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THE PARTICLE-IN-CELL MODEL FOR GAS-DROPLET FLOWS IN SHOCK-TUBES

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ABSTRACT

The present work investigates the propagation of incident and reflected shock and rarefaction waves in a homogeneous mixture of gas and liquid droplets in shock-tubes. Two models describing the break-up process of drops exposed to blasts of air were used. The governing equations were solved using the Particle-In-Cell (pic) method, and was developed specifically to be run on a micro-computer, and to overcome the disadvantages of relatively low speed and limited memory resources of micro-computers compared to main frames. The numerical solution remains stable for low and moderate droplet volume fractions and the predicted velocity,pressure and temperature flow fields for the gas and droplet phases aptly illustrate the capability of the method to treat the complex coupling phenomena associated with multi-phase flows and shows its dependence on the physical properties of both gas and droplets.

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1. INTRODUCTION

In many engineering applications nowadays the flow of compressible gases containing solids or liquid droplets with the possible existence of shock-waves is a common phenomenon notably the flow of atomised droplets in the exhaust gases of liquid propellant rocket motors, jet engines and carburattors. The atomization of a liquid into drops is a complex process in which interrelated aerodynamics and hydrodynamics effects come into play. Many technically important atomization devices such as spray nozzles for combustion chambers inject a liquid under pressure into a stream of air. The action of air friction and pressure causes the deformation of drops and ligaments which subsequently break up in the relative air flow. The transient case exists when a drop is suddenly subjected to a change in relative air velocity. This situation prevails when a drop is supported in a shock-tube and exposed to the so-called hot flow region behind the principal shock-wave.

The basic structure of shock waves incorporating two-phase flow have been studied theoretically by Narkis and Galor(1) and Bales et al.(2). They dealt with stationary waves and calculated the process of the mixture approaching the final equilibrium state behind the wave which is connected by simple algebric relations with the prescribed state ahead of the wave front. The structure and behaviour of shock waves propagation and reflection was investigated theoretically and experimentally by Honda(3), and Rudinger(4). An excellent review works on this type of flow was made by Crowe and Sharama(5) and Andrew(6).

In the present work a procedure for analysing the unsteady flow of gas-droplets suspensions using the PIC method on microcomputers is presented. The PIC method for the numerical solution of problems in fluid dynamics has been extended to the study of incident and reflected shock and rarefaction waves in gas-droplets mixtures. The shock-waves concerned are incident on a mixture of uniformly dispersed liquid droplets in a gas stream in the down-stream part of the driven section of a shock-tube.

2. THE CALCULATION OF SHOCK-WAVES IN GAS-DROPLETS MIXTURES.

2.1 The Differential Equations

The coupled differential equations and the exchange functions that describe the motion of a fluid composed of more than one material, any one of which may be microscopically compressible or incompressible are discussed by Harlow(7). The one-dimensional, two material, plane coordinate version of these equations are summarized below;

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Conservation of mass

$$(\rho_1)_{,t} + (\rho_1 u_1)_{,x} = 0 \qquad (1)$$

Conservation of momentum

$$\rho_1 (u_1)_{,t} + \rho_1 u_1 (u_1)_{,x} = -\epsilon_1 (p)_{,x} + V_1 + K_{1m}(u_m - u_1) \qquad (2)$$

And

$$V_1 = -(q_1)_{,x} \qquad (3)$$

Where, q_1 is the artificial viscous stresses and is given by,

$$q_1 = \rho_1 \nu_1 (u_1)_{,x} \qquad (4)$$

The drag function which controls the exchange of momentum between the two phases can be written in a simplified form

$$K_{1m} = \frac{3}{4} \frac{c_d}{d_1} \epsilon_1 \rho_m |u_1 - u_m| \qquad (5)$$

Conservation of energy

$$\rho_1 (I_1)_{,t} + \rho_1 u_1 (I_1)_{,x} = (\epsilon_1 p + q_1)(u_1)_{,x} + \rho_1 K_{1m} \frac{(u_m - u_1)^2}{\rho_1 + \rho_m} + Q \qquad (6)$$

