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*An Analysis of  
Physical and Chemical Explosions  
Inside a Flow Pathway*

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**Los Alamos** Los Alamos National Laboratory  
Los Alamos, New Mexico 87545

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# An Analysis of Physical and Chemical Explosions Inside a Flow Pathway

P. K. Tang  
W. S. Gregory



**Los Alamos** Los Alamos National Laboratory  
Los Alamos, New Mexico 87545

# AN ANALYSIS OF PHYSICAL AND CHEMICAL EXPLOSIONS INSIDE A FLOW PATHWAY

by

P. K. Tang and W. S. Gregory

## ABSTRACT

This report summarizes work in our analytical investigation of explosions inside a flow network, which emphasizes the explosive event itself. A special finite-difference scheme known as Flux-Corrected Transport has been adapted to solve gas-dynamic problems with large flow gradients, including shocks and contact surfaces. The results of this work can be used to supply the source or driving force for our far-field analysis. A sample model of the problem of shock and contact surface propagation is presented.

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## I. INTRODUCTION

In many industrial facilities the potential exists for both natural and man-caused accidents. Some preventive actions in the areas of design, construction, and operation can reduce the risk, but in practice, any accident still can occur because of the many unforeseen factors involved. The objective of this report is to present a practical tool for analyzing an accident event (in particular, an explosion inside a facility's flow network).

Because of the complexity of the problem, we decided to divide the region of concern into two parts.<sup>1</sup> In the first region, a detailed description of the accident is of little significance--only the accident's effect on remote regions of the facility will be investigated; this is known as the far field. A computer code that can model this problem has been developed and documented.<sup>2</sup> We now must develop some technique to analyze the effects of the

explosive event itself for the region where the accident actually takes place; we call this second region the near field. In this report we are interested mainly in shocks, contact surfaces, and detonations in one-dimensional flow paths; the slower processes of diffusion can be ignored. This report will provide the background information, the physical and chemical principles, the mathematical formulation, the numerical technique, and some simple illustrative examples for the near-field analysis.

## II. FAR-FIELD ANALYSIS

We will review our far-field work briefly to shed some light on the incentive for the current work. Information is available on the basic physical principles and mathematical formulations,<sup>3</sup> improved numerical techniques,<sup>4</sup> and some experimental verifications.<sup>5</sup>

Using the principles of fluid mechanics and thermodynamics, we formulated governing equations for the conservation of mass, energy, and momentum. In applying these equations, we subdivided the complete network into two general components--nodes and branches. The nodes represent boundaries and internal junctions where the conservation of mass and energy applies. The branches can represent ducts, valves, blowers, or filters. The equations for the time rate of change then are transformed into finite-difference equations and are solved numerically.

In the far-field analysis, the explosive event requires some form of simulation where the detail of the event is not significant. Basically, an explosion can be defined by a rapid pressure rise (sometimes along with a rapid temperature rise). These pressure and temperature increases can result from physical, chemical, or nuclear processes; for example, the rupture of a highly pressurized vessel (physical), the combustion or detonation of explosive materials (chemical), or the criticality excursion of fissionable nuclear materials (nuclear) can cause a rapid pressure rise with or without a corresponding rapid temperature rise. All these processes involve a rapid addition of mass and energy to a system, which can be closed or open. Analyses of explosions with rapid mass and energy additions are common and give good results if sufficient rate information is available. These approaches are useful for simulating an explosion inside a system and need detailed mass and

energy source terms in the mass and energy equations. When the energy release rate is not known, we can use other information such as pressure-time or temperature-time profiles at a particular location in combination with mass addition information. The last two approaches require experimental data on the system that can be difficult to obtain. For an explosion outside a system, the pressure- and temperature-time profiles can provide the information needed to investigate a system response. The near-field work described in this report will generate these source terms through a detailed mathematical formulation of the event.

### III. GAS DYNAMICS WITH CHEMICAL REACTIONS

We are interested mainly in explosions caused by physical and chemical processes. The dominant feature of these explosions is the gas flow with or without chemical reactions. Thus, solid particles or liquid droplets can be added to the stream without major complications. However, we will investigate only the gas-phase explosion at this time. We will consider the method of continuum mechanics as adequate to describe the situation without idealizing the explosion front as a discontinuity as long as the physical laws of conservation are satisfied. This approach will lead to a set of partial differential equations that are applicable from deflagration to detonation. Although we will investigate only the one-dimensional detonation problems, the equations given below are general.<sup>6</sup>

The total continuity equation is

$$\frac{\partial \rho}{\partial t} + \rho \frac{\partial u_j}{\partial x_j} + u_j \frac{\partial \rho}{\partial x_j} = 0 \quad , \quad (1)$$

where  $\rho$  and  $u$  are mixture density and velocity, respectively, and  $t$  and  $x$  are time and space, respectively. Cartesian tensor notation is used.

The chemical specie continuity equation is

$$\rho \frac{\partial Y_\alpha}{\partial t} + \rho u_j \frac{\partial Y_\alpha}{\partial x_j} = \omega_\alpha - \frac{\partial}{\partial x_j} (\rho Y_\alpha v_{\alpha j}) \quad , \quad (2)$$

with  $\alpha = 1, \dots, N$  and  $Y_\alpha$  being the mass fraction of specie  $\alpha$ .  $\omega_\alpha$  is the rate of production or destruction, and  $v_\alpha$  is the diffusion velocity of that specie.  $N$  is the total number of species presented. By definition,

$$\sum_{\alpha=1}^N Y_\alpha = 1 \quad . \quad (3)$$

Summing up all  $Y_\alpha$  to a total number of  $N$ , the result must be unity.  
The momentum equation is

$$\rho \frac{\partial u_i}{\partial t} + \rho u_j \frac{\partial u_i}{\partial x_j} = - \frac{\partial p}{\partial x_i} - \frac{\partial}{\partial x_i} \left( \frac{2}{3} \mu \frac{\partial u_k}{\partial x_k} \right) + \frac{\partial}{\partial x_i} \left[ \mu \left( \frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right) \right] , \quad (4)$$

where  $p$  is the pressure and  $\mu$  is the viscosity.

In the internal energy equation,

$$\rho \frac{\partial I}{\partial t} + \rho u_j \frac{\partial I}{\partial x_j} = - \frac{\partial q_k}{\partial x_k} - \left( p + \frac{2}{3} \mu \frac{\partial u_k}{\partial x_k} \right) \frac{\partial u_k}{\partial x_k} + \mu \left( \frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right) \frac{\partial u_j}{\partial x_i} , \quad (5)$$

where  $I$  represents the internal energy, including chemical energy, and  $q$  is the heat flux.

We have neglected body forces and bulk viscosity in the above formulation. Furthermore, we can assume the diffusion velocity,

$$v_{\alpha i} = - D \frac{\partial}{\partial x_i} \ln Y_\alpha , \quad (6)$$

which is the simplest mass diffusion relation, with  $D$  being the diffusion coefficient. Finally, the heat flux is

$$q_i = -\lambda \frac{\partial T}{\partial x_i} + \rho \sum_{\alpha=1}^N h_{\alpha} Y_{\alpha} v_{\alpha i} \quad , \quad (7)$$

where  $\lambda$ ,  $T$ ,  $h_{\alpha}$  are thermal conductivity, temperature, and enthalpy of specie  $\alpha$ , respectively.

