

N66 24952

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ACCESSION NUMBER  
223  
74-727  
NASA GRANT NUMBER

(THRU)  
/ (CODE)  
/ (TITLE)

STUDY OF NONEQUILIBRIUM TWO-PHASE FLOW OF A GAS-PARTICLE MIXTURE

by  
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GPO PRICE \$ \_\_\_\_\_  
CFSTI PRICE(S) \$ \_\_\_\_\_  
6.00  
1.25

#653 1-15-65

Technical Note No. 2  
NASA Grant NsG-702  
Report No. AS-66-5  
March 1966

**COLLEGE OF ENGINEERING**  
**UNIVERSITY OF CALIFORNIA, Berkeley**

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## NOMENCLATURE

Roman Lower Case Symbols

- $a$  - speed of sound  
 $c$  - concentration (moles/unit volume)  
 $c_i$  - coordinate of center of particle  
 $c_p$  - specific heat at constant pressure  
 $c_{pm}$  - specific heat at constant pressure for two-phase mixture  
 $e$  - specific internal energy  
 $e_r = e + \frac{1}{2} v^2$   
 $f$  - arbitrary function  
 $f_i$  - drag force per particle  
 $g$  - arbitrary function  
 $h$  - specific enthalpy  
 $h_A, h_B$  - specific enthalpy of species A or B  
 $h_{gs}$  - specific enthalpy of gaseous species B at particle surface  
 $h_{ref}$  - specific enthalpy of reference  
 $h_m$  - specific enthalpy of two-phase mixture  
 $h_{fg}$  - enthalpy of vaporization  
 $h_{fg}^0$  - enthalpy of vaporization at reference temperature  
 $h_{gi}$  - heat transfer coefficient per particle  
 $i$  - unit vector in  $x$ -direction  
 $i$  - constant in the overall momentum equation  
 $j$  - constant in the overall energy equation  
 $k_{xi}$  - mass transfer coefficient per particle

- $m_i$  - mass of one particle  
 $\dot{m}$  - mass flow rate per unit area  
 $n$  - number density of particles  
 $n_j$  - time- and area-averaged number density of particles  
of group  
 $\underline{n}$  - unit normal vector  
 $p$  - pressure  
 $p_i$  - average pressure across an arbitrary cross-section  
of a particle  
 $p_A, p_B$  - partial pressure of a species (A or B)  
 $p_{Bs}$  - partial pressure of species B at particle surface  
 $\hat{p}_B$  - vapor pressure of pure species B in equilibrium  
with its liquid  
 $\underline{q}$  - heat flux vector  
 $\underline{q}^{(d)}$  - heat flux by diffusion  
 $\underline{q}^{(c)}$  - heat flux by conduction  
 $\underline{q}$  - heat transfer rate for one particle  
 $r$  - radius of a particle  
 $r_j$  - radius of particle size group  $j$   
 $r_0$  - reference radius  
 $\alpha$  - nondimensional distance variable  
 $t$  - time  
 $\underline{v}$  - velocity  
 $\underline{V}$  - velocity vector  
 $\underline{v}_x$  -  $x$ -direction component of the velocity  
 $\underline{v}_k$  - velocity of species K with respect to the mass  
average velocity



- $x$  - distance variable; space coordinate  
 $\chi_A, \chi_B$  - mole fractions of various species  
 $\chi_{Bs}$  - mole fraction of species B at the particle surface  
 $y$  - space coordinate  
 $z$  - space coordinate

Roman Upper Case Symbols

- $A$  - area; surface  
 $A_x$  - cross-section area perpendicular to  $x$ -direction  
 $A_{ge}$  - cross-section of gas at the end of a control volume  
 $A_i$  - arbitrary cross-section area of a particle  
 $A_{i\text{sur}}$  - surface area of a particle  
 $A_{i\text{max}}$  - maximum cross-section area of a particle  
 $C_{Di}$  - drag coefficient per particle  
 $C_p^*$  - nondimensional specific heat  
 $D_{AB}$  - binary diffusion coefficient  
 $F$  - drag force per unit length of flow  
 $F_1, F_2$  - functions defined by equations in the text  
 $H$  - nondimensional enthalpy  
 $I$  - nondimensional constant  
 $J$  - nondimensional constant  
 $\dot{M}$  - nondimensional mass flow rate per unit area  
 $N$  - number of particles  
 $Nu$  - Nusselt number  
 $Nu_D$  - Nusselt number for diffusion  
 $P$  - nondimensional pressure

- $\gamma$  - heat transfer rate per unit length of flow  
 $\delta$  - specific gas constant  
 $Rad_j$  - nondimensional particle radius of group  
 $Ref_j$  - nondimensional reference radius of group  
 $Re_y$  - Reynolds number  
 $S$  - surface  
 $S_{pi}$  - surfaces of particles inside a control volume  
 $S_{pe}$  - cross-section surfaces of particles at the ends  
of the control volumes  
 $Sc$  - Schmidt number  
 $T$  - temperature  
 $\hat{T}_B$  - temperature of pure species B  
 $V$  - volume region; nondimensional velocity  
 $Vol$  - volume  
 $\hat{Y}$  - dummy variable in a constructed function  
 $X$  - nondimensional distance variable

### Script Symbols

- $\hat{F}$  - nondimensional drag force per unit volume  
 $M$  - molecular weight  
 $M_f$  - mean molecular weight for a film  
 $q$  - nondimensional heat rate per unit volume  
 $R$  - gas constant ratio  
 $W_B$  - molar flux of species B

### Greek Symbols

- $\alpha_j$  - group loading factor: mass per unit volume of  
group over the mass of particles per unit  
volume

- $\gamma$  - ratio of specific heats  
 $\delta$  - particle loading factor: density of particles  
 divided by density of gas phase  
 $\epsilon$  - perturbation parameter: liquid density divided  
 by gas density  
 $\eta$  - parameter in the vapor pressure equation  
 $\Theta$  - nondimensional temperature  
 $\vartheta$  - dummy variable in a constructed function  
 $k$  - thermal conductivity  
 $\hat{k}$  - nondimensional conductivity  
 $\lambda$  - second viscosity coefficient  
 $\mu$  - viscosity coefficient  
 $\hat{\mu}$  - nondimensional viscosity group  
 $\mu^*$  - nondimensional viscosity-radius parameter  
 $\xi$  - dummy integration variable  
 $\Pi$  - "continuum" pressure  
 $\rho$  - density  
 $\rho_g$  - nondimensional gas density  
 $\rho_p$  - nondimensional particle density  
 $\tau_{ij}$  - stress tensor  
 $\rho$  - "continuum" density  
 $\tau_{ij}$  - shear stress tensor  
 $\tau_g$  - portion of the time interval  $\tau_0$  that gas occupies  
 a position  $(x, y, z)$   
 $\tau_0$  - time interval required to form average flow  
 properties  
 $\Psi$  - mass transfer rate per unit length  
 $\mathcal{P}$  - nondimensional mass transfer rate per unit volume

$\omega$  - mass fraction

### Subscripts

- $g$  - gas phase
- $i$  - for one particle
- $j$  - size group
- $l$  - liquid (or solid) phase
- $p$  - particles
- $\lambda$  -  $\lambda$ -component;  $\lambda$  cross-section
- $A$  - species A (diluent)
- $B$  - species B (liquid-vapor)
- $k$  - any species
- $S$  - surface of a particle; surface
- $0$  - reference state; initial state
- $1$  - state after the gas shock
- $\infty$  - downstream equilibrium state

### Superscripts

- $*$  - nondimensional quantity
- $\wedge$  - dummy variable; nondimensional quantity
- " - fluctuation of a local property
- $l$  - fluctuation of an area averaged property

### Overbars (time averages)

- $\bar{\quad}$  - time average of a continuous function
- $\sim$  - time average of a function with a limited domain of definition

Brackets (area averages)

- $\langle \rangle$  - quantity averaged over its domain of definition  
in the cross-section
- $\langle \rangle_{\rho}$  - average quantity weighted by the density
- $\langle \rangle_{\dot{m}}$  - average quantity weighted by the mass flux
- $\langle \rangle_{\dot{m}v}$  - average quantity weighted by the momentum flux

## SUMMARY

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The problem of a two-phase nonequilibrium flow of particle suspensions in a gaseous medium is formulated, including the effects brought about by the change of phase that takes place in the case of a liquid-gas mixture. On this basis the relaxation zone behind a shock wave passing through a system of liquid droplets dispersed in a gaseous carrier are analyzed. Allowance is made for the presence of two sizes of particles, but specific effects of drop shattering are neglected. The solution is programmed in Fortran and its application to a particular system is illustrated by the case of n-dodecane droplets in oxygen.

Author

## INTRODUCTION

Presented here is a study of the nonequilibrium flow of a gas-particle mixture. Firstly, basic equations for a two-phase system are derived by a rational transition from locally valid relations of continuum mechanics to the overall description of the flow field. This is accomplished by integrating the conservation equations over a control volume and then defining average flow properties of the gas and particle phase. Limiting the control volume to zero size produces differential equations relating these average properties. In order to treat unsteady flow, the equations are also time-averaged, giving rise to certain terms due to fluctuations of particle velocities which are analogous to Reynolds stresses in turbulent flow.

The final two-phase equations may be viewed as describing two coexistent interacting continua, particles and gas. The averaging processes allow one to neglect many aspects of the detailed flow field. However, several additional variables have been introduced. These are the Reynolds stresses and another group arising from the area-averaging. Sometimes a quantity is simply averaged across an area, while in other instances the density of mass flux is used as a weighting factor. One must assume or deduce additional relations for the new variables. The appropriate assumption depends upon the particular problem.

Similar equations have been developed by several authors for various special problems and under various assumptions.

Among these, especially noteworthy are the contributions of Carrier [1], Kliegel [2], Williams [3], Soo [4], Marble [5], Tien [6], Rannie [7], Zuber [8], and van Deemter and van der Laan [9]. Most of the derivations are based essentially on the application of conservation concepts to a control volume. They presuppose the knowledge of velocities, pressures, and temperatures for each phase. The derivation presented here differs essentially from the others by being strictly deductive in nature.

The second half of the report describes a typical two-phase flow problem: the relaxation zone behind a shock wave. The equilibrium mixture flows into a stationary shock wave which affects only the gas phase. The particles and the gas are then at different states and interact in a relaxation zone behind the shock.

The artificial separation of the problem into a gas-phase shock wave followed by a relaxation zone is produced formally by considering the more general question of the structure of steady-state waves in a two-phase flow. An asymptotic solution, using the density ratio (particle material to gas) as the perturbation parameter, is proposed. The problem is singular in nature and it turns out that the gas shock structure and the relaxation zone structure constitute the first terms in two matched asymptotic expansions as the density ratio approaches infinity. It is also noted that this procedure may be applied to two-phase combustion waves.



The shock wave relaxation zone has been studied previously by Carrier [1], Rudinger [10], and Kriebel [11] for the case of solid particles. In this work liquid droplets which can vaporize or receive condensation are considered. The mass transfer is controlled by diffusion and was investigated in a parametric computer study. The parameters which have most influence on the mass transfer are  $\chi_{B_0}$ , the initial mole fraction of vapor, and  $H_{fg}^\circ$ , the heat of vaporization. Other parameters included in the study were the particle size and the loading factor (mass ratio of liquid to gas). The results are given by graphs of the flow variables as functions of the distance through the relaxation zone. When  $\chi_{B_0}$  is low the mass transfer process may be neglected. This conclusion was also confirmed by a special calculation using n-dodecane at NPT as the liquid. The greatest mass transfer occurs when  $H_{fg}^\circ$  is low and  $\chi_{B_0}$  is high. This combination results in the condensation of a major portion of the gas phase. Several additional computations were made also for the case where two particle sizes were present. If most of the liquid mass is in the larger particles it is possible to vaporize the small particles while the large droplets are growing.

## CHAPTER I

### DERIVATION OF CONTINUITY AND MOMENTUM EQUATIONS

#### A. Introduction

This chapter will be concerned with deriving the equations describing the flow of a two-phase system. The condensed phase is assumed to be small dispersed droplets which are imbedded in a gas. Allowance must be made for disequilibrium between the velocity and temperature of the particles and those of the gas phase. Hence it is necessary to account for mass, momentum, and energy exchanges between the two phases.

Since it would be futile to attempt a detailed description of the flow of a large number of particles in a gas, average properties of the flow should be defined in such a way that simple meaningful equations result. The resulting equations can be considered as describing two coexistent continua, a gas phase and a particle phase. This approach is valid for flow problems where the characteristic length is large compared with the distance between the particles.

The conservation equations governing the two-phase flow are usually derived by physical arguments. The derivation is accomplished by specifying a control volume and then applying a physical principle to the volume. Terms which represent various effects are formulated by physical arguments and analogy with similar terms for single-phase flow. This approach actually amounts to a rederivation of the mathematical laws of fluid

motion for the two-phase system. In such a derivation, the worker is required to formulate each term properly and include all significant factors.

An alternate approach, which is more rigorous and deductive in nature, is possible. It does not appear to have been carried out in the literature. Starting from first principles, the conservation equations, one may proceed mathematically by integrating over a control volume, defining new average variables, and limiting the control volume to zero size. This will produce new differential equations describing the two-phase flow. The advantage of such an approach is twofold: first, the variables appearing in the final equations have explicit definitions in terms of the local flow field variables; second, the assumptions are stated explicitly during the derivation in order to simplify the mathematical expressions and thus the reason and necessity for each assumption is apparent. Together this leads to a clearer understanding of the meaning of each term in the two-phase equations and the applicability of the equations themselves.

The dependent variables in the resulting equations will be area averages of the local time-averaged quantities. In addition, terms appear containing variables which are area averages of the time average of the product of two local fluctuations. These terms are analogous to Reynolds stresses in turbulent flow. The word analogous was used since these terms can exist in two-phase flow even when the flow is laminar. The particle equations also contain the "Reynolds stress" type of term. Some authors have considered that "random" fluctuations constitute a particle phase

pressure. The viewpoint taken in this work interprets the particle phase pressure in a different manner and ascribes the fluctuations their proper role as a Reynolds stress.