The term $(\epsilon_1 p + q_1)(u_1)_{,x}$ is the rate at which work is done by the gas at the boundaries of a differential element of volume, where

$$Q = \frac{1}{2} Nu \, \rho_1 K C_s (T_1 - T_m) / \tau_t \qquad (7)$$

$$\tau_t = \frac{1}{12} (\sigma_s d^2 C_s)/K \qquad (8)$$

The term $\rho_1 K_{1m} \frac{(u_m - u_1)^2}{\rho_m + \rho_1}$ accounts for the dissipation of the droplets kinetic energy into kinetic energy of the gas. Similar equations are written for the second phase.

It must be emphasized that most finite difference methods when applied to problems with discontinuities produce oscillations behind the shock. Von Neuman and Richtmyer (8) developed an artificial viscosity term which was introduced into the Lagrangian form of the equations of gas dynamics. The goal of the artificial viscosity was to reduce the oscillations while allowing the shock transition to occupy only a few mesh points and having negligible effect in the smooth regions. All other forms of artificial viscosity are variations of the one introduced by Neuman. In the present work the artificial viscosity

q_1 in the above equations is introduced as a pressure modification where $q_1 = ac_o$. It was found that taking $ac_o = 1650$ is the best balance between eliminating fluctuations and maintaining a steep enough shock front.

2.2 Numerical Methodology

In the PIC computing technique the spacial domain of duct is subdivided into a set of Eulerian cells, with each is associated such field variables as pressure, specific internal energy and fluid velocity. In addition we superimpose a Lagrangian set of marker droplets. Each droplet represents an element of fluid that moves through the Eulerian mesh and interacts with other elements of fluid in a procedure that couples the two materials together. Each particle carries a fixed mass of material and is tagged to identify the material it represents.

Time duration is divided into a sequence of computational cycles of time δt, and after specifying the initial and boundary conditions the configuration is evoluted through time by a prescribed set of calculational phases in each cycle. These phases are summarized as follows;

Phase 1 : The field variables in each Eulerian cell is calculated as if both materials and the cells follow the fluid motion. Hence no convective terms in the equations are calculated in this phase.

Phase 2 : With the Eulerian cells return to their original positions,the new droplets coordinates are calculated and any resulting transport of a drop from one Eulerian cell to another is accompanied with calculations of mass,momentum,energy and droplet diameter according to the break-up modelling.

Phase 3 : The diffusion of heat and momentum are calculated.

Interaction between phases,when applying this method to suspension flows,are incorporated in phase 1 using all quantities from the previous step.

2.3 Boundary Conditions

The boundary cells calculation of finite differences is rather different than for interior cells in order to satisfy the conservation equations at boundaries. A cell whose right or left boundary is adjacent to the end wall of the shock tube is treated as follows :
In phase 1 calculation, the pressure at the solid boundary is set equal to that in the cell and the work is taken zero.Therefore the velocity at the boundary is set equal to zero.

In phase 2, mass points representing the gas are reflected when colliding with the solid boundary (elastic collision). Consequently the internal energy of the cell and pressure tend to increase. Meanwhile the droplets are assumed to splash and stick to the wall upon collision, hence to be removed from the system.

3. RESULTS AND DISCUSSION

6 At time t=0, the diaphragm separating the two fluid regions is instantaneously removed causing a shock to advance into the lower density region and a rarefaction to propagate back from the contact surface into the higher density region. The properties of the undisturbed gas was chosen to give a sound speed of 340 m/sec., and the pressure ratio across the diaphragm was 5. Calculations were performed in a plane mesh of 100 cells, allowing for 25 cells in the high pressure region. In order to improve the fluctuations on variables profiles and to optimise the time of execution the following initial data were used:

1- The total number of mass points for gas in the high pressure region was 30 and 12 for the droplets.
2- An initial region for calculation was taken and then expansion to the right and left was made at a rate governed by the speed of the shock and rarefaction waves. This expansion provision afforded a considerable saving in time of execution of approximately 30-40% .
3- Cell length of 0.03 mt., time increment of 0.015 m.s. and an artificial viscosity of 1650 were used.
4- The distance a mass point travels in a single time step is less than the spacing between mass points, that is $u\,\delta t < x/m$. This condition also satisfies the Courant-Friedrichs -Lewy condition of stability for flow fields of a compressible fluid.