The equations of state are needed (assuming an ideal gas mixture) to complete the system.

$$p = \rho R_u T \sum_{\alpha=1}^N (Y_{\alpha} / W_{\alpha}) \quad , \quad (8)$$

$$I = \sum_{\alpha=1}^N Y_{\alpha} h_{\alpha} - \frac{p}{\rho} \quad , \quad \text{and} \quad (9)$$

$$h_{\alpha} = h_{\alpha_0} + \int_{T_0}^T C_{p_{\alpha}} dT \quad , \quad (10)$$

where  $R_u$  is the universal gas constant,  $W_{\alpha}$  is the molecular weight,  $C_{p_{\alpha}}$  is the specific heat at constant pressure for specie  $\alpha$ ,  $T_0$  is the reference temperature, and  $h_{\alpha_0}$  is the enthalpy of specie  $\alpha$  at that temperature.  $h_{\alpha_0}$  contains heat of formation. The specie production  $\omega_{\alpha}$  can be defined based on chemical kinetics, but we will not discuss that here.

We frequently would like to write an equation for the total energy instead of the internal energy:

$$e = I + \frac{u^2}{2} \quad . \quad (11)$$

We can obtain a kinetic energy equation by multiplying Eq. (4) by  $u_i$ . After some manipulation,

$$\begin{aligned} \rho \frac{\partial}{\partial t} \left( \frac{u_i^2}{2} \right) + \rho u_j \frac{\partial}{\partial x_j} \left( \frac{u_i^2}{2} \right) = & - \frac{\partial(\rho u_k)}{\partial x_k} + p \frac{\partial u_k}{\partial x_k} - \frac{\partial}{\partial x_i} \left( \frac{2}{3} \mu u_i \frac{\partial u_k}{\partial x_k} \right) + \frac{2}{3} \mu \left( \frac{\partial u_k}{\partial x_k} \right)^2 \\ & + \frac{\partial}{\partial x_i} \left[ \mu u_i \left( \frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right) \right] - \mu \left( \frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right) \frac{\partial u_j}{\partial x_i} . \end{aligned} \quad (12)$$

Adding Eqs. (5) and (12), we have

$$\rho \frac{\partial e}{\partial t} + \rho u_j \frac{\partial e}{\partial x_j} = - \frac{\partial(\rho u_k)}{\partial x_k} - \frac{\partial q_k}{\partial x_k} - \frac{\partial}{\partial x_i} \left( \frac{2}{3} \mu u_i \frac{\partial u_k}{\partial x_k} \right) + \frac{\partial}{\partial x_i} \left[ \mu u_i \left( \frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right) \right] , \quad (13)$$

which is the equation for the total energy.

Finally, Eqs. (1), (2), (4), and (13) can be rewritten in the conservative form:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_j) = 0 , \quad (14)$$

$$\frac{\partial(\rho Y_\alpha)}{\partial t} + \frac{\partial}{\partial x_j} (\rho Y_\alpha u_j) = \omega_\alpha - \frac{\partial}{\partial x_j} (\rho Y_\alpha v_{\alpha j}) , \quad \alpha = 1, \dots, N , \quad (15)$$

$$\frac{\partial(\rho u_i)}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_i u_j) = - \frac{\partial p}{\partial x_i} - \frac{\partial}{\partial x_i} \left( \frac{2}{3} \mu \frac{\partial u_k}{\partial x_k} \right) + \frac{\partial}{\partial x_i} \left[ \mu \left( \frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right) \right] , \quad (16)$$

and

$$\begin{aligned} \frac{\partial(\rho e)}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_j e) = & - \frac{\partial(\rho u_k)}{\partial x_k} - \frac{\partial q_k}{\partial x_k} - \frac{\partial}{\partial x_i} \left( \frac{2}{3} \mu u_i \frac{\partial u_k}{\partial x_k} \right) \\ & + \frac{\partial}{\partial x_i} \left[ \mu u_i \left( \frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right) \right]. \end{aligned} \quad (17)$$

The interesting feature of this formulation is that if the right-hand side is zero, the product of the flow element volume and  $\rho$ ,  $\rho Y_\alpha$ ,  $\rho u_i$ , or  $\rho e$  will not change following the movement of the flow element, which can be seen in the total mass balance equation [Eq. (14)]. Accordingly, the right-hand sides of all these equations are considered as the sources that cause the changes in the respective quantities within that element. This feature will have a strong bearing on the numerical technique.

#### IV. FINITE-DIFFERENCE TECHNIQUE

After an extensive literature survey, we have concluded that the Flux-Corrected Transport method<sup>7</sup> is the numerical technique to use in the development of the near-field code. Basically, this method has the feature of handling sharp gradients such as shocks and flames without using artificial viscosity or an upwind technique, which would introduce excessive damping. The governing equations become

$$\frac{\partial(\rho A)}{\partial t} + \frac{\partial}{\partial x} (\rho u A) = 0, \quad (18)$$

$$\frac{\partial(\rho Y_\alpha A)}{\partial t} + \frac{\partial}{\partial x} (\rho Y_\alpha u A) = A \omega_\alpha, \quad \alpha = 1, \dots, N, \quad (19)$$

$$\frac{\partial(\rho u A)}{\partial t} + \frac{\partial}{\partial x} (\rho u^2 A) = - \frac{\partial(\rho A)}{\partial x} , \text{ and} \quad (20)$$

$$\frac{\partial(e A)}{\partial A} + \frac{\partial}{\partial x} (\rho u e A) = - \frac{\partial}{\partial x} (\rho u A) . \quad (21)$$

The above equations have the form of

$$\frac{\partial(\psi A)}{\partial t} + \frac{\partial}{\partial x} (\psi u A) = S , \quad (22)$$

where  $\psi$  can be  $\rho$ ,  $\rho Y_\alpha$ ,  $\rho u$ , or  $\rho e$  and is called the generalized density.  $A$  is the flow cross-section area;  $S$  can be considered as the generalized source term. We will describe the numerical technique using the Eulerian approach.

As can be seen in Eq. (22), the most prominent effect on the change of the generalized density inside a flow element is a result of convection, so we obtain

$$V_i \psi_i^* = V_i \psi_i^0 - \delta t \psi_{i+1/2}^0 A_{i+1/2} u_{i+1/2} + \delta t \psi_{i-1/2}^0 A_{i-1/2} u_{i-1/2} , \quad (23)$$

with

$$u_{i+1/2} = \frac{1}{2} (u_i + u_{i+1}) . \quad (24)$$

$V_i$  is the volume of cell  $i$ ;  $\psi_i^0$  and  $\psi_i^*$  are the generalized density in cell at the previous time and the updated value with the convective effect only, respectively.  $\delta t$  is the time step used. Note that the half-index means that the quantities are evaluated at the cell interface location.