## B. Physical Background

In order to simplify the work and emphasize the important concepts, consider a flow where gravity and electrical effects are negligible and where the flow is one-dimensional. By "one-dimensional" it is meant that certain time- and area-averaged quantities, to be defined later, are only functions of one space coordinate  $x$ . The particles will be thought of as spherical liquid droplets; however, the definitions will usually remain unchanged or be simplified for solid particles. The nonparticle phase, sometimes called the continuous phase, will be taken as a compressible gas but the extension of the equations to any fluid should not be difficult.

Consider a flow containing numerous dispersed liquid particles. The  $x$ -direction velocity across a typical cross-section is depicted in Figure 1-1. In this figure, the gas phase velocity is arbitrarily assumed to be higher than that of the liquid. The gas velocity decreases in the neighborhood of the droplet surface in order to "stick" to the wall. At positions inside the droplet the velocity is the liquid velocity. The same situation exists for the temperature and density variables. Now as time goes on the particles move past the cross-section and the position previously occupied by the liquid is now occupied by the gas. The velocity at the former time has changed from a value corresponding

to the gas. Thus, the two-phase flow is essentially unsteady and three-dimensional in its detailed structure.

The main theme of this chapter is to establish meaningful definitions of spatially and time-averaged properties which will also result in simple conservation equations. The area averaging will be done in much the same way that one formulates average quantities for pipe flow. The time-averaging process will be similar to that used in turbulence theory. Even though the flow may be laminar, the time averaging is necessary because of the essential unsteady nature of the flow. The difficulty comes from the fact that each phase occupies only a portion of the flow field for a portion of the time and each phase is typified by different magnitudes of temperatures, velocity, etc.

The equations relating the averaged properties may be viewed as conservation laws for two coexistent continua, the gas and the particles. This viewpoint can be taken, of course, only when one is concerned with problems whose characteristic length and time are large compared with the lengths and times required to form suitable average properties. The concept of two coexistent continua is used, for example, when two different molecular species constitute a gas. The distinguishability of the species and the fact that the molecules are dispersed allow this description (see Morse and Feshbach, ref. [12], for a general discussion of the representation of matter as continuous). In the two-phase problem the distinction between the two phases and the fact (assumption) that both phases are dispersed allow a continuum formulation. The gas phase and the particle phase

interact by exchanging mass, momentum, and energy between each phase. These interchanges depend upon the particle radius and because of this it is expedient to consider a set of distinct particle sizes and regard each size as a separate distinguishable continuum. The advantage of this view will become clearer during the derivation.

In formulating the derivation one of the important aspects is the mass, momentum, and energy transfer between the phases. To clarify the assumptions regarding these processes we consider the situation around a single drop, as depicted in Figure 1-2. The gas stream, which may be laminar or turbulent, approaches the particle and stagnates at some point. Depending on the Reynolds number it may or may not be appropriate to consider that a boundary layer exists in the gas around the particles. In any case the gas velocity decreases so that the tangential liquid velocity and gas velocity are equal at the surface of the particle. For large Reynolds numbers a wake exists behind the particle. The pressure and viscous stresses at the particle surface provide the mechanism for accelerating the particle. The shear forces at the particle surface also induce an internal flow of the liquid. This flow has a circulation pattern as indicated in the figure. In addition to this, one must remember that the flow field is unsteady. As the disequilibrium between the particles and gas changes, the detailed flow around the particles is altered appropriately.

What has been said concerning the velocity field is also true for the temperature field and the concentration distribution of various chemical species, if need be.

In the discussion above it has been assumed that a discontinuity of zero thickness exists between the gas and the liquid. The state of affairs at the liquid-gas interface is very complicated and constitutes a subject in itself (see Fig. 1-3). Gibbs [13, p. 219] formulated the thermodynamics of an interface in a rigorous manner. A recent review of this subject with particular emphasis on water droplets is given in Dufour and Defay [14].

It is widely known that a tension force exists in the surface region and that from static equilibrium conditions the pressure within a drop is much higher than that on the outside. A figure for a drop of water, radius  $10^{-4}$  cm (1 micron), is

$$P_{r,l} - P_{gas} = 1.46 \text{ bar (1 atm} = 0.76 \text{ bar)}$$

(all numerical estimates are taken directly from Dufour and Defay [14]). In addition to this, other thermodynamic properties may be attributed to the surface region--a surface enthalpy, entropy, adsorbed mass of a particular species, etc. In general, these properties are dependent upon the radius of the particle. Hence, in a rigorous analysis, changes in the thermodynamic state of the surface region must be considered. Several examples comparing properties at a plane interface and those at an interface of a droplet of water of  $r = 10^{-4}$  cm will be given. The vapor pressure ratio at 273° K is

$$P_r / P_\infty = 1.001$$

The ratio of latent heats of vaporization is

$$h_{fg,r} / h_{fg,\infty} = 1.000$$

And finally for a partial pressure of 6.1 mb the equilibrium temperature of the droplet is 272.98° K, compared with 273° K for a plane surface. These figures show that for particles larger than 1 micron in radius these effects can be ignored; except for the excessive internal pressure within the droplet.

The discussion above concerns the static properties of an interface region. The interface also has a dynamic character and it can be viewed as a two-dimensional world in which a two-dimensional flow is taking place. Two recent papers on the formulation of the equations of motion in a surface are Scriven [15] and the commentary of Slattery [16]. The problem requires a full tensorial treatment and this subject has been included as Chapter 10 in Aris [17]. For flow in a surface, the surface tension plays a role analogous to pressure in the three-dimensional world. Likewise, one can propose a surface viscosity coefficient and indeed in some liquids the surface behavior is non-Newtonian. The important aspect of the detailed study of surface flow, as far as this work is concerned, is that the stress tensor differs from one phase to the other not only because of the surface tension but because of the viscous effects in the surface flow.

The thermodynamics and fluid mechanics of surfaces have been briefly discussed above in order to indicate the complexity of the subject and point out when certain of the assumptions



will become invalid. As far as this work is concerned, the gas-liquid interface will be characterized by a surface across which fluid properties may be discontinuous. Properties on either side of the surface will be taken as those of the bulk fluid just outside the interfacial region. The density is the distinguishing property of each phase and hence is discontinuous across the surface. On the other hand, the temperature will be assumed as continuous. The surface will have one property, a tension force which varies with the radius and maintains the mechanical equilibrium of the surface. Therefore, the pressure is discontinuous across the surface. Sometimes it will be necessary to consider an arbitrary cross-section of a particle. The cross-section would also cut the interface surface. When the forces are integrated over a cross-section, the contribution of the tension force will be associated with the liquid inside the particle. It is also assumed that the surface contains no mass, momentum, or energy and hence these quantities are conserved across the surface. With regard to the motion of the fluid, the tangential components of the velocity and of the stress tensor on each side are assumed equal across the surface.

### C. Scheme for the Derivations

Consider a flow field consisting of a gas and dispersed particles of liquid. At each point in the flow, inside the particles and out, the velocity, temperature, etc., are given in the usual continuum sense. The surfaces of the particles are discontinuities for some properties like density, but other properties such

as temperature are continuous across the particle surface. The usual differential equations for the conservation of mass, momentum, and energy are valid and these may be integrated over a volume in space  $V(t)$  whose boundary  $S(t)$  moves with an arbitrary velocity  $\underline{v}_s$ . This has been carried out by Thorpe [18] and his equations are used here as a starting point. An example of the method of obtaining the integral forms is given in section C of the next chapter.

The continuity equation indicates that the rate of change of the mass within  $V(t)$  is equal to the net flux of mass across the boundary:

$$\frac{d}{dt} \int_{V(t)} \rho dV = - \int_{S(t)} \rho (\underline{v} - \underline{v}_s) \cdot \underline{n} dS \quad (1-1)$$

Variables without subscripts denote local values without specifying the particular phase. The momentum equation states that the rate of change of the momentum within  $V(t)$  is equal to the net flux across the boundary plus the net surface forces. We specifically neglect body forces of any kind:

$$\frac{d}{dt} \int_{V(t)} \rho \underline{v} dV = - \int_{S(t)} \rho \underline{v} (\underline{v} - \underline{v}_s) \cdot \underline{n} dS + \int_{S(t)} \underline{n} \cdot \underline{\sigma} dS \quad (1-2)$$

The energy of the fluid (neglecting external fields) is the sum of the internal energy,  $e$ , and the kinetic energy,  $\frac{1}{2} v^2$ . The rate of change for the control volume  $V(t)$  equals the net flux across the boundary plus the work of the surface forces and the flux of the heat.

$$\frac{d}{dt} \int_{V(t)} \rho e_T dV = - \int_{S(t)} \rho e_T (\underline{v} - \underline{v}_s) \cdot \underline{n} dS - \int_{S(t)} \underline{q} \cdot \underline{n} dS - \int_{S(t)} \underline{n} \cdot (\underline{\sigma} \cdot \underline{v}) dS \quad (1-3)$$

where

$$e_T = e + \frac{1}{2} v^2$$

These three equations provide a fundamental point of departure for the derivation.

To apply the equations, it is first necessary to choose a control volume and specify its motion. For a one-dimensional flow in the  $\chi$ -direction, attention is focused on the matter between two stations  $\chi$  and  $\chi + \Delta\chi$ . The elemental control volume is pictured in Figure 1-4. Since there is a distinction between the gas phase and the particle phase, it can be further specified that the control volume consists of only the gas phase between  $\chi$  and  $\chi + \Delta\chi$ . This control volume resembles a piece of Swiss cheese where the holes are regions to be occupied by the particles. The planes at  $\chi$  and  $\chi + \Delta\chi$  are stationary. The holes move with a speed  $\underline{v}_s$  at each point on their surface. Across the end surfaces  $\chi$  and  $\chi + \Delta\chi$ , there are fluxes of mass, momentum, and energy due to the gas phase. Fluxes across the holes represent interchanges between the particles and gas phase. The equations derived by considering this control volume are called gas phase equations.

In a similar manner, a particle or liquid control volume can be distinguished and defined as all the particles or portions thereof between  $\kappa$  and  $\kappa + \Delta\kappa$ . This control volume consists of a finite number of disjoint control volumes, one for each particle. The surface of the control volume moves with velocity  $\underline{v}$ , except for the particles cut into by the planes at  $\kappa$  and  $\kappa + \Delta\kappa$ . At these positions the control volume is stationary. Again, across the surface of the particles, there are mass, momentum, and energy fluxes as the gas interacts with the particles. The principal restriction on this control volume is that the dimension of the discrete volumes, the particle radius, must be a macroscopic length.

To be complete, a third control volume would be needed for the matter in the interfacial region between the gas and particle regions. As discussed previously, the interfacial region will be idealized, and changes in the state and motion of the interface will be neglected.

The notation for the derivations is very extensive and will be introduced as it is needed. To begin, several surfaces of the control volume are denoted by special symbols. The surface of a particle is denoted by  $S_p$ ;  $S_p^i$  if the surface is inside of, or interior to, the sections at  $\kappa$  and  $\kappa + \Delta\kappa$ , and  $S_{pe}$  if the surface is an end surface located at  $\kappa$  or  $\kappa + \Delta\kappa$ . All other surfaces are denoted by  $A$ .  $A_x$  indicates an arbitrary cross-section across both the gas and liquid phases;  $A_{gx}$  is that portion of  $A_x$  which is occupied by gas, and  $A_{lx}$  that portion occupied by liquid. The cross-section occupied by the

gas and located at  $x$  and  $x + \Delta x$ , i.e.,  $A_{g,x}(x)$  and  $A_{g,x}(x + \Delta x)$ , is given the additional symbol  $A_{ge}$  for gas end cross-section.

The local values of velocity, temperature, density, etc., are designated by the usual symbols  $v$ ,  $T$ ,  $\rho$ , etc. If the gas occupies the position  $x$ ,  $y$ ,  $z$ ,  $t$ , then a subscript  $g$  is added; if the liquid occupies the position, then  $l$  is subscripted. The integrals of the local properties will appear naturally from the integral form of the conservation equations applied to the control volume. These integrals will define area-averaged, density-averaged, or mass-flux-averaged quantities which will be functions of  $x$  and  $t$ . When the length of the control volume is limited,  $\Delta x \rightarrow 0$ , a differential equation results in which the dependent variables are the average quantities.

The area-averaged quantities above are not useful variables because they average the instantaneous local values of  $v$ ,  $\rho$ , etc., and the flow is essentially unsteady. Dependent variables which are area averages of the local time-averaged property are better both for physical insight and experimental verification. In order to time-average the equations, one proceeds in a manner similar to turbulent flow theory; however, some peculiarities are introduced by the existence of two phases.

#### D. Area Averaging of Continuity and Momentum Equations

The continuity and momentum equations for the gas phase will be considered first, and then the same equations for the liquid phase. The energy equations and overall gas-plus-liquid equations will be treated in the next chapter.

For the gas-phase control volume, the integrated continuity equation may be applied with the following result:

$$\frac{d}{dt} \int_x^{x+\Delta x} \int_{A_{gx}} \rho_g dS dx = - \int_{A_{ge}} \rho_g \underline{v}_g \cdot \underline{n}_g dS - \sum_i \int_{S_{vi} + S_{pe}} \rho_g (\underline{v}_g - \underline{v}_s) \cdot \underline{n}_g dS \quad (1-4)$$

The integration over  $A_{ge}$  actually consists of two integrals, one for  $x$  and one for  $x + \Delta x$ . Likewise, the symbol summation over  $i$  means that the integrals over all particles are added;  $i$  is not used as a dummy index. This equation will be reduced to a differential equation for the gas phase of the two-phase mixture by defining suitably averaged quantities and then limiting the control volume by letting  $\Delta x \rightarrow 0$ .