Fig.1 shows the velocity, pressure and temperature profiles f a single phase flow at 1.5,3.0,4.5 and 6.0 m.s. The calculatio time is enlarged to allow for the shock and rarefaction waves to reflect from both ends of the shock-tube. From the figure it is noted that artificial viscosity does not spread the contact discontinuity. The smearing of the contact discontinuity is due to the truncation error of the scheme and the smearing of the shock is due to the truncation error of the scheme as well as the artificial viscosity.

Within the framework of the basic multiphase model, the treatment of liquid droplets or solid particles is essentially the same except that different values of the drag coefficient are appropriate and droplets may fragment under the action of shock-waves.

Figs.2,3 give the graph of the various flow profiles for air and water droplets when the initial droplet diameter is 500 microns. These show the typical shock-tube profiles seen earlier for the single phase shock-tube calculations and illustrate the slower speed of shock propagation and reflection.

In fig.2 the breakup model adopted is that for the droplet to break up when the Weber number exceeds a critical value of 22.0 (9) . The Weber number is defined as;

$$We = \frac{\rho_g |u_g - u_l| r_p}{\sigma}$$

The droplet break up happens immediately behind the shock since the model gives instantaneous break-up of drops. This has the

effect of substantially increasing the drag and reducing the phase relative velocity until the Weber number criteria is satisfied. The velocity difference gradually disappears as phase relaxation takes place.

The other break-up model used is that derived emperically by Hanson et al. (10), for the break up of drops exposed to blasts of air in shock-tubes, in which the critical break-up curve for water was defined by the emperical equation:

$$|u_g - u_l|^2 \, d_p = 6.21 * 10^6$$

Where $|u_g - u_l|$ is in ft/sec and d_p is in microns.
The radius of the droplet is calculated automatically by the program until the above condition is satisfied.

Fig.3 clearly shows that the shock front using that break-up model is sharper than the Weber number model and that the shock is smeared out over fewer number of grid nodes. There is however a slight overshoot in the velocity profile behind the shock. Comparing these results with those of gas-solids flows (11) it appears that the droplet break up mechanism acts as a stabilising mechanism since it prevents the velocity differences becoming too large. This is a physical stability mechanism and can also act against any unphysical instability arising from the model.

Fig.4 shows the profiles for methyl alcohol droplets where the break-up model is defined by the emperical equation;

$$|u_g - u_l|^2 \, d_p = 2.71 * 10^6$$

It is clearly shown that the relative phase velocity is much smaller immediately behind the shock front than in the case of water droplets. This increases the drag which greatly aids the stability of the numerical calculations.

4. CONCLUSION

The following conclusions are drawn from the present study:
1- The newly modified PIC method can give plausible predictions of the structure and behaviour of incident and reflected shock and rarefaction waves.
2- The droplet break-up mechanism acts as a physical stabilising agent since it prevents the velocity differences becoming too large which aids the numerical calculations for the damping of perturbations.
3- The use of this method is not restricted to liquid droplets but it could be applied to the small particles in shock-tubes.
4- The study could be extended to strongly nonequilibrium circumstances when metal fragments ablate. Such a study would require calculational model for the phase transition and possible burning that could take place in such an interaction.