After convection, the generalized density is modified because of the source term,

$$V_i \psi_i^T = V_i \psi_i^* + \delta t V_i S_i \quad . \quad (25)$$

$\psi_i^T$  is the generalized density with the source effect; the expression in the last term assumes that the source is a volumetric effect. Other forms can be used if the source is a result of gradients, divergences, and so on. A combination of all these effects can be added up to obtain the total contribution.

The next step is to add a diffusion stage so that the numerical solution will be stable. The equation is

$$V_i \tilde{\psi}_i = V_i \psi_i^T + v_{i+1/2} V_{i+1/2} (\psi_{i+1}^0 - \psi_i^0) - v_{i-1/2} V_{i-1/2} (\psi_i^0 - \psi_{i-1}^0) \quad . \quad (26)$$

$\tilde{\psi}_i$  is the new cell generalized density (still a temporal value), and  $v$  is defined by

$$v_{i+1/2} = \frac{1}{6} + \frac{\epsilon_{i+1/2}^2}{3} \quad , \quad (27)$$

with

$$\epsilon_{i+1/2} = A_{i+1/2} u_{i+1/2} \frac{\delta t}{2} \left( \frac{1}{V_i} + \frac{1}{V_{i+1}} \right) \quad . \quad (28)$$

The expression used in Eq. (27) is to reduce the phase errors.

Because the diffusion process of Eq. (26) is an artificial one, we must counteract that by an antidiffusion step. The flux is

$$F_{i+1/2} = \eta_{i+1/2} V_{i+1/2} \left( \psi_{i+1}^T - \psi_i^T \right) , \quad (29)$$

before any correction is made;  $\eta$  is defined by

$$\eta_{i+1/2} = \frac{1}{6} - \frac{\epsilon^2}{6} \eta_{i+1/2} . \quad (30)$$

The generalized density used here is the one before the diffusion stage.  $F$  is further modified by using

$$F_{i+1/2}^c = s_{i+1/2} \max \left\{ 0, \min \left[ |F_{i+1/2}| , s_{i+1/2} V_{i+1} \left( \tilde{\psi}_{i+2} - \tilde{\psi}_{i+1} \right) , \right. \right. \\ \left. \left. s_{i+1/2} V_i \left( \tilde{\psi}_i - \tilde{\psi}_{i-1} \right) \right] \right\} . \quad (31)$$

$s_{i+1/2}$  has the value of unity and the sign of  $\left( \tilde{\psi}_{i+1} - \tilde{\psi}_i \right)$ .  $F_{i+1/2}^c$  is known as the corrected antidiffusion flux. Finally, the new generalized density is obtained.

$$V_i \psi_i^n = V_i \tilde{\psi}_i - F_{i+1/2}^c + F_{i-1/2}^c , \quad (32)$$

with  $\psi_i^n$  being the new generalized density at the new time in element  $i$ .

The preceding procedure forms the basis of the current near-field analysis code. In fact, the integration is performed at a half-time step  $\left( \frac{\delta t}{2} \right)$  from which

the source terms can be calculated before we carry out the full-time step ( $\delta t$ ) integration. This process results in greater accuracy in time. Other variations are possible, but we will not discuss them here.

Although the above procedure gives excellent numerical stability without excessive damping, its accuracy still depends on the element size, particularly in the region where the gradient is large. The refinement of the cell size must be incorporated as the condition requires, and it also should follow the movement of shock, flame, or any contact surface. The current code does not have any rezoning technique to accomplish this goal, but we will add this in the future.

## V. BURSTING DIAPHRAGM PROBLEM

We will use the classical problem of the bursting diaphragm that generates moving shock and contact surfaces to illustrate the capability of our computer code, which is based on the technique we discussed earlier. A pipe is divided into two regions with different pressures and densities by a diaphragm, and the diaphragm is set to break. The pressure and density distributions at specific time intervals following the break are shown in Figs. 1--14. Except for the initial disturbance, the shock front is well defined (pressure and density distribution plots), as is the contact surface, which is moving at a slower speed (density plots); the reflection of the shock from the solid boundary on the right is shown clearly in Figs. 3--6. Later, we see the interaction of the reflected shock and the contact surface. The result is that the reflected shock slows down (Figs. 7 and 8), and the contact surface becomes practically stationary. A weak compression wave is traveling to the right after the interaction. As the diaphragm breaks, a rarefaction wave travels to the left, reflecting back from the solid boundary on the left. Eventually, the reflected shock and the reflected rarefaction wave interact. This weakens the reflected shock substantially; it becomes about the same strength as the initial shock except that it is traveling toward the left boundary (Figs. 9--12). Because there is no dissipation (physical or numerical), a shock can travel back and forth inside the pipe with the same strength. The shock reflection from the left boundary is shown in Figs. 13 and 14.

We also can run a case with one end of the pathway open; the results should include the mass and energy fluxes leaving that end, which are the source terms we need to drive the far-field code. However, we will not discuss the work here.

## VI. FUTURE WORK

The computer code that we now have will provide the framework for our future near-field explosion investigation. Some refinements will be made to improve the numerical interpolation. The rezoning scheme will be added to adjust for the variation in gas-dynamic gradients, and we will add the capability to simulate chemical reactions so that we can study the propagation of detonation.

Even with all the refinements we have cited, the near-field work should not be limited to the areas we have discussed so far. In fact, a capability of analyzing general detonation and deflagration for two- and three-dimensional configurations and for multicomponent and multiphase flow should be developed. Efforts will be made toward this goal.

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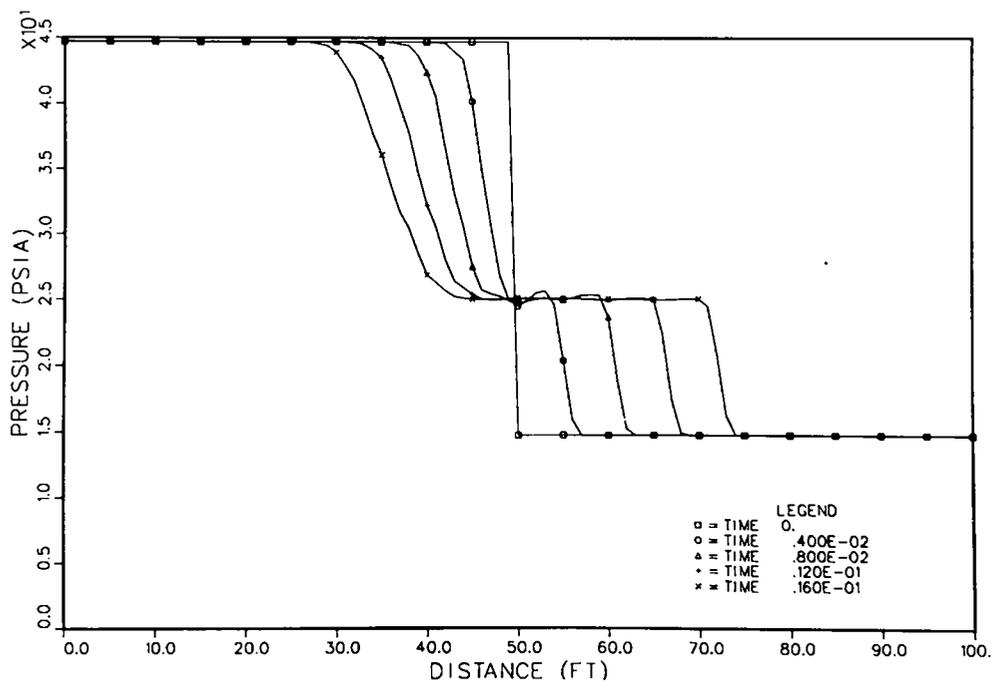


Fig. 1.  
Pressure distribution (time from 0 to 0.016 s).