The symbol  $\langle \rangle$  will designate a simple area average. The symbol  $\langle \rangle_\rho$  will imply that the density has been used as a weighting factor. These definitions are exemplified by the density and velocity as given below:

$$\langle \rho_g \rangle = \frac{1}{A_{gx}} \int_{A_{gx}} \rho_g dS \quad (1-5)$$

$$\langle \underline{v}_{gx} \rangle_\rho = \frac{1}{\langle \rho_g \rangle A_{gx}} \int_{A_{gx}} \rho_g \underline{v}_g \cdot \underline{i} dS \quad (1-6)$$

Consider the left-hand side of the continuity equation; the differentiation with respect to time may be moved inside the

integration over  $x$  and then the mean-value theorem for integrals applied. The first term on the right-hand side is identified as an increment in the average mass flow rate. The equation now reads

$$\frac{\partial}{\partial t} (A_{gx} \langle \rho_g \rangle) \Big|_{x=x_0}^{x=x_0+\Delta x} = - \frac{1}{\Delta x} \left[ \langle \rho_g \rangle \langle v_{gx} \rangle A_{gx} \right]_{x_0}^{x_0+\Delta x} - \frac{1}{\Delta x} \sum_i \int_{S_{pi}} \rho_g (v_g - v_s) \cdot n_g dS \quad (1-7)$$

The last term represents the net mass interchange between the gas phase and the condensed phase per unit length of flow direction. This term will be denoted by  $\Psi$  :

$$\Psi = - \lim_{\Delta x \rightarrow 0} \frac{1}{\Delta x} \sum_i \int_{S_{pi}} \rho_g (v_g - v_s) \cdot n_g dS \quad (1-8)$$

Letting  $\Delta x \rightarrow 0$  in equation (1-7) gives the continuity equation for the area-averaged quantities:

$$\frac{\partial}{\partial t} (A_{gx} \langle \rho_g \rangle) = - \frac{\partial}{\partial x} (\langle \rho_g \rangle \langle v_{gx} \rangle A_{gx}) + \Psi \quad (1-9)$$

With regard to the function  $\Psi$  it will be assumed that droplets of a given size  $j$  could be grouped together and a  $\Psi_j$  defined for each distinct size:

$$\Psi = \sum_j \Psi_j = - \sum_j \left\{ \lim_{\Delta x \rightarrow 0} \frac{1}{\Delta x} \sum_i \int_{S_{pi}} \rho_g (\underline{v}_g - \underline{v}_s) \cdot \underline{n}_g dS \right\} \quad (1-10)$$

where  $j$  is a finite number (there are only finite number of drops in consideration!).

The momentum equation for the gas is derived by considering the same control volume as for the continuity equations. The momentum theorem states that the rate of change of momentum within the control volume is equal to the sum of the net flux of momentum across the surface and the net force on the surface. Body forces will be neglected:

$$\frac{d}{dt} \int_{V(t)} \rho \underline{v} dV = - \int_{S(t)} \rho \underline{v} (\underline{v} - \underline{v}_s) \cdot \underline{n} dS + \int_{S(t)} \underline{n} \cdot \underline{\underline{\sigma}} dS \quad (1-11)$$

For the gas-phase control volume, the  $x$ -component of this equation is

$$\begin{aligned} \frac{d}{dt} \int_x^{x+\Delta x} \int_{A_{gx}} \rho_g v_{gx} dS dx = & - \int_{A_{ge}} \rho_g v_{gx} (\underline{v}_g \cdot \underline{n}_g) dS \\ & - \sum_i \int_{S_{pi}} \rho_g v_{gx} (\underline{v}_g - \underline{v}_s) \cdot \underline{n}_g dS + \int_{A_{ge} + A_{gs}} (\underline{n}_g \cdot \underline{\underline{\sigma}}_g) dS + \sum_i \int_{S_{pi}} (\underline{n}_g \cdot \underline{\underline{\sigma}}_g)_x dS \end{aligned} \quad (1-12)$$

The left-hand side is reduced as follows:



$$\begin{aligned} \frac{d}{dx} \int_x^{x+\Delta x} \int_{A_{gx}} \rho_g v_{gx} dS dx &= \int_x^{x+\Delta x} \frac{\partial}{\partial t} \int_{A_{gx}} \rho_g (v_g \cdot \eta_g) dS dx \\ &= \left. \frac{\partial}{\partial t} (\langle \rho_g \rangle \langle v_{gx} \rangle A_{gx}) \right]_{x-x_f} \cdot \Delta x \end{aligned} \quad (1-13)$$

The first term on the right-hand side of equation (1-12) is the momentum flux of the gas through the ends of the control volume. This motivates the definition of a "density average of the velocity squared" as opposed to the "density-averaged velocity" defined by equation (1-6):

$$\langle v_{gx}^2 \rangle = \frac{1}{\langle \rho_g \rangle \langle A_{gx} \rangle} \int_{A_{gx}} \rho_g (v_g \cdot \underline{i})^2 dS \quad (1-14)$$

thus

$$- \int_{A_{ge}} \rho_g v_{gx} (v_g \cdot \eta_g) dS = - \left. \langle \rho_g \rangle \langle v_{gx}^2 \rangle A_{gx} \right]_x^{x+\Delta x} \quad (1-15)$$

The second term on the right-hand side of equation (1-12) is the  $x$ -direction momentum is transferred between the two phases. The mass flux  $\rho_g (v_g - v_s) \cdot \eta_g$  into or out of the droplet surfaces is multiplied by the  $x$ -component of the gas velocity at the surface of the droplet. Then this product is integrated over the droplet surface and the integrals are summed over the

distinct droplets. A precise evaluation of this term would require a detailed knowledge of the flow field around the droplet (and this requires a knowledge of the flow on the surface and inside the droplet). Since an overall continuum description of the spray is the present goal, one seeks simplifying assumptions that will allow this term to be expressed by the overall mass transfer function  $\Psi$  and the overall droplet velocity. Two assumptions seem to be required: the mass flux from a droplet is uniform around the surface, and the droplet moves without distorting in (surface only) translational motion. The proof of this is involved and will be given in the appendix. For the present, only the result will be stated:

$$-\lim_{\Delta x \rightarrow 0} \frac{1}{\Delta x} \sum_i \int_{S_{pi}} v_{gx} (v_g - v_s) \cdot \underline{n}_g dS = \sum_j \langle v_{xj} \rangle \Psi_j \quad (1-16)$$

If only one size of particles is in the problem,

$$\langle v_{x,x} \rangle \Psi = \sum_j \langle v_{xj} \rangle \Psi_j \quad (1-17)$$

The last two terms in the momentum equation (1-12) are the results of surface forces. The surface forces on the particles are used to define a drag function:

$$-F_x = + \lim_{\Delta x \rightarrow 0} \frac{1}{\Delta x} \sum_i \int_{S_{pi}} (\underline{n}_g \cdot \underline{\sigma}_g)_x dS \quad (1-18)$$

If more than one size of particle is present, the integrals may be grouped according to particle size and a drag function for each size  $j$  defined:

$$F_x = \sum_j F_{xj} \quad (1-19)$$

The drag function represents the forces on the particles in the particular flow field at a specific time. Formally the drag force does not separate into a steady-state part, a part due to heat or mass transfer, a part due to unsteady motion, a part due to a gas phase pressure gradient, and so forth. This separation can occur only when one considers a specific situation. Zuber [8] has given some interesting ideas on the detailed representation of the drag for slow laminar flow.

Another aspect of the drag force arises when one considers two particles passing each other. As the two particles approach each other, the gas flow field between them changes and the surface forces on the particles, and hence the drag, changes. The particles need not touch each other for the encounter to have a significant effect on the drag function. On the other hand, a physical collision causes an almost instantaneous transfer of momentum between the particles. Consideration of collisions at the boundary of the control volume has been excluded from this analysis. A thoughtful paper on this subject has been given recently by Marble [19].

The surface forces on the gas portion of the control volume are divided into pressure and viscous forces:

$$\begin{aligned}
 - \int_{A_{j^c} + A_{j^s}} (\underline{n}_j \cdot \underline{\sigma}_j)_x dS &= - \int_{A_{j^c}} [\rho_j (\underline{n}_j \cdot \underline{i}) + (\underline{n}_j \cdot \underline{\sigma}_j)_x] dS \\
 &\quad - \int_{A_{j^c}} [\rho_j (\underline{n}_j \cdot \underline{i}) + (\underline{n}_j \cdot \underline{\sigma}_j)_x] dS
 \end{aligned}
 \tag{1-20}$$

The viscous forces on the side wall will be dropped. The pressure on the side wall does not contribute to the  $x$ -direction forces. (If a variable flow area  $A_x$  is considered an additional term  $\rho_j dA_x / dx$  will occur).

The integrals over the ends of the control volume give

$$- \int_{A_{j^c}} (\underline{n}_j \cdot \underline{\sigma}_j)_x dS = - A_{j^c} \langle \rho_j \rangle \Big|_x^{x+\Delta x} - A_{j^c} \langle \tau_{xx} \rangle \Big|_x^{x+\Delta x}
 \tag{1-21}$$

where the area-averaged properties are

$$\begin{aligned}
 \langle \rho_j \rangle &= \frac{1}{A_{j^c}} \int_{A_{j^c}} \rho_j dS \\
 \langle \tau_{xx} \rangle &= \frac{1}{A_{j^c}} \int_{A_{j^c}} (\underline{i} \cdot \underline{\sigma}_j)_x dS
 \end{aligned}
 \tag{1-22}$$

The viscous stress  $\langle \tau_{xx} \rangle$  will be retained because it has application in the shock wave problem; usually it would be neglected.

Substituting the results that are discussed above into the momentum equation (1-12) yields

$$\begin{aligned} \frac{\partial}{\partial t} (\langle \rho_g \rangle \langle v_{gx} \rangle A_{gx}) \\ = - \frac{\partial}{\partial x} (\langle \rho_g \rangle \langle v_{gx}^2 \rangle A_{gx}) - \frac{\partial}{\partial x} (A_{gx} \langle p_g \rangle)_{(1-23)} \\ - \frac{\partial}{\partial x} (A_{gx} \langle \tau_{xx} \rangle) + \sum_j \Psi_j \langle v_{xj} \rangle - \sum_j F_{xj} \end{aligned}$$

The effect of the particles shows up in two terms:  $F_x$ , the drag force and  $\Psi \langle v_{ex} \rangle$ , the momentum added to the gas phase by the vaporizing liquid. Note that the velocity  $\langle v_{ex} \rangle$  is characteristic of this momentum whether the liquid is vaporizing or the gas is condensing. In either case the matter that is about to change phase is located at the interface surface where the local velocity of the gas and the liquid differ only by a small component normal to the surface.

The equations referring to the particles are derived by integrating the appropriate conservation law over the volume occupied by the particles between  $x$  and  $x + \Delta x$ . The overall continuity equation is

$$\sum_i \frac{d}{dt} \int_{V_i} \rho_i dV = - \sum_i \int_{S_i + S_e} \rho_i (\underline{v}_i - \underline{v}_s) \cdot \underline{n}_i dS \quad (1-24)$$

The liquid will be assumed to have a uniform density. Suppose the cross-section area of the particles at any station  $x$  is called  $A_{lx}$ ; then the volume integrals are rewritten to give

$$\int_x^{x+\Delta x} \left[ \frac{\partial}{\partial t} \rho_l \sum_i \int_{A_{lx}} dS \right] dx \quad (1-25)$$

$$= - \sum_i \int_{S_{pe}} \rho_l (\underline{v}_e \cdot \underline{n}_e) dS - \sum_i \int_{S_{pi}} \rho_l (\underline{v}_e - \underline{v}_s) \cdot \underline{n}_e dS$$

The particle velocity averaged over the area is defined as

$$\langle \underline{v}_{lx} \rangle = \langle \underline{v}_{lx} \rangle_\rho = \frac{1}{A_{lx}} \sum_i \int_{S_{px}} \underline{v}_e \cdot \underline{i} dS \quad (1-26)$$

then

$$- \rho_l A_{lx} \langle \underline{v}_{lx} \rangle \Big|_x^{x+\Delta x} = - \rho_l \sum_i \int_{S_{pe}} \underline{v}_e \cdot \underline{n}_e dS \quad (1-27)$$

The last term on the right-hand side of equation (1-25) is the mass transferred between the gas and liquid phases. This is shown by noting that across the liquid-gas interface the mass conservation law requires that

$$\rho_l (\underline{v}_l - \underline{v}_s) \cdot \underline{n}_l = - \rho_g (\underline{v}_g - \underline{v}_s) \cdot \underline{n}_g \quad (1-28)$$

Substituting this into the integral of the last term in equation (1-25) shows that this term is  $-\Psi$  as defined by equation (1-8).

The continuity equation is derived from equation (1-25) by using the mean value theorem for the integral over on the left-hand side. Then dividing by  $\Delta x$  and limiting  $\Delta x \rightarrow 0$ , the result is

$$\frac{\partial}{\partial t} (\rho_e A_{ex}) = - \frac{\partial}{\partial x} (\rho_e A_{ex} \langle v_{ex} \rangle) - \Psi \quad (1-29)$$

Note that for the constant density particles,  $\rho_e$  may be taken from under the differentiation sign.