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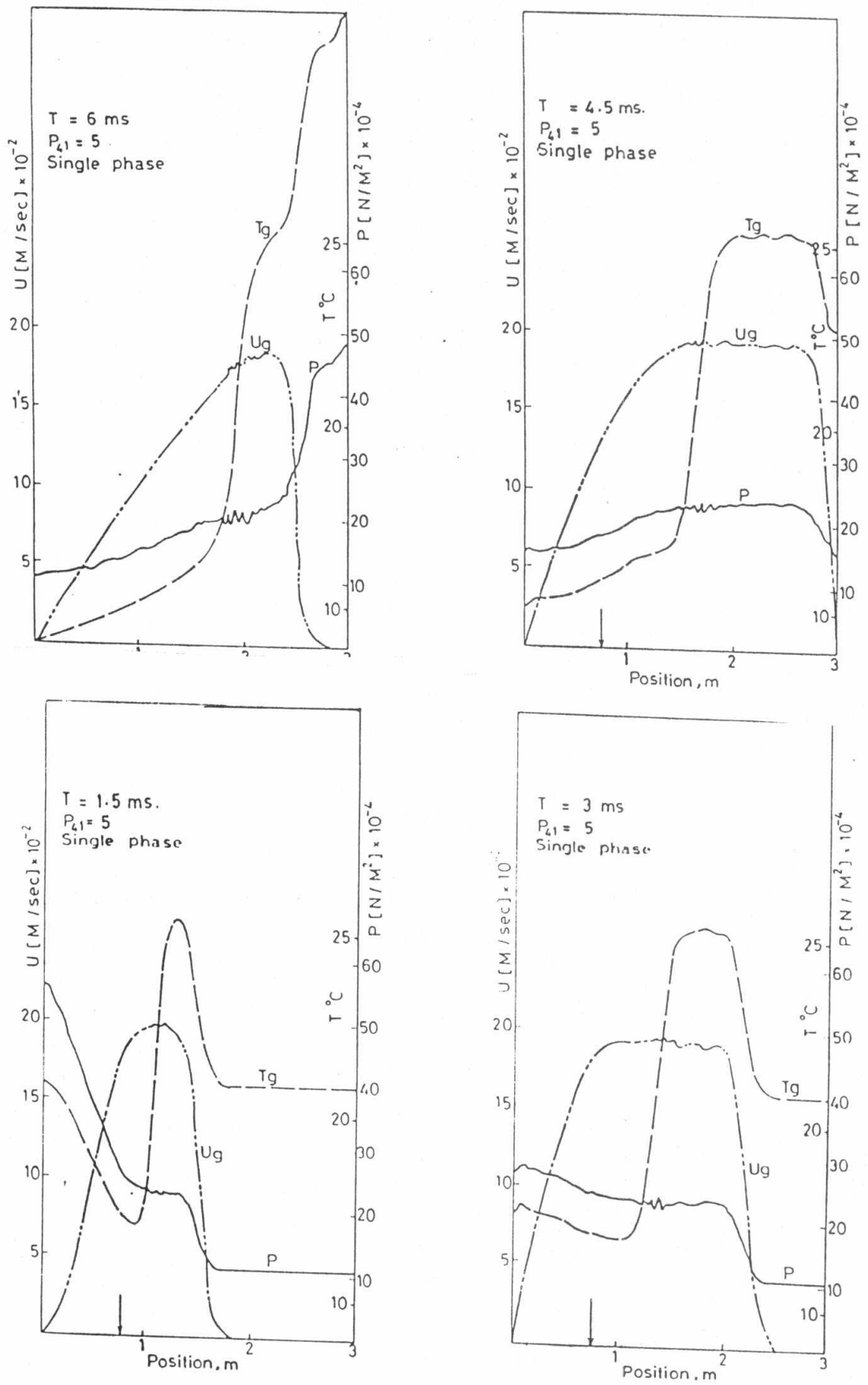

Fig. 1 Pressure, Velocity and Temp. profiles for a shock-tube containing gas only.