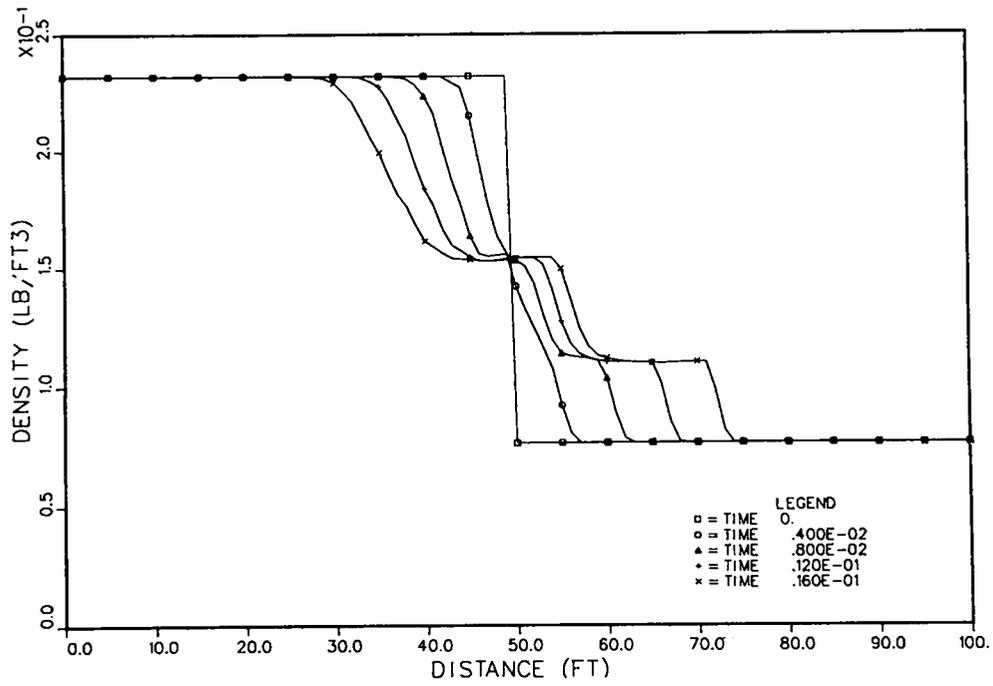


Fig. 2.  
Density distribution (time from 0 to 0.016 s).

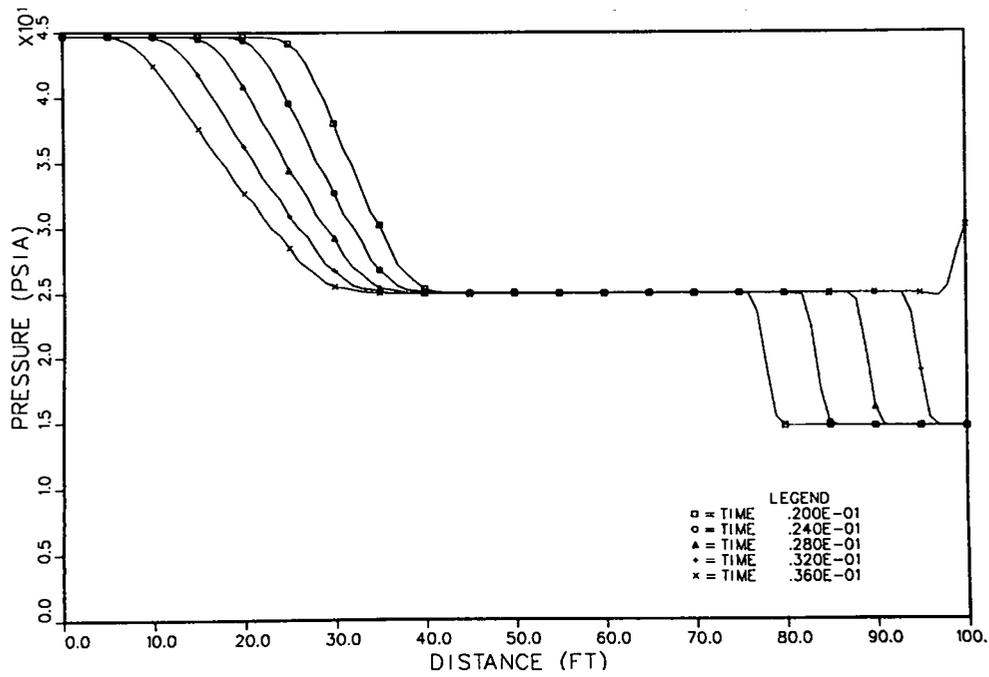


Fig. 3.  
Pressure distribution (time from 0.02 to 0.036 s).

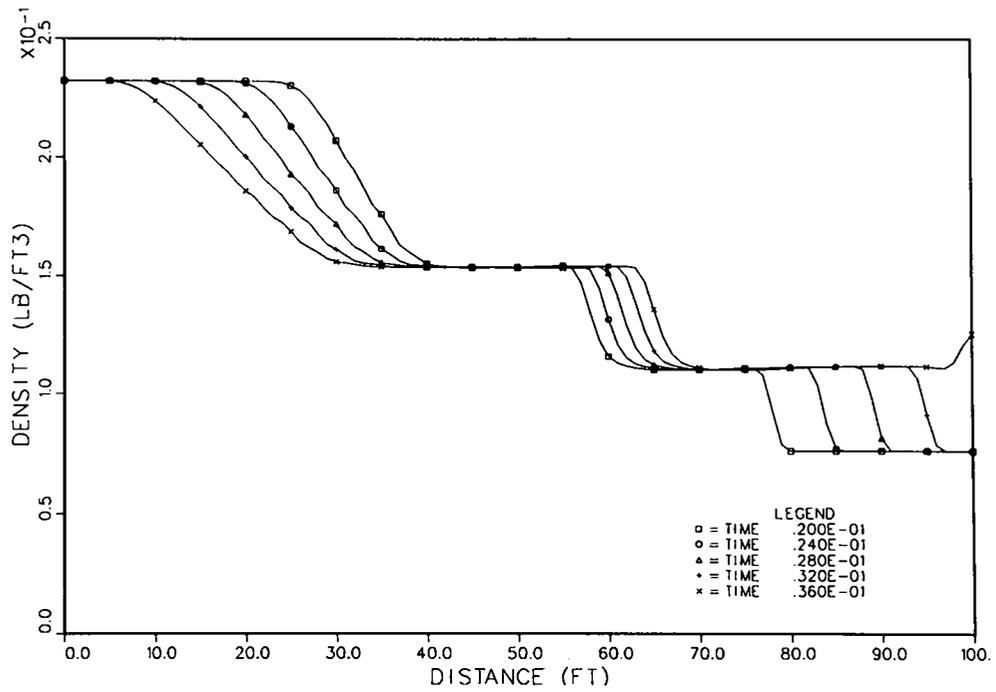


Fig. 4.  
Density distribution (time from 0.02 to 0.36 s).