For several distinct sizes of particles, the equation above is valid for each particular size, i.e.,

$$\frac{\partial}{\partial t} \rho_{ej} A_{exj} = - \frac{\partial}{\partial x} (\rho_{ej} A_{exj} \langle v_{exj} \rangle) - \Psi_j \quad (1-30)$$

Proceeding in a way similar to the derivation of the continuity equation, the momentum theorem is written for the sum of the particles between  $x$  and  $x + \Delta x$ . For the  $x$ -direction,

$$\sum_i \frac{d}{dt} \int_{V_i} \rho_e v_{ex} dV = - \sum_i \int_{S_{pi} + S_{pe}} \rho_e v_{ex} (v_x - v_s) \cdot n_x dS + \sum_i \int_{S_{pi} + S_{pe}} (n_x \cdot \underline{\sigma}_e)_x dS \quad (1-31)$$

Since the particles are composed of an incompressible fluid, the left-hand side is

$$\rho_l \int_x^{x+\Delta x} \left[ \frac{d}{dt} \sum_i \int_{A_{lx}} \underline{v}_i \cdot \underline{n}_i dS \right] dx \quad (1-32)$$

$$= \rho_l \left. \frac{d}{dt} (\langle v_{lx} \rangle A_{lx}) \right|_{x=x_0} \cdot \Delta x$$

The first term on the right-hand side accounts for fluxes of momentum across the control surfaces. The "interior" droplet surfaces account for momentum leaving the liquid phase:

$$-\sum_i \int_{S_{pi}} \rho_l v_{lx} (\underline{v}_i - \underline{v}_s) \cdot \underline{n}_i dS$$

$$= \sum_i \int_{S_{pi}} \rho_g (v_{gx} - v_{sx}) \cdot \underline{n}_i v_{lx} dS \quad (1-33)$$

$$= -\sum_j \psi_j \langle v_{lxj} \rangle = -\psi \langle v_{lx} \rangle$$

The steps for arriving at the last equation are given in the appendix.

The liquid momentum flux across the ends of the control volume at  $x$  and at  $x + \Delta x$  is by definition an increment in the mass-flux-averaged droplet velocity:



$$-\sum_i \int_{S_{pe}} \rho_x v_{ix} (\underline{v}_i \cdot \underline{n}_i) dS = -\rho_x \langle v_{ix}^2 \rangle A_{ix} \Big]_x^{x+\Delta x} \quad (1-34)$$

where

$$\langle v_{ix}^2 \rangle = \langle v_{ix}^2 \rangle = \frac{1}{A_{ix}} \sum_i \int_{S_{pe}} (v_{ix} \cdot \underline{i})^2 dS \quad (1-35)$$

The terms representing the surface forces in the  $x$ -direction will be considered next (equation 1-31). At a point on a particle surface, the force from the liquid side upon the gas side is  $\underline{n}_i \cdot \underline{\sigma}_i$ . This force can be broken into two components, along the surface and normal to the surface.

It was previously assumed that the tangential stress on the liquid side was the same as that on the gas side; however, the normal stress was discontinuous because of the surface tension. Suppose that the surface tension is uniform around the surface of the particle; then the jump in the normal stress across the surface is uniform. The integral of the  $x$ -component of a constant over the surface of the particle will be zero. These arguments show that the drag force of the gas upon the particles is the same as the drag of the particles upon the gas:

$$\begin{aligned}
& \int_{S_p} (\underline{n}_x \cdot \underline{\sigma}_x)_x dS \\
&= \int_{S_p} [(\underline{n}_x \cdot \underline{\sigma}_x)_{\text{tan}} + (\underline{n}_x \cdot \underline{\sigma}_x)_{\text{norm}}]_x dS \quad (1-36) \\
&= \int_{S_p} [-(\underline{n}_g \cdot \underline{\sigma}_g)_{\text{tan}} + (\underline{n}_g \cdot \underline{\sigma}_g)_{\text{norm}} + (\text{SUR TEN})]_x dS \\
&= - \int_{S_p} (\underline{n}_g \cdot \underline{\sigma}_g)_x dS
\end{aligned}$$

$$F_x \cdot \Delta x = \sum_i \int_{S_{pi}} (\underline{n}_x \cdot \underline{\sigma}_x)_x dS \quad (1-37)$$

In addition to the surface tension there is actually an additional jump in the normal stress because of the vaporization. This slight recoil pressure can be handled in the same way as the surface tension, by assuming a uniform vaporization rate around the particle.

The last term to be considered is the forces upon the liquid cross-sections cut by the planes at  $x$  and  $x + \Delta x$ . This term

constitutes the pressure force for the liquid phase:

$$\sum_i \int_{S_{pe}} (\underline{n}_i \cdot \underline{\sigma}_i)_x ds = -A_{ex} \langle P_i \rangle \Big|_x^{x+\Delta x} \quad (1-38)$$

where

$$\langle P_i \rangle = \frac{1}{A_{ex}} \sum_i \int_{S_{pe}} P_i ds \quad (1-39)$$

This pressure is the force of the liquid on one side of the control volume upon the liquid on the other; thus this is not part of the drag. The integrals above include the surface forces or surface tension in the particles. For droplets in a static situation the surface tension is a force proposed to maintain the mechanical equilibrium of the curved surface. The integral over the cross-section of the droplet plus the surface tension is balanced by the integral of the external pressure (see Fig. 1-5). Thus, the average particle pressure defined above would be the same as the gas pressure. If the stagnant gas around the particle is increased in pressure, the internal particle pressure is increased proportionally. The internal particle pressure is a mechanical variable since the thermodynamic state, as specified by the temperature and density, is unchanged by the increase in pressure.

When a particle is accelerated there exists a pressure gradient within the liquid in the direction of the acceleration. This gradient is easily envisioned if one imagines the horizontal acceleration of a tray of water. Upon acceleration, the free surface assumes a sloping position showing that a pressure gradient exists within the liquid on any horizontal plane. Since the gradient of particle pressure appears in the particle momentum equation, it might be expected that particle acceleration has an important influence on this term. This is not the case, however, as will now be shown.

Figure 1-4 is a schematic of the flow field with a plane at  $x$  (or  $x + \Delta x$ ) cutting through the droplets. The term that is of interest here is the gradient of the particle pressure times the liquid cross-section:

$$\frac{d}{dx} A_{Lx} \langle p_i \rangle = \frac{d}{dx} \sum_i \int_{S_{pi}} p_i dS \quad (1-40)$$

The summation over the distinct particles changes with  $x$ , so one cannot simply differentiate the separate integrals. Let the integral across a particle be denoted by an average pressure and the particle cross-section area:

$$\int_{S_{pi}} p_i dS = A_i p_i \quad (1-41)$$

Next  $p_i$  is expanded to two terms about the center of the particle:

$$p_i = p(c_i) + \frac{dp}{dx}(x - c_i) + \dots \quad (1-42)$$

$p(c_i)$  is the average pressure at the center of the particle and  $dp/dx$  is the gradient caused by acceleration of the particle. Now by definition of the derivative, the particle pressure force can be computed:

$$\frac{d}{dx} (A_{2x} \langle p_2 \rangle) = \lim_{\Delta x \rightarrow 0} \left\{ \sum_i A_i(x+\Delta x) \left[ p(c_i) + \frac{dp}{dx} \Big|_{c_i} (x+\Delta x - c_i) \right] - \sum_i A_i(x) \left[ p(c_i) + \frac{dp}{dx} \Big|_{c_i} (x - c_i) \right] \right\} \quad (1-43)$$

The first sum is for particles cut by the plane at  $x + \Delta x$  and the second, for those at  $x$ . Each sum may have some particles in common with the other but there are undoubtedly particles which belong to only one of the groups. Consider one of the groups, say those located at  $x$ . The group can be further divided into plus particles whose centers are on the right of  $x$ , and minus particles whose centers are on the left. There are just as many particles on the left of  $x$  as on the right and the particles are paired according to the distance between their centers and the plane at  $x$ . Thus, for a paired + and - particle couplet,

$$(\alpha - c_{i+}) = -(\alpha - c_{i-}) = (\alpha - c_{i\pm}) \quad (1-44)$$

and

$$A_{i+} = A_{i-} = A_{i\pm} \quad (1-45)$$

With this pairing, the sum at  $\alpha$  is written as the sum  $i\pm$  over pairs:

$$\begin{aligned} & \sum_{i+, i-} \left\{ A_{i+} P_+ + A_{i-} P_- + A_{i+} \left. \frac{dP}{d\alpha} \right|_{c_{i+}} (\alpha - c_{i+}) + A_{i-} \left. \frac{dP}{d\alpha} \right|_{c_{i-}} (\alpha - c_{i-}) \right\} \\ & = 2 \sum_{i\pm} A_{i\pm} \left\{ \left( \frac{P_+ + P_-}{2} \right) + \left( \left. \frac{dP}{d\alpha} \right|_{c_{i+}} - \left. \frac{dP}{d\alpha} \right|_{c_{i-}} \right) \frac{(\alpha - c_{i\pm})}{2} \right\} \end{aligned} \quad (1-46)$$

The average of the center pressures is taken as the center pressure at  $\alpha$ ,  $p_c(\alpha)$ ; the particle acceleration (which causes  $\left. \frac{dP}{d\alpha} \right|_{c_i}$ ) does not change significantly over the distance equal to a particle diameter. The expression above then reduces to

$$2 \sum_{i\pm} A_{i\pm} p_c(\alpha) = p_c(\alpha) \cdot 2 \sum_{i\pm} A_{i\pm} = p_c(\alpha) A_{2\alpha} \quad (1-47)$$

Finally, one can substitute into equation (1-43) and compute the results:

$$\begin{aligned} \frac{d}{dx} (A_{ex} \langle p_e \rangle) &= \lim_{\Delta x \rightarrow 0} \left\{ A_{ex}(x+\Delta x) p_c(x+\Delta x) - A_{ex}(x) p_c(x) \right\} \\ &= \frac{d}{dx} (A_{ex} p_c(x)) \end{aligned} \tag{1-48}$$

The derivative of the particle pressure is the same as the derivative of the average pressure of the center of the particles. But it was found previously that the average internal pressure in a droplet was dependent upon the pressure of the surrounding gas when in static equilibrium. When there is a flow field around the particle causing an acceleration force, the average external pressure might deviate from the "free stream" gas pressure. A calculation for inviscid irrotational flow around a sphere gives  $p_{ave} = 3 p_\infty$  (computed for the most severe assumption that the minimum local pressure is zero). In any event, the particle pressure defined here is of the order of magnitude of the gas phase pressure, its exact value depending upon the details of the motion.

The final momentum equation is formed by substituting equations (1-32), (1-33), (1-34), (1-37), and (1-38) into equation (1-31), then dividing by  $\Delta x$  and limiting  $\Delta x \rightarrow 0$  :

$$\frac{\partial}{\partial t} (\rho \langle v_{xx} \rangle A_{xx}) = - \frac{\partial}{\partial x} \left[ (\rho \langle v_{xx}^2 \rangle A_{xx}) + \langle p_x \rangle A_{xx} \right] - \Psi \langle v_{xx} \rangle + F_x \quad (1-49)$$

### E. Time Averaging of Continuity and Momentum Equations

The continuity and momentum equations derived in the preceding section represent instantaneous area-averaged equations. The flow is not actually steady and it is necessary to time-average the equations in a manner similar to turbulent flow theory. Let an overbar denote the time average (see Hinze [20] for a general discussion of this topic):

$$\bar{f}(x,t) = \frac{1}{\tau_0} \int_0^{\tau_0} f(x,t+\xi) d\xi \quad (1-50)$$

The time average is independent of further averaging:

$$\bar{\bar{f}} = \bar{f} \quad (1-51)$$



Averaging also satisfies the following relations:

$$\begin{aligned} \overline{f+g} &= \bar{f} + \bar{g} & \overline{f \cdot g} &= \bar{f} \cdot \bar{g} \\ \frac{\partial \overline{f}}{\partial x} &= \frac{\partial \bar{f}}{\partial x} & \frac{\partial \overline{f}}{\partial t} &= \frac{\partial \bar{f}}{\partial t} \end{aligned} \quad (1-52)$$

A fluctuation component is defined by the equation below, and its time average can be shown to be zero by applying the relations above:

$$\begin{aligned} f &= \bar{f} + f' \\ \overline{f'} &= 0 \end{aligned} \quad (1-53)$$

A useful relationship for the product of two quantities in terms of the average values and the fluctuations may also be derived:

$$\overline{f \cdot g} = \bar{f} \cdot \bar{g} + \overline{f' g'} \quad (1-54)$$

An equation may be time-averaged by integrating from 0 to  $\tau_0$  and dividing by  $\tau_0$ . Then the relations above are employed to express the equation in the desired variables.

The time-averaged continuity equation for the gas phase is

$$\frac{\partial}{\partial t} (\overline{A_{gx} \langle \rho_g \rangle}) = - \frac{\partial}{\partial x} (\overline{A_{gx} \langle \rho_g \rangle \langle v_{gx} \rangle}) + \bar{\Psi}$$

$$\begin{aligned}
& \frac{\partial}{\partial t} (\overline{A_{gx}} \overline{\rho_g}) + \overline{A'_{gx} \rho'_g} \\
&= - \frac{\partial}{\partial x} \left[ \overline{A_{gx} \rho_g} \overline{v_{gx}} + \overline{A_{gx} \rho'_g} \overline{v'_{gx}} \right] \\
&+ \overline{\rho_g} \overline{A'_{gx} v'_{gx}} + \overline{v_{gx}} \overline{A'_{gx} \rho'_g} \\
&+ \overline{A'_{gx} \rho'_g v'_{gx}} \Big] + \overline{\Psi} \tag{1-55}
\end{aligned}$$

This equation contains five new terms which concern the fluctuating quantities. As discussed by Hinze [20, pp. 19 and 368], the fluctuations in density can usually be neglected when the Mach number of the turbulence is small. Making this assumption allows one to discard four of the five new terms; the fifth term contains the gas cross-section area fluctuation  $A'_{gx}$ . If the particles remain dispersed and do not collect into temporary bunches or voids, then the fluctuations in  $A_{gx}$  will be small compared with the average value  $\overline{A_{gx}}$ . Employing these two assumptions gives

$$\frac{\partial}{\partial t} (\overline{A_{gx}} \overline{\rho_g}) = - \frac{\partial}{\partial x} (\overline{\rho_g} \overline{A_{gx}} \overline{v_{gx}}) + \overline{\Psi} \tag{1-56}$$

This equation has the same form as the usual continuity equation when the terms have been replaced by the time average of the area-averaged properties.

The assumption that  $A_{gx}' / \bar{A}_{gx} \ll 1$  is akin to the assumption that the gas density fluctuations are incompressible ( $\langle \rho_g \rangle' / \langle \rho_g \rangle \ll 1$ ). The gas cross-section actually depends upon the number of particles at the cross-section ( $A_{gx} + A_{lx} = A_x$ ), so, in discussing  $A_{gx}$ , one is really discussing the behavior of the particles. This leads to the central point, which is that of considering the particles and gas phases as two coexistent continua.