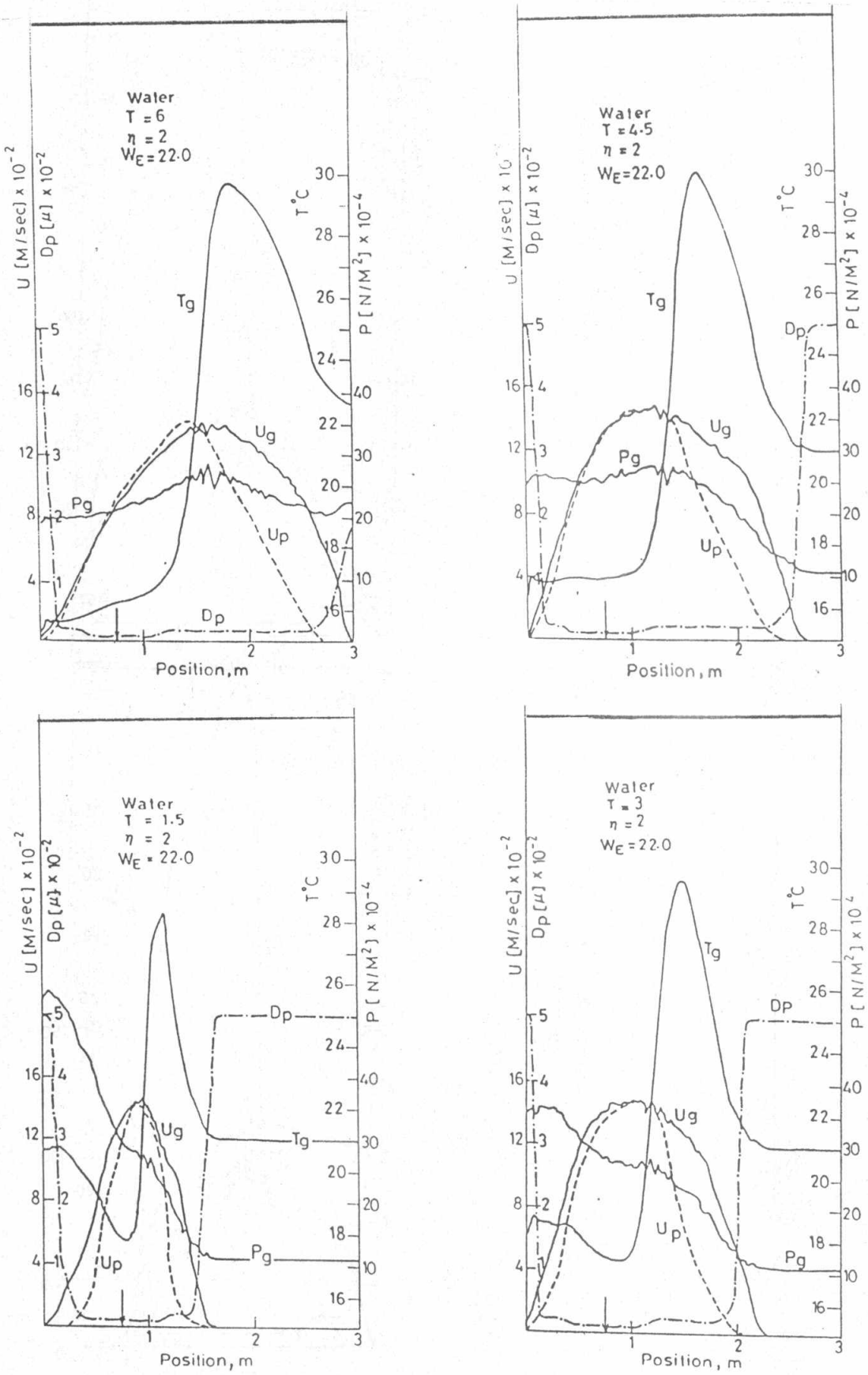

Fig.2 Pressure, Velocity, Temp. and droplet size profiles for a shock-tube containing gas-droplet mixture.