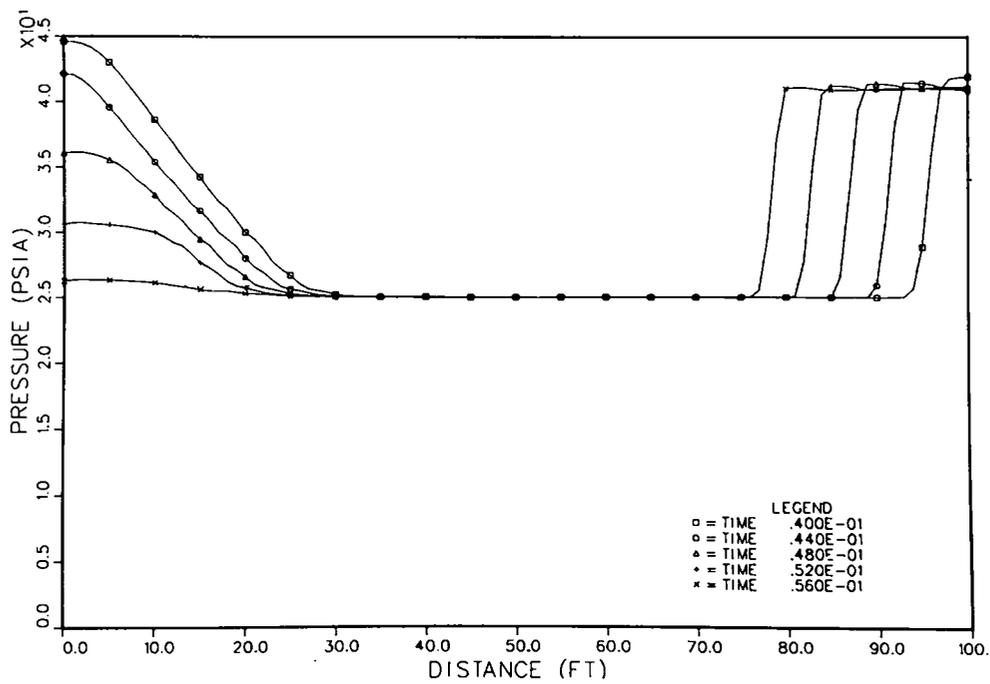


Fig. 5.  
Pressure distribution (time from 0.04 to 0.056 s).

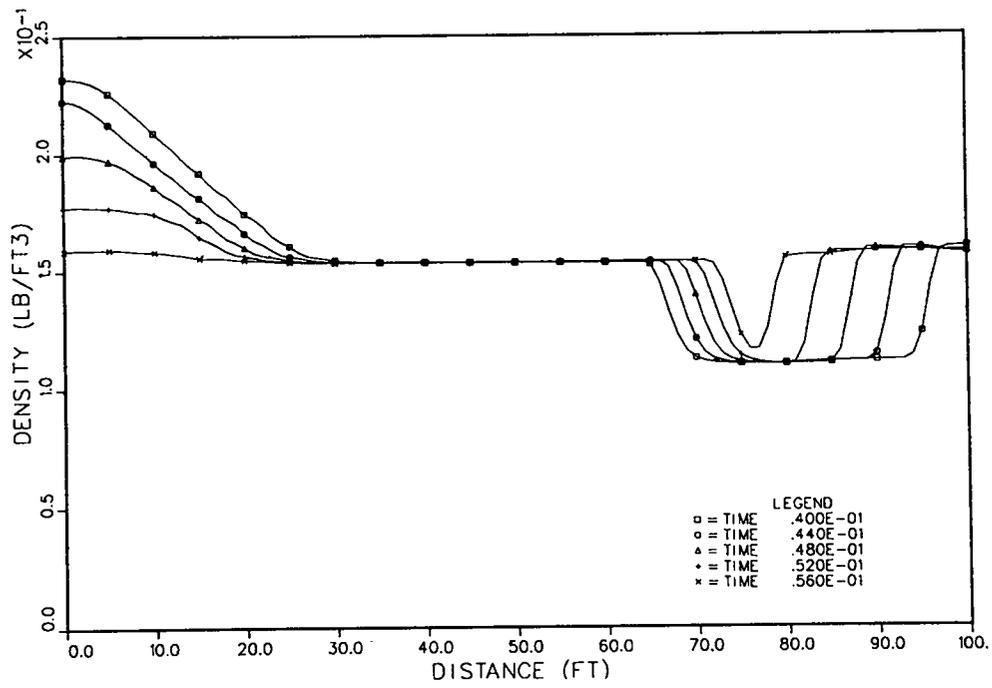


Fig. 6.  
Density distribution (time from 0.04 to 0.056 s).

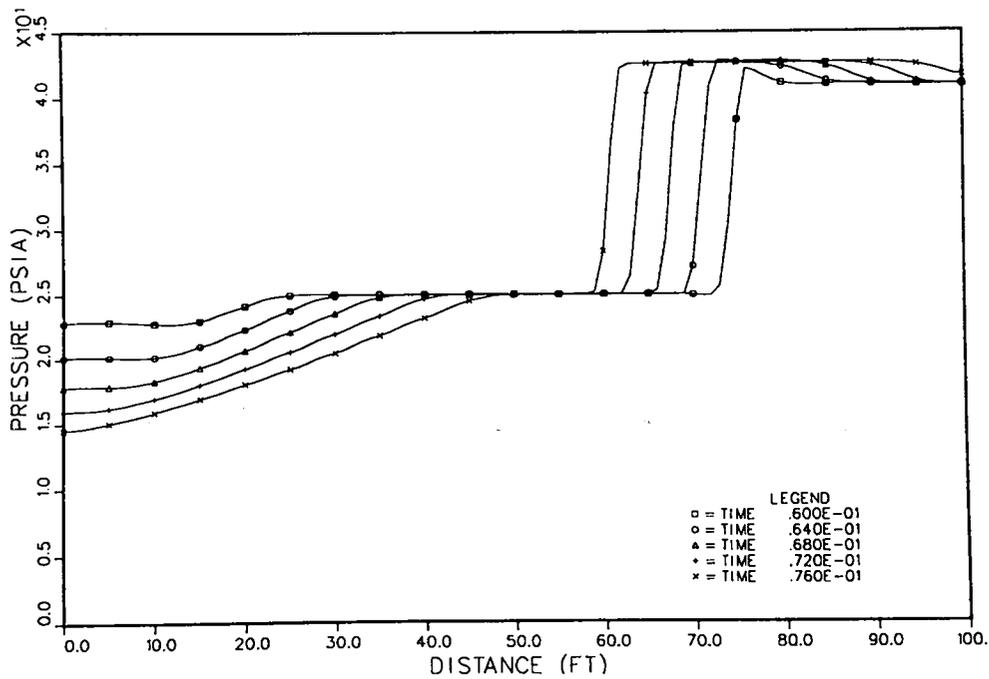


Fig. 7.  
Pressure distribution (time from 0.06 to 0.076 s).