The particles may be considered as a "continuum" if they are "numerous" and "dispersed." To make these notions more precise, a number density of particles is defined

$$n(x, y, z, t) = \lim_{\Delta V \rightarrow 0} \frac{N}{\Delta V} \quad (1-57)$$

by taking the ratio of the number of particles  $N$  in an arbitrary cube  $\Delta V$  around the point  $x, y, z$ , at  $t$ . If the particles are dispersed and numerous, then the value of  $N/\Delta V$  is closely  $n$  even when  $N$  is small and the characteristic dimension of  $\Delta V$  is small compared with a characteristic dimension of the problem.

The continuum density of the particles is then given by the following for spherical particles:

$$\sigma_p = \frac{4}{3} \pi r^3 \rho_p n \quad (1-58)$$

Another relation for the average density across the flow area is found to relate to the actual liquid density and the liquid cross-section:

$$\langle \sigma_p \rangle A_x = A_{lx} \rho_l \quad (1-59)$$

Thus, the number density, the liquid and gas cross-sections, and the overall particle density are all directly related:

$$\langle \sigma_p \rangle = \frac{4}{3} \pi r^3 \rho_l \langle n \rangle = \frac{A_{lx} \rho_l}{A_x} = \frac{A_x - A_{gx}}{A_x} \rho_l \quad (1-60)$$

Assuming that the number density has only small fluctuations implies that the fluctuations in  $A_{gx}$ ,  $A_{lx}$ , and  $\sigma_p$  are also negligible. This could be summarized by stating that the particles considered as a continuum undergo incompressible fluctuations. This assumption is necessary in order to produce tractable conservation equations for two-phase flow, and it will be made in all subsequent equations.

Next, the time-averaging process is applied to the gas phase momentum equation (1-23), and density fluctuations (gas and particles) are assumed to be negligible. The result is

$$\begin{aligned}
& \frac{\partial}{\partial t} \left[ \overline{\rho_g} \overline{A_{gx}} \overline{v_{gx}} \right] \\
&= - \frac{\partial}{\partial x} \left[ \overline{\rho_g} \overline{A_{gx}} \overline{v_{gx}^2} \right] \\
&\quad - \frac{\partial}{\partial x} \left[ \overline{A_{gx}} (\overline{p_g} + \overline{\tau_{xx}}) \right] \qquad (1-61) \\
&\quad + \overline{\Psi} \overline{v_{gx}} + \overline{\Psi' v_{gx}'} - \overline{F_x}
\end{aligned}$$

The dotted underlined term can be dropped by assuming negligible fluctuation in the mass transfer rate  $\Psi$ . This assumption is usually reasonable; in fact, the term  $\overline{\Psi} \overline{v_{gx}}$  is usually small compared with other terms in the equation.

The momentum and continuity equation for the gas phase looks deceptively simple. Actually, more new variables have been gained in the process of defining time- and area-averaged properties. The original differential equation has  $v_{gx}$  as one of the dependent variables; now two velocities,  $\overline{v_{gx}}$  and  $\overline{v_{gx}^2}$ , appear. The relation between these two quantities depends upon the velocity profiles. We can ignore the detailed structure of the flow field but we must have some knowledge or make some assumption connecting the density-averaged velocity and the mass-flux-averaged velocity. An analogous situation occurs in the one-dimensional treatment of laminar pipe flow of a single fluid. In this case a direct calculation using the exact result (a parabolic profile) shows that  $\overline{v_{gx}^2} = \frac{4}{3} \overline{v_{gx}}^2$ .

Besides the area averaging, we have introduced a time-averaging process. Time averaging introduces additional variables by splitting the quantities into a steady or average quantity and a fluctuation; an example is the momentum flux in incompressible turbulent flow:

$$\overline{v_{gx} v_{gx}} = \overline{v_{gx}} \overline{v_{gx}} + \overline{v'_{gx} v'_{gx}} \quad (1-62)$$

The last term is the Reynolds stress, and finding a relation for it is a central problem of turbulent flow theory. The velocities appearing in the two-phase equations have been both area- and time-averaged, so the problem is doubly difficult, or anyway doubly tedious.

Consider the velocity of the gas at a particular point in the flow. Plotted against time the function has breaks in it for those intervals when a particle occupies the particular point under consideration. Suppose that, by some suitable averaging process, it is possible to find a local average for the gas velocity at  $x, y, z, t$  (see Fig. 1-6). This average is zero at times when a particle occupies the position just as the gas velocity is zero. The local gas velocity fluctuation is defined by the difference between the instantaneous and the mean values:

$$v_{gx}(x, y, z, t) = \tilde{v}_{gx}(x, y, z, t) + v''_{gx}(x, y, z, t) \quad (1-63)$$

The average is denoted by the symbol  $\sim$  since it is a local average, whereas the previous time average, denoted by the symbol  $-$ , was applicable to quantities which were continuous functions of  $x$  and  $t$  only. If the local velocity is integrated over time and divided by the interval of time occupied by gas,  $\tau_g(x, y, z, t)$ , then the result should be the time-averaged gas velocity, provided, of course, that the time interval is appropriately chosen:

$$\tilde{v}_g(x, y, z, t) = \frac{1}{\tau_g(x, y, z, t)} \int_{\tau_g} v_g(x, y, z, t + \tau) d\tau \quad (1-64)$$

As before, the local time average is considered independent of subsequent averaging, the average fluctuation is zero, and the process is distributive. But now these statements are true only when  $f$  and  $g$  have the same domain of definition:

$$\tilde{\tilde{f}} = \tilde{f}$$

$$\tilde{\tilde{f} \cdot g} = \tilde{f} \cdot \tilde{g}$$

$$\tilde{\tilde{f} + g} = \tilde{f} + \tilde{g}$$

(1-65)

$$f = \tilde{f} + f''$$

$$\tilde{f''} = 0$$

The relationship between this time average, the bar time average, and the area average must be considered more carefully.

Now, attention will be focused on the gas properties at a particular cross-section of the flow. The domain in which gas properties are defined is represented by a volume in  $y, z, t$  space. When a particle passes the cross-section at some location  $y, z$  and some time  $t$ , the gas properties are undefined and this leaves a hole in the domain. In Figure 1-6 the black regions represent the passage of particles past the cross-section. Consider a cylinder which is  $\tau_0$  time units long and excludes the black regions.  $\tau_0$  is assumed long enough to form valid average properties of the flow. Call this region VOL. Choose a point  $(y, z)$ ; then  $\tau_g$  is the time from 0 to  $\tau_0$  which lies within VOL in which the gas properties are defined. Next consider a cross-section of VOL at some specific time; this region is merely the gas cross-section previously defined,  $A_{gx}(x, t)$ . Now the volume of the cylinder minus the "particle holes" can be computed in two ways:

$$VOL = \int_0^{\tau_0} A_{gx}(x, t+s) ds = \int_{A_x} \tau_g(x, s) dS \quad (1-66)$$

The first integral is  $\tau_0 \bar{A}_{gx}$  by the definition (1-50). The right-hand side is easily identified so that equation (1-66) reduces to

$$\tau_0 \bar{A}_{gx} = A_x \langle \tau_g \rangle \quad (1-67)$$



$\overline{A_{gx}}$  is a bar average in this equation since it is only a function of  $x$  and  $t$ .

Next, the integral of a function defined on the cylinder VOL is computed. This can be done by alternate ways also:

$$\begin{aligned} \int_{Vol} f dy dz dt &= \int_{A_x} \int_{\tau_g(x,s)} f(x,s,t+s) dS dS \\ &= \int_{\tau_0} \int_{A_{gx}(x,t)} f(x,s,t+s) dS dS \end{aligned} \quad (1-68)$$

Substituting from equation (1-64) gives

$$\int_{A_x} \tau_g(x,s) \tilde{f}(x,s) dS = \int_{\tau_0} A_{gx}(x,t) \langle f \rangle(x,t+s) dS \quad (1-69)$$

and using equation (1-50) results in

$$A_x \cdot \langle \tau_g \cdot \tilde{f} \rangle = \tau_0 \overline{(A_{gx} \langle f \rangle)} \quad (1-70)$$

$$\frac{A_x}{\tau_0} \langle \tau_g \cdot \tilde{f} \rangle = \overline{A_{gx} \langle f \rangle} \quad (1-71)$$

It would be desirable to remove  $\tau_g$  from the area-averaging process. Now  $\tau_g$  is, in general, a function of  $y, z$ ; however, if the number density of particles is uniform across the area  $A_x$ , then a uniform value of  $\tau_g$  independent of the area averaging can be expected. This assumption is not expected to hold where the number density changes appreciable, near a physical wall for instance. Taking  $\tau_g$  from under the area averaging and employing equation (1-67) gives the following result:

$$\overline{\langle f \rangle} = \langle \tilde{f} \rangle \quad (1-72)$$

The time average of an area-averaged quantity is equal to the area average of the local time average.

In order to treat flows where the number density varies over the cross-section one takes advantage of the arbitrary nature of  $A_x$ . The area  $A_x$  is chosen as a small region about a point in the flow. Then it is proposed that the number density is uniform and that equation (1-72) holds locally. Now  $\langle \tilde{f} \rangle$  is a definition of a local average property and dependent upon the point about which  $A_x$  is chosen and another averaging over the entire cross-section is required.

Equation (1-72) is only valid for an area-averaged property. In order to apply it to the equations given previously, the density-averaged properties are converted as given below:

$$\begin{aligned} \langle \rho_g \rangle \langle v_{gx} \rangle_\rho &= \langle \rho_g v_{gx} \rangle \\ \langle \rho_g \rangle \langle v_{gx}^2 \rangle_\rho &= \langle \rho_g v_{gx}^2 \rangle \end{aligned} \quad (1-73)$$

These relations conclude the preliminary work necessary to time average the conservation equations.

The continuity equation for the gas is given by equation (1-55). The terms in this equation are reduced as follows:

$$\begin{aligned}
 \overline{A_{g^x} \langle \rho_g \rangle} &= \overline{(A_{g^x} + A'_{g^x}) \langle \tilde{\rho}_g + \rho_g'' \rangle} \\
 &= \overline{A_{g^x} \langle \tilde{\rho}_g \rangle} \\
 &= \overline{A_{g^x} \langle \tilde{\rho}_g \rangle}
 \end{aligned} \tag{1-74}$$

$$\begin{aligned}
 \overline{A_{g^x} \langle \rho_g \rangle \langle v_{g^x} \rangle} &= \overline{A_{g^x} \langle \rho_g v_{g^x} \rangle} \\
 &= \overline{A_{g^x} \langle \tilde{\rho}_g \tilde{v}_{g^x} \rangle} \\
 &= \overline{A_{g^x} \langle \tilde{\rho}_g \tilde{v}_{g^x} + \rho_g'' v_{g^x}'' \rangle} \\
 &= \overline{A_{g^x} \langle \tilde{\rho}_g \tilde{v}_{g^x} \rangle} \\
 &= \overline{A_{g^x} \langle \rho_g \rangle \langle \tilde{v}_{g^x} \rangle}
 \end{aligned} \tag{1-75}$$

The definition of the density-averaged velocity is analogous to the previous definition. Substituting into equation (1-55) gives the final form for the gas phase continuity equation:

$$\frac{\partial}{\partial t} (\overline{A_{g^x} \langle \tilde{\rho}_g \rangle}) = - \frac{\partial}{\partial x} (\overline{A_{g^x} \langle \tilde{\rho}_g \rangle \langle \tilde{v}_{g^x} \rangle}) + \overline{\Psi} \tag{1-76}$$

The significant difference between this equation and equation (1-56) is that the properties  $\langle \tilde{\rho}_g \rangle$  and  $\langle \tilde{v}_{gx} \rangle$  are time-averaged locally before being integrated.

In a similar manner, the necessary terms for the momentum equation are computed. Consider the convective momentum term:

$$\begin{aligned}
 \overline{\rho_g \langle v_{gx}^2 \rangle} &= \overline{\rho_g v_{gx}^2} = \overline{\rho_g \widetilde{v_{gx}^2}} \\
 &= \overline{\rho_g \widetilde{v_{gx} v_{gx}}} \\
 &= \overline{\rho_g \widetilde{v_{gx}^2} + \rho_g \widetilde{v_{gx}'' v_{gx}''}} \quad (1-77) \\
 &= \overline{\rho_g} [\langle \widetilde{v_{gx}^2} \rangle + \langle \widetilde{v_{gx}'' v_{gx}''} \rangle] \\
 &= \overline{\rho_g} [\langle \tilde{\rho}_g \rangle \langle \tilde{v}_{gx}^2 \rangle + \langle \tilde{\rho}_g \rangle \langle \widetilde{v_{gx}'' v_{gx}''} \rangle]
 \end{aligned}$$

Substituting into the time-averaged form of equation (1-23) gives the gas phase momentum equation. Again, the assumption that is small is employed:

$$\begin{aligned}
 \frac{\partial}{\partial t} [\overline{\rho_g \langle \tilde{\rho}_g \rangle \langle \tilde{v}_{gx} \rangle}] \\
 &= -\frac{\partial}{\partial x} \left\{ \overline{\rho_g \langle \tilde{\rho}_g \rangle} [\langle \tilde{v}_{gx} \rangle + \langle \widetilde{v_{gx}'' v_{gx}''} \rangle] \right\} \quad (1-78) \\
 &\quad - \frac{\partial}{\partial x} \left\{ \overline{\rho_g} [\langle \tilde{\rho}_g \rangle + \langle \tilde{\tau}_{xx} \rangle] \right\} \\
 &\quad + \Psi \langle \tilde{v}_x \rangle - \overline{F_x}
 \end{aligned}$$

This equation contains the local Reynolds stress,  $\overline{v_{gx}'' v_{gx}''}$  averaged over the cross-section. This term was previously hidden in the term  $\overline{v_{gx}^2}$  in the form of the momentum equation given in equation (1-61). That is,  $\overline{v_{gx}^2}$  contains both the contribution of the momentum flux due to the local time-averaged velocity and that due to the fluctuations. This points out the importance of displaying the equations in terms of local time-averaged velocities (which are also measurable) and the fluctuations. The continuity and momentum equations above have been derived assuming that the particles are numerous, dispersed uniformly across the cross-section, and that they undergo incompressible fluctuations when considered as a continuum. The major assumption regarding the gas phase is that it also has negligible density fluctuations.

