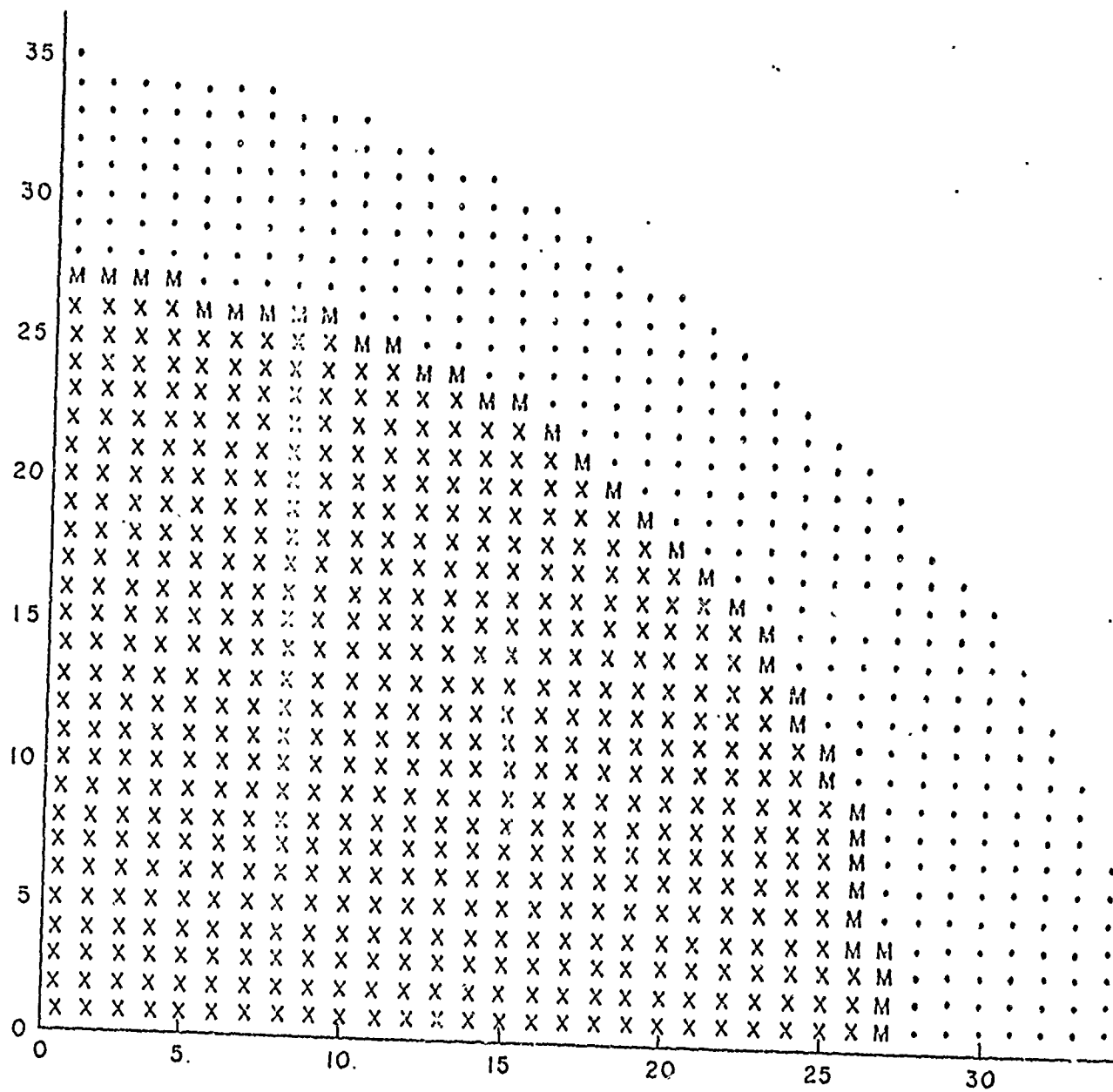


Fig. 13--Cell configuration for the TOIL code at 2.25 μ sec

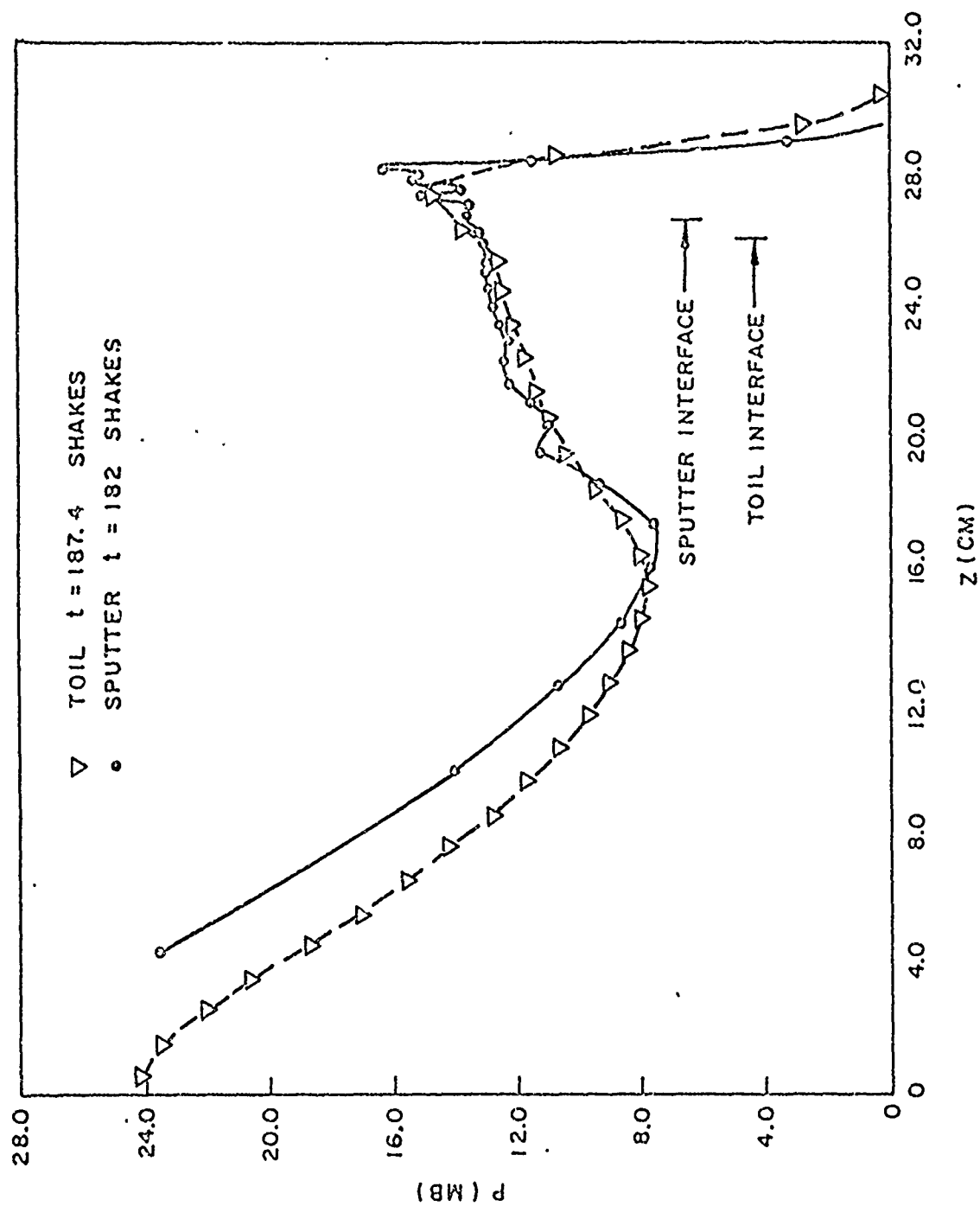


Fig. 14--Pressure versus distance for the TOIL-SPUTTER
(one-dimensional Lagrangian) comparison

REFERENCES

1. Johnson, W. E., "OIL--A Continuous Two-dimensional Eulerian Hydrodynamic Code," General Atomic Report GAMD-5580(Revised), June 1965, AD-477-240.

2. Johnson, W. E., J. M. Walsh, et al, "Theory of Hypervelocity Impact," General Atomic Report GA-5119, March 31, 1964, AD-436-251.