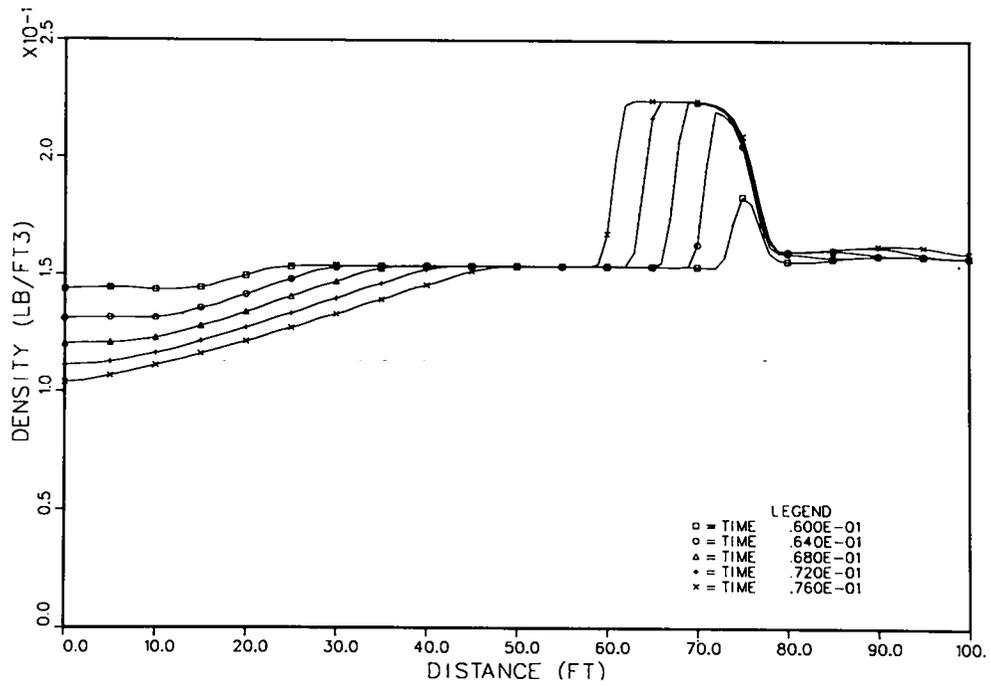


Fig. 8.  
Density distribution (time from 0.06 to 0.076 s).

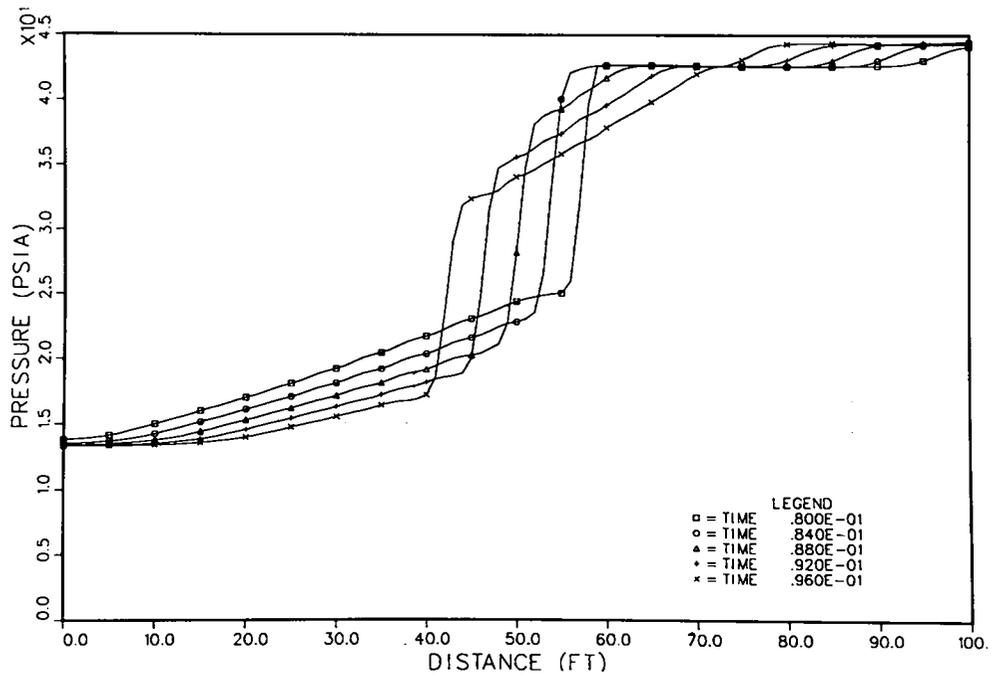


Fig. 9.  
Pressure distribution (time from 0.08 to 0.096 s).

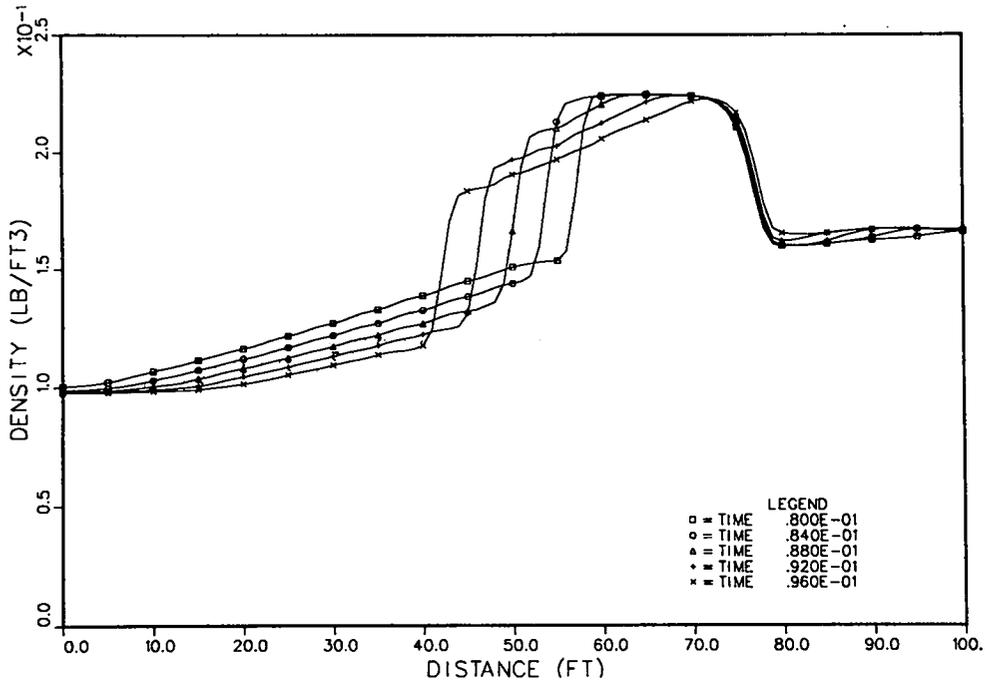


Fig. 10.  
Density distribution (time from 0.08 to 0.096 s).