A few remarks concerning the various average velocities are in order. These averages must be performed because the flow is essentially three-dimensional and unsteady. The gas velocity at a point fluctuates because periodically a particle comes along and occupies that position. As a particle approaches, the gas velocity drops (or rises) to the velocity of the particle surface. This happens in order to satisfy the boundary condition on the velocity at the droplet surface. Thus, even though the gas flow field may be laminar, the velocity fluctuates. The same is true with respect to the area-averaging process. The flow may have a certain overall uniformity across each cross-section; however, a difference between the mass- and momentum-averaged velocities may exist because of the detailed gas velocity profile between

each particle. Finally, a true turbulent flow situation may exist because of the interaction of the gas and the particles. When the difference between the gas and particle velocities is large the flow will separate and vortices will be shed from the particle. Likewise, the particle velocities would be expected to fluctuate.

The continuity and momentum equation for the particles can be handled by the same method employed for the gas phase. The main difference between the definitions for the particles and the corresponding definition for the gas phase is that the integrals are summed over the distinct particles. For instance,

$$\langle v_{ex} \rangle = \frac{1}{A_{ex}} \sum_i \int_{S_{pi}} \underline{v}_e \cdot \underline{i} \, dS \quad (1-79)$$

There are only a finite number of particles so from a mathematical viewpoint one could simply denote the disjoint domain of integration as  $\sum_i S_{pi}$  and proceed with the usual mathematical operations,

$$\langle v_{ex} \rangle = \frac{1}{A_{ex}} \int_{\sum_i S_{pi}} \underline{v}_e \cdot \underline{i} \, dS \quad (1-80)$$

Reviewing the definitions of local time-averaged properties and area-averaged properties shows that all the formulas regarding the averages are still valid with the domain of definition changed.

Using the same assumptions as before ( $\psi'/\bar{\psi} \ll 1$ ,  $\rho_g''/\bar{\rho}_g \ll 1$ ,  $\rho_s''/\bar{\rho}_s \ll 1$ , and uniformly dispersed particles across  $A_x$ ), one can derive the equations for the particles:

$$\frac{\partial}{\partial t} (\rho_s \bar{A}_{ex}) = - \frac{\partial}{\partial x} (\rho_s \bar{A}_{ex} \langle \tilde{v}_{ex} \rangle) - \bar{\psi} \quad (1-81)$$

$$\begin{aligned} \frac{\partial}{\partial t} (\rho_s \bar{A}_{ex} \langle \tilde{v}_{ex} \rangle) &= - \frac{\partial}{\partial x} \left\{ \rho_s \bar{A}_{ex} \left[ \langle \tilde{v}_{ex}^2 \rangle + \langle \tilde{v}_{ex}'' \tilde{v}_{ex}'' \rangle \right] \right. \\ &\quad \left. - \frac{\partial}{\partial x} (\bar{A}_{ex} \langle \tilde{p}_x \rangle) - \bar{\psi} \langle \tilde{v}_{ex} \rangle \right. \\ &\quad \left. + \bar{F}_x \right. \end{aligned} \quad (1-82)$$

In the momentum equation a term appears because of the turbulence, fluctuations, or random motion of the particles. This is a Reynolds stress for the particle continuum. Frequently the random motion of the particles is viewed as a particle pressure in analogy with the kinetic theory of a gas (although the corresponding temperature analogy is never used). Equation (1-82) displays the random motion in its proper role in the continuum viewpoint of the particle motion.

The equations for the gas and particle continuum may be added to obtain overall mixture equations. These equations are very useful and are given in the appendix where all equations are summarized. In the overall equations, if one assumes the

temperature and the velocities of both phases to be the same, then the two phases are represented as a single fluid with pseudo-physical properties. This is called the homogeneous flow model in the literature.



## CHAPTER II

## DERIVATION OF ENERGY AND STATE EQUATIONS

A. Introduction

The energy equations may be developed for the separate phases as was done in the previous chapter for the continuity and momentum equations. This process is lengthy and will not be carried out here. Instead, an equation was derived describing the overall conservation of energy of both phases and another equation describing the thermal energy of the particles. These two equations are more valuable for solving practical problems than equations describing the energy of each phase.

Once the conservation equations are established, attention is turned to the appropriate form of the equations of state from the viewpoint of two "coexistent continua." This leads naturally to a discussion of the number density and phase cross-section equations. A short discussion of three-dimensional equations then closes the chapter.

B. Overall Energy Equation

For this derivation the control volume is taken as all the matter between  $x$  and  $x + \Delta x$ . This is essentially the sum of the gas and liquid control volumes previously considered. The integrated energy equation is written excluding gravitational and electrical effects and neglecting radiation:

$$\frac{d}{dt} \int_{V(t)} \rho (e + \frac{1}{2} v^2) dV = - \int_{S(t)} \rho (e + \frac{1}{2} v^2) (\underline{v} - \underline{v}_j) \cdot \underline{n} dS$$

$$- \int_{S(t)} \underline{q} \cdot \underline{n} dS - \int_{S(t)} \underline{n} \cdot \underline{p} \underline{v} dS - \int_{S(t)} \underline{n} \cdot [\underline{T} \cdot \underline{v}] dS \quad (2-1)$$

The symbol  $\underline{q}$  denotes the transport of energy because of temperature gradients and also the transport by diffusion if several species are present. The integrals are divided into portions referring to the liquid and portions referring to the gas phases. Instead of distinguishing area-averaged and density-averaged properties at this stage, the general area-averaging process defined by equation (1-5) is employed. Otherwise, the derivation follows the familiar pattern established by Chapter I: the volume integral on the left is broken into an integral over  $x$  and one over the area  $A_x$ ; the time derivative is independent of the  $x$  integral which is then estimated by the mean value theorem; then dividing by  $\Delta x$  and limiting  $\Delta x \rightarrow 0$  produces the final equation:

$$\frac{\partial}{\partial t} \left\{ A_{gx} [\langle \rho_g \epsilon \rangle + \frac{1}{2} \langle \rho_g v_g^2 \rangle] + A_{lx} [\langle \epsilon_l \rangle + \rho_l \frac{1}{2} \langle v_l^2 \rangle] \right\}$$

$$= - \frac{\partial}{\partial x} \left\{ A_{gx} [\langle \rho_g v_{gx} h_g \rangle + \frac{1}{2} \langle \rho_g v_{gx} v_g^2 \rangle] \right. \quad (2-2)$$

$$+ \langle q_{gx} \rangle + \langle \underline{\dot{e}} \cdot \underline{T} \cdot \underline{v}_g \rangle$$

$$\left. + A_{lx} [\rho_l \langle v_{lx} h_l \rangle + \frac{1}{2} \rho_l \langle v_{lx} v_l^2 \rangle] \right\}$$

The heat transfer and viscous terms for the liquid phase have been dropped.

This equation is to be time-averaged assuming incompressible fluctuations of the particles and the gas. Finally, the various average quantities are defined in accord with the previous development. The time-averaged terms for the gas phase are listed separately below:

$$\overline{\langle \rho_g \epsilon_g \rangle} = \langle \widetilde{\rho_g \epsilon_g} \rangle = \langle \widetilde{\rho_g} \widetilde{\epsilon_g} \rangle = \langle \widetilde{\rho_g} \rangle \langle \widetilde{\epsilon_g} \rangle$$

$$\overline{\langle \rho_g v_g^2 \rangle} = \langle \widetilde{\rho_g v_g v_g} \rangle = \langle \widetilde{\rho_g} \widetilde{v_g^2} + \widetilde{\rho_g} \widetilde{v_g'' v_g''} \rangle$$

$$= \langle \widetilde{\rho_g} \rangle \langle \widetilde{v_g^2} \rangle + \langle \widetilde{\rho_g} \rangle \langle \widetilde{v_g'' v_g''} \rangle$$

$$\overline{\langle \rho_g v_{gx} h_g \rangle} = \langle \widetilde{\rho_g v_{gx} h_g} \rangle = \langle \widetilde{\rho_g} \widetilde{v_{gx} h_g} + \widetilde{\rho_g} \widetilde{v_{gx}'' h_g''} \rangle$$

$$= \langle \widetilde{\rho_g} \rangle \langle \widetilde{v_{gx}} \rangle \langle \widetilde{h_g} \rangle + \langle \widetilde{\rho_g} \rangle \langle \widetilde{v_{gx}'' h_g''} \rangle$$

(2-3)

$$\overline{\langle \rho_g v_{gx} v_g^2 \rangle} = \langle \widetilde{\rho_g v_{gx} v_g^2} \rangle = \langle \widetilde{\rho_g} [\widetilde{v_{gx} + v_{gx}''}] [\widetilde{v_g + v_g''}]^2 \rangle$$

$$= \langle \widetilde{\rho_g} [\widetilde{v_{gx} v_g^2} + \widetilde{v_{gx} v_g'' v_g''} + 2 \widetilde{v_{gx} v_g'' v_g''} + \widetilde{v_{gx}'' v_g'' v_g''}] \rangle$$

$$= \langle \widetilde{\rho_g} \rangle [ \langle \widetilde{v_{gx} v_g^2} \rangle + \langle \widetilde{v_{gx} v_g'' v_g''} \rangle$$

$$+ 2 \langle \widetilde{v_{gx} v_g'' v_g''} \rangle + \langle \widetilde{v_{gx}'' v_g'' v_g''} \rangle ]$$

There is a similar set of terms for the particle phase. Substitution of these equations into equation (2-2) above yields the final energy equation. The final equation contains a great many terms resulting from fluctuations, and it is obvious that the solution of a practical problem will require several simplifications. Another thing to note is that the internal energy  $\langle e_g \rangle$ , is a density-averaged quantity while the enthalpy  $\langle h_g \rangle_n$  is averaged by weighting it with the mass flux.

When the fluctuation terms are neglected (or assumed independent of  $x$ ) and the steady state is assumed, the equation can be integrated to give the familiar form (neglecting  $q_r$  and  $(\frac{d\Gamma}{dx}) \cdot v_g$ ):

$$\bar{A}_{gx} \langle \tilde{p}_g \rangle \langle \tilde{v}_{gx} \rangle \left[ \langle \tilde{h}_g \rangle_n + \frac{1}{2} \frac{\langle \tilde{v}_{gx}^2 \tilde{v}_g^2 \rangle}{\langle \tilde{v}_{gx} \rangle} \right] + \bar{A}_{px} \langle \rho_p \rangle \langle v_{px} \rangle \left[ \langle \tilde{h}_p \rangle_n + \frac{1}{2} \frac{\langle \tilde{v}_{px}^2 \tilde{v}_p^2 \rangle}{\langle v_{px} \rangle} \right] = \text{Const} \quad (2-4)$$

This is an overall gas-plus-particle equation. A gas-phase equation may be obtained by eliminating all variables which refer to the particles. To do this, it is necessary to have the particle thermal energy equation which will be the subject of the next section.

### C. Thermal Energy Equation for the Particles

The thermal energy differential equation is well known and widely used. The integral form of this equation will be derived

since this was not done by Thorpe [18]; this will display the method of arriving at the integral forms. Thermal energy is integrated over a volume with arbitrary motion. The time rate of change of this integral must be found and the Leibnitz formula applied:

$$\frac{d}{dt} \int_{V(t)} \rho e dV = \int_{V(t)} \frac{\partial}{\partial t} \rho e dV + \int_{S(t)} \rho e \underline{v}_s \cdot \underline{n} dS \quad (2-5)$$

Now the differential equation for thermal energy is (ref. [21], p. 323, eq. Q):

$$\frac{\partial}{\partial t} (\rho e) = -\nabla \cdot (\rho e \underline{v}) - \nabla \cdot \underline{q} - p \nabla \cdot \underline{v} - \underline{\tau} : \nabla \underline{v} \quad (2-6)$$

This is substituted into the integral of the first term on the right-hand side of equation (2-5). The divergence theorem can be applied to the first two terms, i.e.,

$$\int_{V(t)} \nabla \cdot (\rho e \underline{v} + \underline{q}) dV = \int_{S(t)} \underline{n} \cdot (\rho e \underline{v} + \underline{q}) dS \quad (2-7)$$

Carrying this out and collecting terms yields the final equation:

$$\begin{aligned} \frac{d}{dt} \int_{V(t)} \rho e dV = & \int_{S(t)} \rho e (\underline{v} - \underline{v}_s) \cdot \underline{n} dS - \int_{S(t)} \underline{n} \cdot \underline{q} dS \\ & - \int_{V(t)} [(p \nabla \cdot \underline{v}) + \underline{\tau} : \nabla \underline{v}] dV \end{aligned} \quad (2-8)$$

The equation demonstrates that thermal energy is not conserved. The rate of change of internal energy within  $V$  is equal to the sum of the net flux convected across the boundary and the heat crossing the boundary plus the production of internal energy within the volume (compression and viscous dissipation). Ordinarily the production terms would be hard to determine but for an incompressible flow  $\nabla \cdot \underline{v} = 0$ , and the dissipation term is ignored. This drops the last term on the right-hand side.