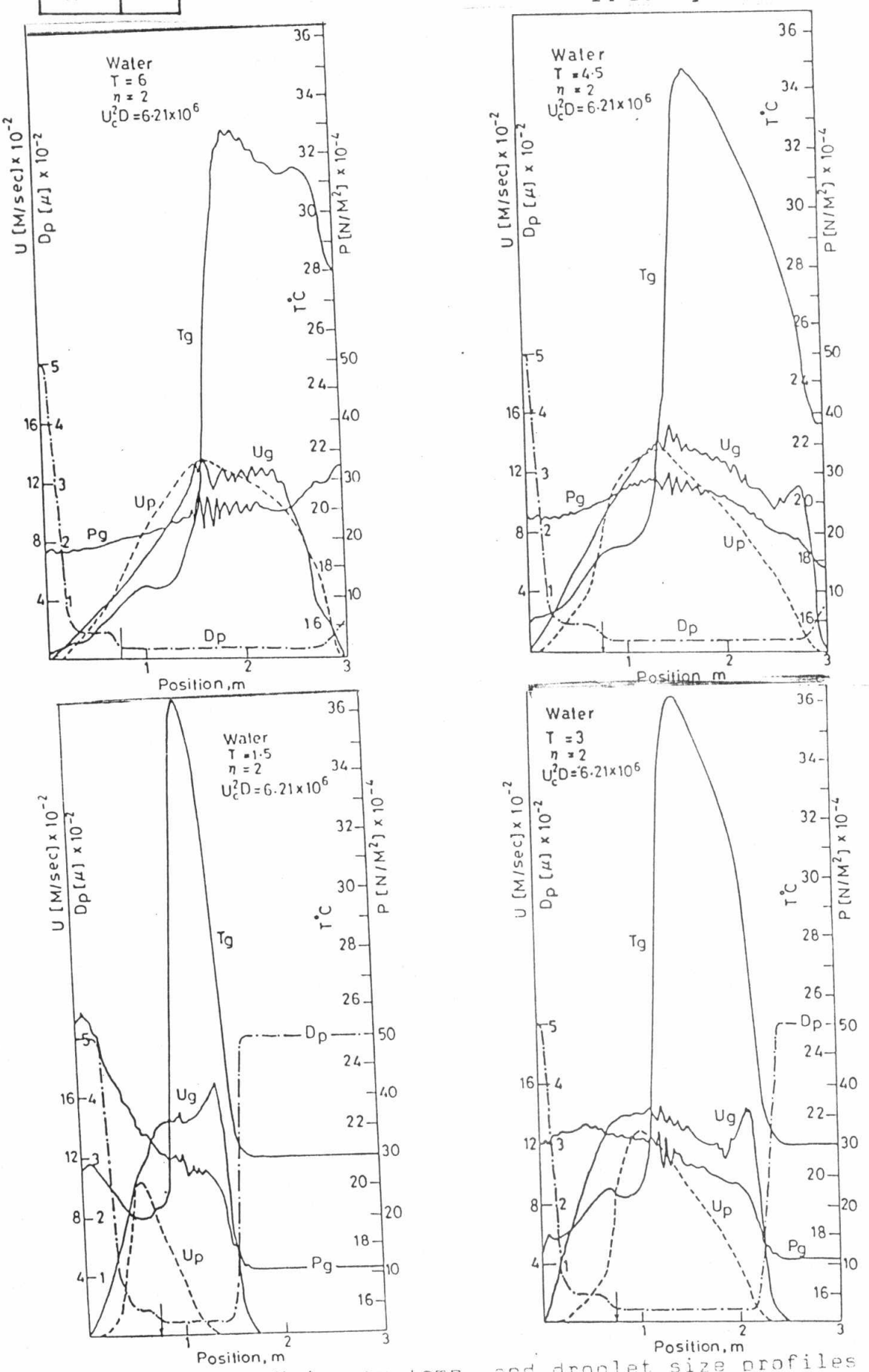

Fig.3 Pressure, Velocity, Temp. and droplet size profiles for a shock-tube containing gas-droplet mixture.