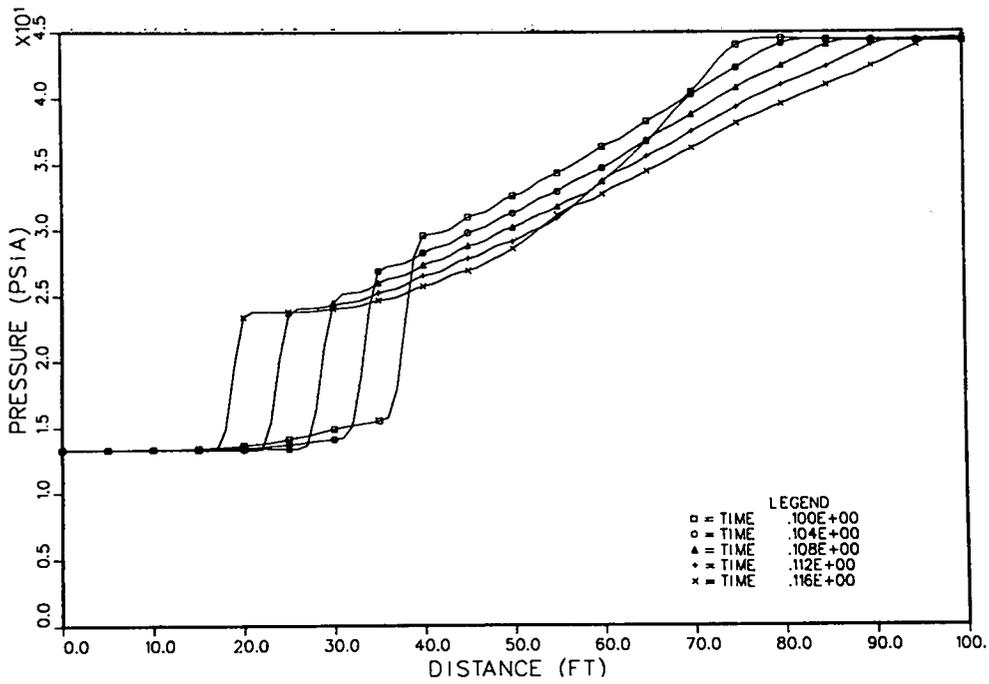


Fig. 11.  
Pressure distribution (time from 0.1 to 0.116 s).

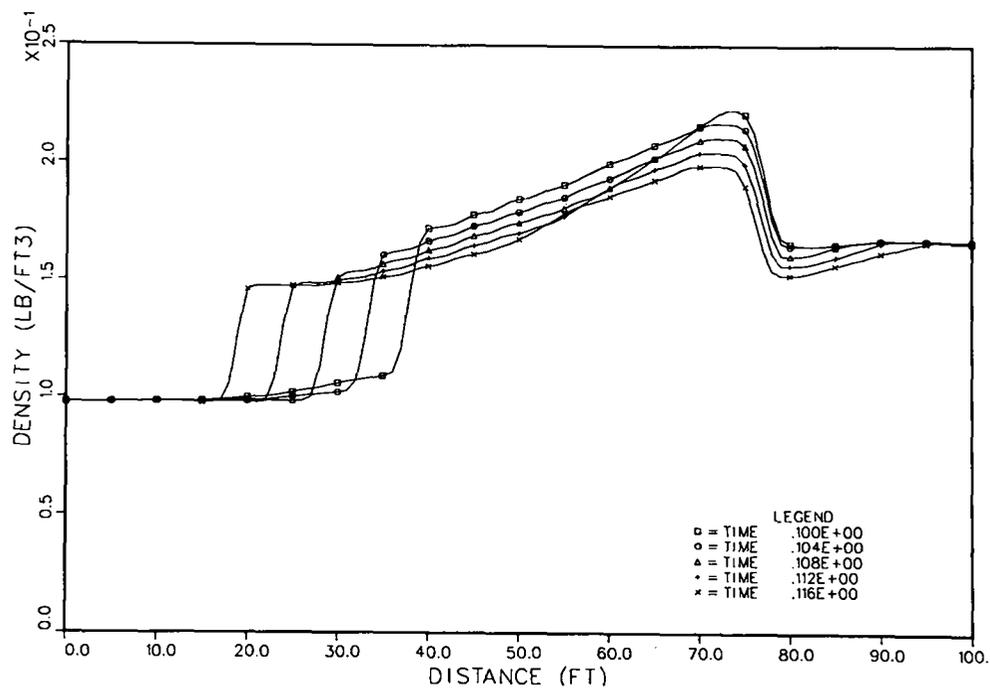


Fig. 12.  
Density distribution (time from 0.1 to 0.116 s).

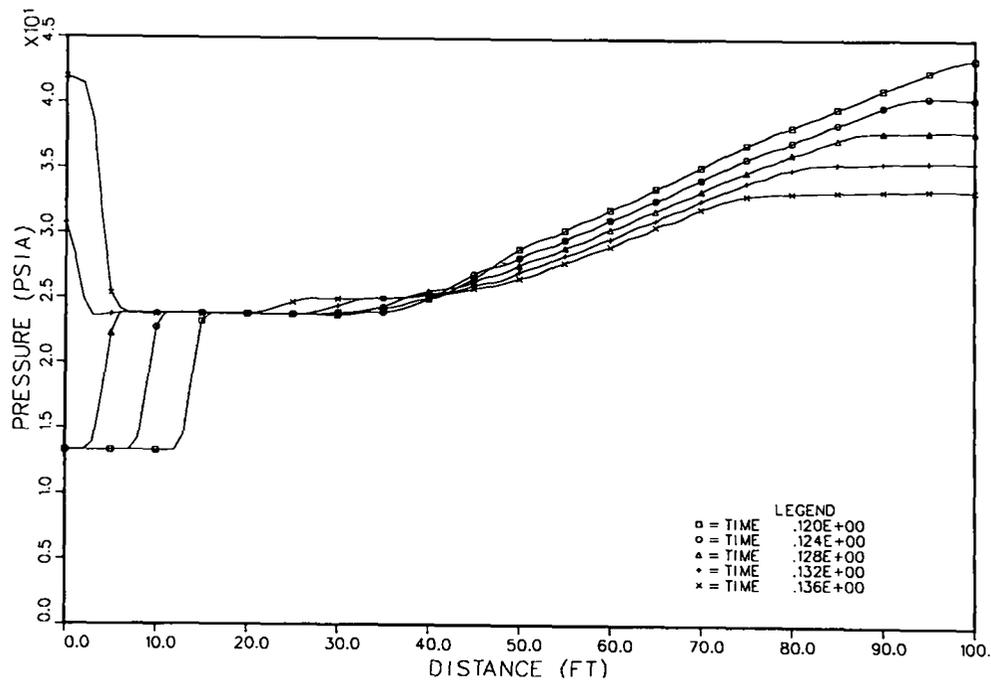


Fig. 13.  
Pressure distribution (time from 0.12 to 0.136 s).