When the "incompressible" thermal energy equation is written for the particles, we get

$$\frac{d}{dt} \int_x^{x+\Delta x} \int_{A_{\Delta x}} \rho_e e_e dV = - \sum_i \int_{S_{pi}} (\rho_e e_e (\underline{v}_e \cdot \underline{v}_s) \cdot \underline{n}_e + q_e \cdot \underline{n}_e) dS - \int_{A_{le}} \rho_e e_e \underline{v}_e \cdot \underline{n}_e dS \quad (2-9)$$

The integrals over the surfaces of the particles contain the properties on the liquid side of the interface discontinuity. It would be desirable (especially because of the heat flux ) to change to the gas side properties. To do this, consider that energy is conserved across the interface:

$$\begin{aligned} \rho_e e_e (\underline{v}_e - \underline{v}_s) \cdot \underline{n}_e + q_e \cdot \underline{n}_e + \rho_e \underline{v}_e \cdot \underline{n}_e \\ = - \rho_g e_g (\underline{v}_g - \underline{v}_s) \cdot \underline{n}_g - q_g \cdot \underline{n}_g - \rho_g \underline{v}_g \cdot \underline{n}_g \end{aligned} \quad (2-10)$$

This expression contains a pressure term which does not appear in the integral above. The equation is rearranged as follows:

$$\begin{aligned} \rho_e \left( e_e + \frac{p_e}{\rho_e} \right) (\underline{v}_e - \underline{v}_s) \cdot \underline{n}_e + q_e \cdot \underline{n}_e \\ = -\rho_g \left( e_g + \frac{p_g}{\rho_g} \right) (\underline{v}_g - \underline{v}_s) \cdot \underline{n}_g - \underline{q}_g \cdot \underline{n}_g - (p_g - p_e) \underline{v}_s \cdot \underline{n}_g \end{aligned} \quad (2-11)$$

The last term on the right-hand side is nonzero because of the surface tension forces; it is neglected primarily because it would introduce the droplet radius into the equations. For very small particles this term could be significant. Likewise, on the left-hand side, it is assumed that  $p_e / \rho_e \ll e_e$ . This is usually true because  $\rho_e$  is high even though the pressure inside the particle may be double that for a plane interface. Introducing these simplifications into the thermal energy equation gives

$$\begin{aligned} \int_x^{x+\Delta x} \frac{\partial}{\partial t} \int_{A_{ex}} \rho_e e_e dV \\ = \sum_i \int_{S_i} (\rho_g h_g (\underline{v}_g - \underline{v}_s) \cdot \underline{n}_g + \underline{q}_g \cdot \underline{n}_g) dS \\ - \int_{A_{ec}} \rho_e e_e \underline{v}_e \cdot \underline{n}_e dS \end{aligned} \quad (2-12)$$

The heat flux  $\underline{q}$  contains a conduction flux  $\underline{q}^{(c)}$  and a flux due to molecular diffusion  $\underline{q}^{(d)}$ . The molecular diffusion flux is (ref. [21] p. 566)

$$\underline{q}^{(d)} = \sum_k h_k \rho_k (\underline{v}_k - \underline{v}) \quad (2-13)$$

where  $h_k$  is the partial enthalpy of species  $k$  per unit mass,  $\rho_k$  is the density of species  $k$ , and  $\underline{v}_k$  is the velocity of species  $k$  with respect to the mass-averaged velocity  $\underline{v}$ . The diffusion flux and the gas enthalpy flux can be combined together and this is done for the special case of a binary mixture in the gas phase. Say species A will be "inert" and only species B will cross the interface of the particle:

$$\begin{aligned} & \left[ \underline{q}^{(d)} + \rho_g h_g (\underline{v}_g - \underline{v}_s) \right] \cdot \underline{n}_g \\ &= \left[ \rho_A h_A (\underline{v}_A - \underline{v}_g) + \rho_B h_B (\underline{v}_B - \underline{v}_g) + \rho_g h_g (\underline{v}_g - \underline{v}_s) \right] \cdot \underline{n}_g \\ &= \left[ \rho_A h_A (\underline{v}_A - \underline{v}_s) + \rho_B h_B (\underline{v}_B - \underline{v}_s) + \rho_A h_A (\underline{v}_s - \underline{v}_g) \right. \\ & \quad \left. + \rho_B h_B (\underline{v}_s - \underline{v}_g) + \rho_g h_g (\underline{v}_g - \underline{v}_s) \right] \cdot \underline{n}_g \end{aligned} \quad (2-14)$$



Since only species B crosses the interface,

$$\rho_B (\underline{v}_B - \underline{v}_s) \cdot \underline{n}_g = \rho_g (\underline{v}_g - \underline{v}_s) \cdot \underline{n}_g \quad (2-15)$$

and species A does not (actually species A could be a mixture in itself),

$$\rho_A (\underline{v}_A - \underline{v}_s) \cdot \underline{n}_g = 0 \quad (2-16)$$

also, the enthalpy is given by

$$\rho_g h_g = \rho_A h_A + \rho_B h_B \quad (2-17)$$

Utilizing these expressions gives the simple result:

$$\left[ \dot{q}^{(d)} + \rho_g h_g (\underline{v}_g - \underline{v}_s) \right] \cdot \underline{n}_g = \rho_g (\underline{v}_g - \underline{v}_s) \cdot \underline{n}_g h_B \quad (2-18)$$

The integral terms over the particles in the thermal energy equation now describe two effects: heat transferred by conduction on the gas side of the interface, and the transport of partial enthalpy of the condensing material:

$$\sum_i \int_{S_{pi}} \left[ q_{Tg}^{(c)} \cdot \underline{n}_g + h_{Bsg} \rho_g (\underline{v}_g - \underline{v}_s) \cdot \underline{n}_g \right] dS \quad (2-19)$$

The heat transferred from the gas to the particles per unit length of flow is called  $Q$  :

$$Q = \lim_{\Delta x \rightarrow 0} \frac{1}{\Delta x} \sum_i \int_{S_{pi}} q_{Tg}^{(c)} \cdot \underline{n}_g dS \quad (2-20)$$

Also, if one assumes that the temperature of the gas at the particle surface is uniform, then

$$\sum_i \int_{S_{pi}} \rho_g h_B (\underline{v}_g - \underline{v}_s) \cdot \underline{n}_g dS = - h_{Bsg} \Psi \Delta x \quad (2-21)$$

Since the gas enthalpy appears in the equation above, it is convenient to use the liquid enthalpy in the remaining terms. That is, the approximation  $h_g \approx c_g$  is used. The final area-averaged thermal energy equation is

$$\begin{aligned} \frac{\partial}{\partial t} (A_{ex} \rho_e \langle h_e \rangle) = & - \frac{\partial}{\partial x} (A_{ex} \rho_e \langle v_{ex} h_e \rangle) \\ & + Q - \Psi h_B \end{aligned} \quad (2-22)$$

This equation is time-averaged in the usual manner:

$$\begin{aligned} \frac{\partial}{\partial t} (\bar{A}_{lx} \tilde{\rho}_l \langle \tilde{h}_l \rangle) \\ = - \frac{\partial}{\partial x} \left[ \bar{A}_{lx} \rho_l (\langle \tilde{v}_{lx} \rangle \langle \tilde{h}_l \rangle_m + \langle \overline{v_{lx}'' h_l''} \rangle) \right] \quad (2-23) \\ + \bar{Q} - \bar{\Psi} h_{BS} \end{aligned}$$

Also, in interpreting  $h_l(x, y, z, t)$  it is interesting to note that a nonuniform temperature distribution within the particle would cause a fluctuation as the particle passes the point  $x, y, z$ .

Before leaving the particle thermal energy equation it is noted that one can differentiate by parts, assume  $\langle \tilde{h}_l \rangle = \langle \tilde{h}_l \rangle_m$ , and substitute the particle continuity equation to get a differential equation for the particle enthalpy:

$$\rho_l \bar{A}_{lx} \left[ \frac{\partial}{\partial t} + \langle \tilde{v}_{lx} \rangle \frac{\partial}{\partial x} \right] \langle \tilde{h}_l \rangle = \bar{Q} - \bar{\Psi} (h_{BS} - \langle \tilde{h}_l \rangle) \quad (2-24)$$

When the average particle temperature is the same as the surface temperature, the last expression is simply the latent heat of vaporization  $h_{fg}$ .

#### D. Thermodynamics

The conservation equations developed thus far are not a complete set for the solution of problems. The thermodynamic equations of state must be included to determine the problem. First the gas phase is considered. The conservation equations contain the gas density  $\rho_g$  and one notes that it is always associated with the gas cross-section flow area  $A_{gx}$ . Considering the two phases as two coexistent continua, the natural definition for gas-phase density would be the mass of gas per unit volume of gas-plus-liquid mixture. This is given the symbol  $\sigma_g$  and one notes that the following relation connects  $\sigma_g$  and  $\rho_g$ :

$$\langle \tilde{\sigma}_g \rangle A_x = \langle \tilde{\rho}_g \rangle \bar{A}_{gx} \quad (2-25)$$

Next one observes that the gas pressure  $\langle \tilde{p}_g \rangle$  also appears in combination with  $A_{gx}$  in the momentum equation. The perfect gas law is assumed,

$$p_g = \rho_g R T_g \quad (2-26)$$

and the fluctuations in the density are taken to be small. The gas constant is also assumed constant; if there are significant variations in the molecular weight, it would probably be best to work in terms of concentrations instead of densities:

$$\tilde{p}_g = \tilde{\rho}_g R \tilde{T}_g \quad (2-27)$$

Integrating across the cross-section gives

$$\langle \tilde{p}_g \rangle = \langle \tilde{\rho}_g \rangle R \langle \tilde{T}_g \rangle \quad (2-28)$$

A continuum gas phase pressure  $\langle \tilde{\pi}_g \rangle$  is defined in analogy with the density:

$$\langle \tilde{\pi}_g \rangle A_x = \bar{A}_{gx} \langle \tilde{p}_g \rangle \quad (2-29)$$

then the perfect gas law is

$$\langle \tilde{\pi}_g \rangle = \langle \tilde{\sigma}_g \rangle R \langle \tilde{T}_g \rangle \quad (2-30)$$

Hence, the gas cross-section area  $A_{gx}$  can be eliminated from the conservation statements in favor of the prescribed flow area

$A_x$ , by utilizing the new variables  $\tilde{\pi}_g$  and  $\tilde{\sigma}_g$ . The pressure  $\langle \tilde{\pi}_g \rangle$  and density  $\langle \tilde{\sigma}_g \rangle$  are the "coexistent continuum" properties of the gas phase and are related by the perfect gas law above.

The next question is to determine how the average gas temperature fits into the second equation of state. The gas-phase enthalpy is given by

$$\tilde{h}_g = c_p \tilde{T}_g + \tilde{h}_{REF} \quad (2-31)$$

Weighting the enthalpy with the density,

$$\begin{aligned} \langle \tilde{h}_g \rangle_\rho &= \langle c_p \tilde{T}_g \rangle_\rho + h_{REF} \\ &= c_p \langle \tilde{T}_g \rangle_\rho + h_{REF} \end{aligned} \quad (2-32)$$

Thus, if the gas-phase specific heat is constant, then the density-averaged enthalpy is related to the density-weighted temperature as defined in the perfect gas law. The mass-flux-averaged enthalpy  $\langle \tilde{h}_g \rangle_m$  also appears in the energy equation. The relationship between  $\langle \tilde{h}_g \rangle_\rho$  and  $\langle \tilde{h}_g \rangle_m$  depends upon the detailed temperature profiles.

So the thermodynamic properties of the gas-phase continuum are  $\pi_g$ ,  $\sigma_g$ , and  $T_g$ . The temperature  $T_g$  is the actual local gas temperature; however, the pressure and density include the gas-phase cross-section  $A_{gx}$  in their definitions. If the volume occupied by the particles is small, then  $\langle \tilde{\pi}_g \rangle \approx \langle \tilde{p}_g \rangle$  and  $\langle \tilde{\sigma}_g \rangle \approx \langle \tilde{\rho}_g \rangle$ .

The thermodynamic equations of state for an incompressible fluid are

$$\rho_e = \text{constant}$$

$$h_e = c_{pe} T_e + h_{\text{REF}} \quad (2-33)$$

The pressure is a mechanical variable. The conservation equations indicate that the "coexistent continuum" density, enthalpy, and pressure should be defined as follows:

$$\begin{aligned} \langle \tilde{\sigma}_p \rangle &= \frac{\overline{A_{ex}}}{A_x} \rho_e \\ \langle \tilde{\pi}_p \rangle &= \frac{\overline{A_{ex}}}{A_x} \langle \tilde{p}_e \rangle \\ \langle \tilde{h}_e \rangle &= c_{pe} \langle \tilde{T}_e \rangle + h_{\text{REF}} \end{aligned} \quad (2-34)$$

Although the particles are incompressible, the "coexistent continuum" particle density is a variable. There is no equation of state relating  $\sigma_p$  and  $\pi_p$  and it cannot be obtained since the fluid is incompressible. The pressure  $\pi_p$  depends upon  $A_{ex}$  and  $p_e$ , the internal particle pressure. As discussed previously, the pressure of the gas phase influences  $p_e$ , but the detailed flow around the particle must be known before it is possible to be more specific. The assumption regarding  $p_e$  must be made depending upon the problem at hand, but usually it would be reasonable to say that  $p_e \approx p_g$  and then neglect  $\pi_p$  when  $A_{ex} \ll A_x$ . Whatever the assumption is, it takes the place of an equation of state between  $\sigma_p$  and  $\pi_p$ .

An additional quantity  $h_{BS}$  appears in the particle thermal energy equation. This is the enthalpy of species B (the liquid) in the gas phase at the surface of the particle. Since the temperature is assumed continuous across the interface,  $h_{BS}$  is the enthalpy of gaseous species B at the temperature of the liquid next to the surface.