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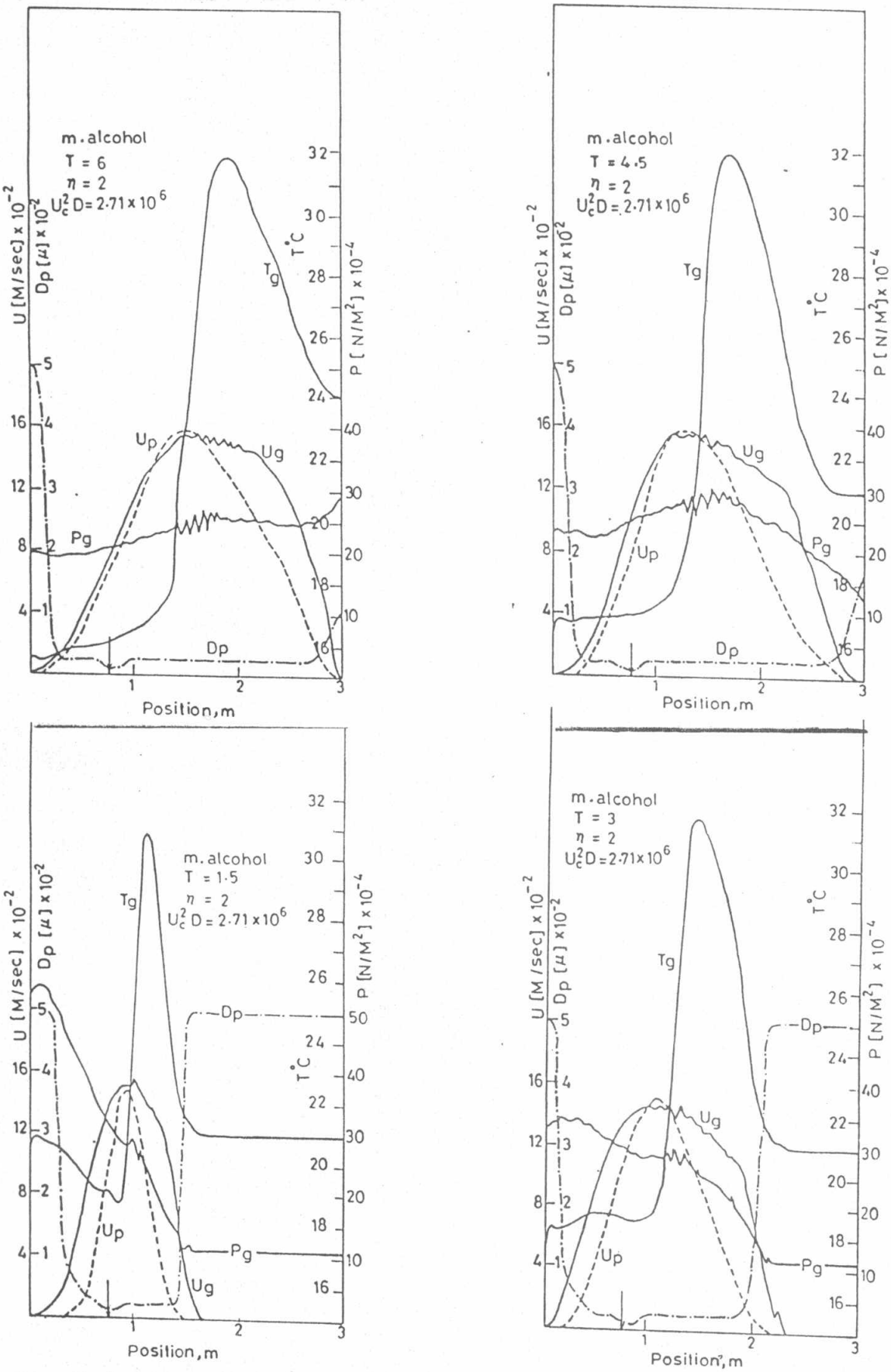

Fig.4 Pressure, Velocity, Temp. and particle size profiles for a shock-tube containing gas-droplet mixture.