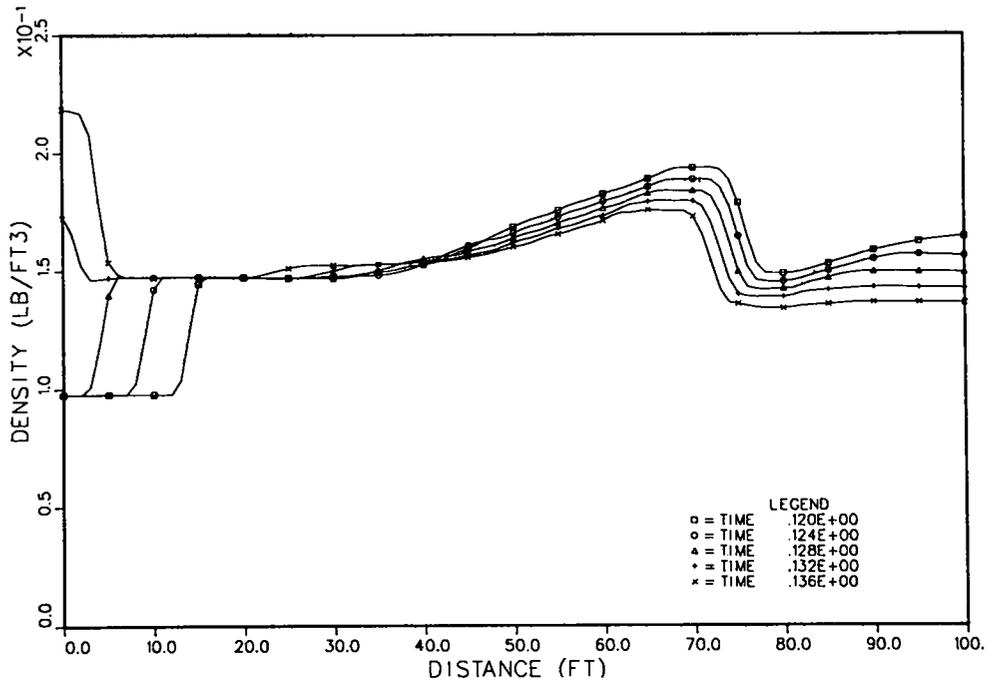


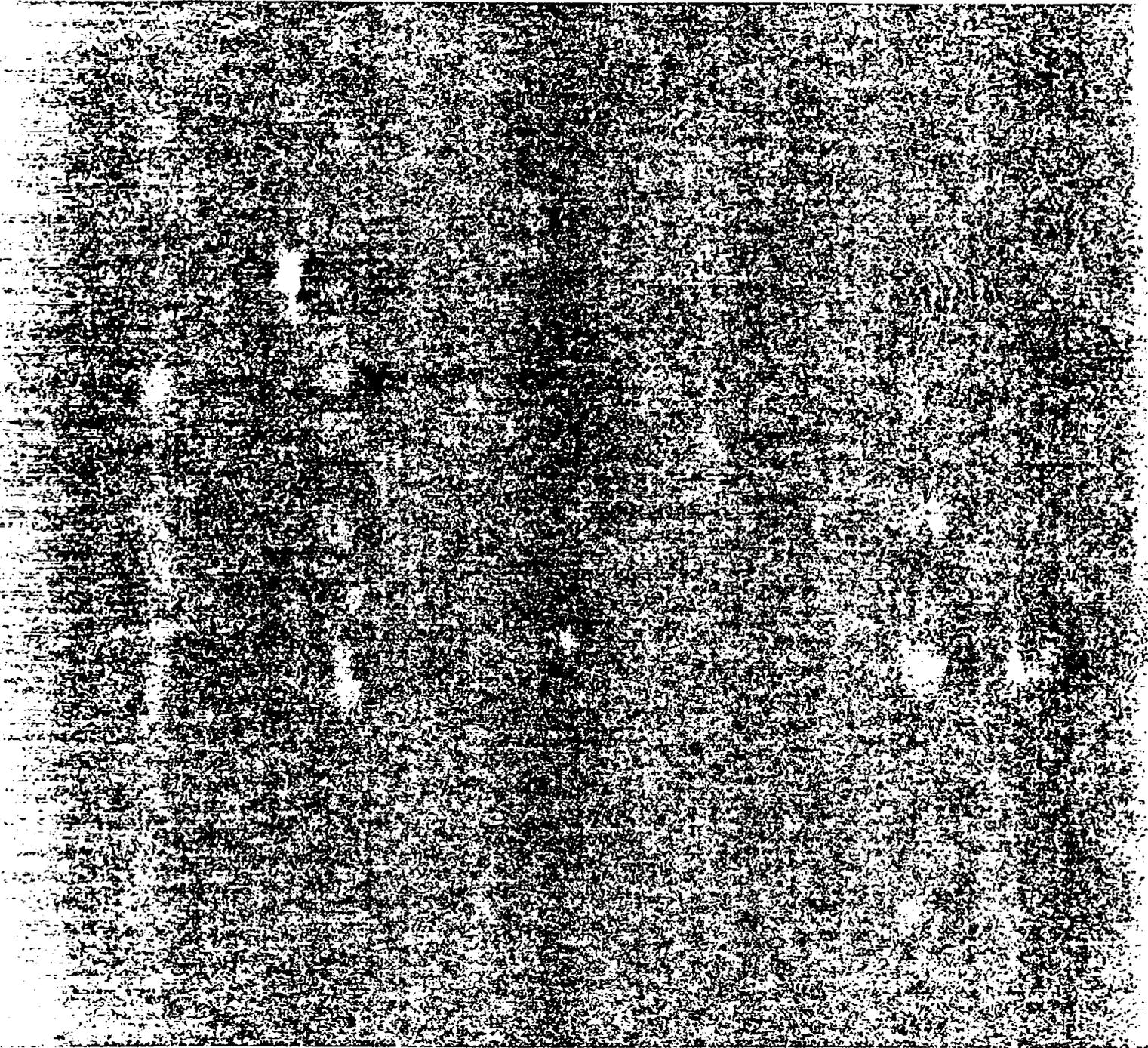
Fig. 14.  
Density distribution (time from 0.12 to 0.136 s).

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051-075	A04	201-225	A10	351-375	A16	501-525	A22
076-100	A05	226-250	A11	376-400	A17	526-550	A23
101-125	A06	251-275	A12	401-425	A18	551-575	A24
126-150	A07	276-300	A13	426-450	A19	576-600	A25
						601-up*	A99

\*Contact NTIS for a price quote.



Los Alamos