As a further indication of the reasonableness of the definitions given above, consider the equilibrium state. Suppose that the particles and the gas are in equilibrium and a sample is enclosed by imaginary planes. The temperature of the liquid and the gas is the same; otherwise heat transfer would alter the temperatures. Likewise, the partial pressure of the vapor of the liquid species corresponds to the equilibrium value at that temperature in order that the mass transfer go to zero. Finally, the velocities of the gas and particles are the same. Let the pressure of the gas be  $p_g = \langle \hat{p}_g \rangle$ . The particle pressure was defined to be the sum of the integrals of the cross-section of the particles cut by the planes and the contribution of the surface forces. Because the particles are not accelerating, the average pressure across the particle cross-section is the same as the gas pressure. The pressure for the mixture is then the sum of the constituent pressures in analogy with the Dalton rule for ideal mixtures:

$$\begin{aligned} \langle \hat{\pi}_m \rangle &= \langle \hat{\pi}_p \rangle + \langle \hat{\pi}_g \rangle = \frac{\bar{A}_{Lx}}{A_x} \langle p_L \rangle + \frac{\bar{A}_{gx}}{A_x} \langle p_g \rangle \\ &= \frac{\bar{A}_{Lx} + \bar{A}_{gx}}{A_x} p_g = p_g \end{aligned} \quad (2-35)$$



Similarly, the mixture density is the sum of the separate phase densities:

$$\sigma_m = \sigma_p + \sigma_g \quad (2-36)$$

The enthalpy of the mixture is computed (unit mass basis) as follows:

$$\sigma_m h_m = \sigma_g \langle \tilde{h}_g \rangle + \sigma_p \langle \tilde{h}_p \rangle \quad (2-37)$$

When a mixture specific heat is introduced, we get

$$\sigma_m c_{pm} T_m = \sigma_g c_{pg} \langle \tilde{T}_g \rangle + \sigma_p c_{pe} \langle \tilde{T}_p \rangle \quad (2-38)$$

But all the temperatures are the same, so

$$c_{pm} = \frac{\sigma_g}{\sigma_m} c_{pg} + \frac{\sigma_p}{\sigma_m} c_{pe} \quad (2-39)$$

This is the customary formula for the specific heat of an ideal mixture when  $\sigma_g / \sigma_m$  is recognized as the mass fraction of the constituent.

#### E. Particle Flow Cross-section and Number Density

The conservation equations for the gas and particle continuum contained thermodynamic properties discussed above. They also contain terms relating to the interphase transport of mass  $\Psi$ , momentum  $F_x$ , and energy ( $Q$  for instance). These terms could

be expected to be proportional to the number of particles times an interphase transport function per particle. Hence, in formulating  $\Psi$ ,  $F$ , and  $Q$ , one needs to know the number density. Let  $n(x, y, z, t)$  be the number of particles (of a specific size group) per unit mixture volume, and  $m_i$  the nominal mass of a particle. Then the particle phase density is given by

$$\langle \tilde{\sigma}_p \rangle A_x = \int_e \bar{A}_{ex} = m_i \langle \tilde{n} \rangle A_x \quad (2-40)$$

Substituting into the continuity equation for the particles, we have

$$\frac{\partial}{\partial t} (m_i \langle \tilde{n} \rangle A_x) = - \frac{\partial}{\partial x} (m_i \langle \tilde{n} \rangle A_x \langle \tilde{v}_{px} \rangle) - \bar{\Psi} \quad (2-41)$$

This can be differentiated by parts to obtain the following:

$$m_i \left[ \frac{\partial}{\partial t} \langle \tilde{n} \rangle A_x + \frac{\partial}{\partial x} \langle \tilde{n} \rangle A_x \langle \tilde{v}_{px} \rangle \right] + \langle \tilde{n} \rangle A_x \left[ \frac{\partial m_i}{\partial t} + \langle \tilde{v}_{ex} \rangle \frac{\partial m_i}{\partial x} \right] = \bar{\Psi} \quad (2-42)$$

Recall that  $\Psi$  represented the mass flux leaving or entering the particle holes per unit length of flow direction. Then  $\Psi / A_x$  is a volumetric source and is equal to the number density of

particles times the substantial derivative of the particle mass. Subtracting this from the equation above results in the number density equation:

$$\frac{\partial}{\partial t} \langle \tilde{n} \rangle A_x + \frac{\partial}{\partial x} \langle \tilde{n} \rangle A_x \langle \tilde{v}_{ix} \rangle = 0 \quad (2-43)$$

For a constant area and steady flow, equation (2-43) reduces to the simple but very useful equation

$$\langle \tilde{n} \rangle \langle \tilde{v}_{ix} \rangle = \text{constant} \quad (2-44)$$

The differential equation for the number density above was developed from a continuity equation which implied a conservation of particles. When a source or sink of droplets (and mass) exists, the right-hand side of equation (2-41) (and eq. (2-43)) should be modified to include the net production of particles per unit length of distance.

For the actual formation of a particle drag force or heat or mass transfer rate, it is necessary to know the particle radius. Equivalently, the particle mass could be used since the particles have constant density:

$$m_i = \frac{4}{3} \pi r^3 \rho_p \quad (2-45)$$

The equation for  $m_i$  was actually described above but not explicitly written:

$$\frac{\partial m_i}{\partial t} + \langle \tilde{v}_{ix} \rangle \frac{\partial m_i}{\partial x} = \frac{1}{A_x \langle \tilde{n} \rangle} \Psi \quad (2-46)$$

When the flow is steady, a much simpler method of computing the particle radius is available. In this case the mass flow rate is used as a variable instead of the density. By definition:

$$\langle \tilde{\sigma}_p \rangle = m_i \langle \tilde{n} \rangle \quad (2-47)$$

so

$$m_i = \frac{\langle \tilde{n} \rangle}{\langle \tilde{\sigma}_p \rangle} = \frac{\langle \tilde{n} \rangle \langle \tilde{v}_{ix} \rangle}{\langle \tilde{\sigma}_p \rangle \langle \tilde{v}_{ix} \rangle} = \frac{\text{Constant}}{\dot{m}_p} \quad (2-48)$$

Thus, the particle mass is inversely related to the particle mass flow rate.

#### F. Extension to Three-dimensional Flow

Thus far, the conservation equations and other relations have been developed for quasi one-dimensional flow. The scheme was to integrate over an elemental volume. This provided the motivation to define area-averaged properties of the particles and of the gas. Some of the properties were averaged by themselves, some were weighted by the density, and some were weighted by the mass flux. Limiting the length of the control volume resulted in differential equations for the average properties.

In addition to being essentially nonuniform in space, the two-phase flow is also nonuniform in time. By performing a time-averaging process, it was possible to refine the definitions of the properties of the gas and produce differential equations for the area average of the time-smoothed properties. In addition to the time-smoothed terms, the equations contained Reynolds stress terms, that is, the time average of two fluctuations multiplied together. In the one-dimensional derivation, the cross-section area  $A_x$  was allowed to vary and it was assumed that there was no interaction with the wall; that is, no mass, momentum, or energy left the control volume through the sides.

A relatively simple way to derive the three-dimensional equation for two-phase flow would be to extend the one-dimensional analysis. In order to do this, consider an elemental volume  $\Delta x \Delta y \Delta z$  and apply the same arguments with the variable area  $A_x$  replaced by  $\Delta y \Delta z$ . One significant difference is that now mass, momentum, and energy are convected across the side walls of the control volume. Thus the convective terms which were simple derivatives with respect to  $x$  will now appear behind a  $\nabla$  operator. In a similar manner, it is necessary to account for heat flow, pressure, and viscous forces on the side walls. The liquid portions of these terms could be dropped, as was done before, and the gas portion would result in the usual heat and viscous terms.

The interphase transport between the particles and the gas was previously formulated in terms of functions with the following format:

$$\lim_{\Delta x \rightarrow 0} \frac{1}{\Delta x} \sum_i \int_{S_{pi}} \dots dS \quad (2-49)$$

In three dimensions the definitions would be made on a per volume basis:

$$\lim_{\substack{\Delta x \rightarrow 0 \\ \Delta y \rightarrow 0 \\ \Delta z \rightarrow 0}} \frac{1}{\Delta x \Delta y \Delta z} \sum_i \int_{S_{pi}} \dots dS \quad (2-50)$$

A careful consideration would be expected to show that the time average could be interchanged with the area averaging if the particles were uniformly dispersed in  $\Delta x \Delta y \Delta z$ . The remaining Reynolds stresses for the gas and the particles should come out of this operation (only  $\langle \overline{v_x'' v_x''} \rangle$  appeared in the one-dimensional case).

Another possible way to derive the three-dimensional equations would be to integrate over a volume of arbitrary shape. Then one would make use of the definition of the operator given by Milne-Thomson [22]:

$$\nabla * f = \lim_{\Delta V \rightarrow 0} \int_S n * f dS \quad (2-51)$$

The function  $f$  and the multiplication  $*$  are arbitrary tensor calculus operations. Since  $f$  must be defined all over the surface  $S$ , it is obvious that the formula above can only be applied after one defines the average gas or particle velocities at an arbitrary point.

## CHAPTER III

## A TYPICAL RELAXATION PROCESS, THE TWO-PHASE SHOCK STRUCTURE

A. Description of the Problem

In this chapter the problem of the relaxation between two phases will be formulated in detail. In general, one phase consists of dispersed particles of liquid or solid and the other phase is gaseous. The flow is one-dimensional and steady. Initially, the gas and particles are at given states, but they are not in equilibrium and they move at different velocities. The mixture proceeds to its final equilibrium state by a relaxation process in which the gas and particles interact with each other. The initial state can be specified arbitrarily and the properties of the gas and particles computed, using the distance along the relaxation zone as the independent variable.

Physically, several situations might be imagined which would produce the initial state: the acceleration of a static mixture to the entrance of a pipe, the injection of droplets into a flowing gas stream, or the support of the particles by a screen as in a fluidized bed. In this chapter the initial conditions are assumed to be produced by a shock wave in the gas phase. This problem has been treated for the case of solid particles by Carrier [1], Rudinger [10], and Kriebel [11]. Extending the problem to liquid drops involves the consideration of mass transfer between the phases, in addition to the momentum and heat transfer.

Viewed from a coordinate system on the shock wave, the particles and gas approach with the same supersonic velocity (see Fig. 3-1). The particles, which are much more dense than the gas,



penetrate the gas shock because of their high momentum. Likewise, the heat-transfer and mass-transfer rates to the drop are slow and the particles emerge from the gas shock without being altered in mass, temperature, or velocity. The gas shock wave, on the other hand, is assumed to be unaffected by the presence of the particles. Thus, the initial disequilibrium conditions for the particles are the velocity and temperature in front of a gas shock wave, and, for the gas phase, the velocity and temperature behind a gas shock wave. The proper jump conditions are for a shock wave in a gas with the specific heat ratio of the initial gas phase.

The gas phase will be assumed to consist of two species: a diluent, A, which is insoluble in the liquid drops, and the droplet vapor denoted by B. The gas phase will be treated as a perfect gas mixture. Upstream of the shock, the gas and liquid phases are in equilibrium and thus the partial pressure of species B in the gas phase is the equilibrium pressure corresponding to the droplet temperature. Immediately after passing through the gas shock, the temperature of the drop is unchanged and therefore the vapor pressure of species B at droplet surface is unchanged. On the other hand, the vapor of species B in the gas phase has been compressed by the shock to a higher value. This partial pressure (or mole fraction) gradient between the main gas stream and the surface of the particle results in the diffusion of species B from the gas to the surface of the particle where it condenses. The diffusion of species B through the gas surrounding the particle is taken as the rate-controlling process, i.e., the rate of condensation (or vaporization) is much faster

than the diffusion rate. The droplet supplies or consumes species B so that the partial pressure of species B at the surface is in equilibrium with the liquid (as determined by the liquid temperature). This partial pressure is then a boundary condition at the particle surface for the diffusion of species B from the main gas stream. The condensation of species B immediately after the gas shock is only the initial behavior; frequently the mass transfer changes sign and vaporization occurs further on in the relaxation zone.

The two-phase flow can be described by several choices of dependent variables; the motion of the gas is given by the velocity  $v_g$  and that of the particles by  $v_{pj}$ . The thermodynamic state is described by  $T_g$  and  $T_{pj}$ ; however, instead of another thermodynamics variable, the mass flow rates  $\dot{m}_g$  and  $\dot{m}_{pj}$  will be chosen as dependent variables. Knowledge of the mass flow rates is equivalent to knowledge of the density since the velocities are known. From a knowledge of these six quantities any other properties of the flow can be computed by simple algebraic formula.

### B. Algebraic Formulation

The conservation equations for a two-phase gas-particle system consists of nine equations, namely, three mass, momentum, and energy balances: for the gas, for the particles, and for the overall mixture. Only six of these are independent since the conservation equation referring to the mixture may be obtained by adding the equations for the gas phase and the liquid

phase. For the problem at hand, it is most convenient to use the overall conservation equations and the equations for the liquid phase. The particle phase and gas phase equations were derived in the previous chapters. The overall equations are obtained by simple addition. The dependent variables in these equations are averages of the local time-averaged flow properties. It is assumed that the flow region under consideration is free of any wall effects and thus the time averaged property is independent of the area averaging, i.e.,  $\langle \tilde{f} \rangle = \langle \tilde{f} \rangle_r = \langle \tilde{f} \rangle_m$ .

A coordinate system is chosen with the origin on the shock wave. The upstream equilibrium state is denoted by 0, the state immediately behind the shock by 1, and the equilibrium state for downstream by  $\infty$ .

Let  $n_j$  be the number density of spherical particles of a size group  $j$  of radius  $r_j$  and density  $\rho_j$ . The density is assumed to be constant. The density of liquid per unit volume of two-phase mixture is the sum of the densities of each size group:

$$\sigma_p = \sum_j \sigma_{pj} \quad (3-1)$$

Each size group has a velocity  $v_{pj}$ . Thus the mass flow rate of particles per unit flow area is sum of the mass flow rates of each size:

$$\dot{m}_p = \sum_j \dot{m}_{pj} = \sum_j \sigma_{pj} v_{pj} \quad (3-2)$$

It is convenient to introduce a coefficient  $\alpha_j$  which denotes the fraction of the mass flux initially in each size divided by the initial total partial mass flux,  $\dot{m}_{p0}$ :

$$\alpha_j = \dot{m}_{pj0} / \dot{m}_{p0} \quad (3-3)$$

It will be assumed that there is no creation or destruction of particles in any size group. Hence we explicitly ruled out breakup and shattering. This means the solutions will be limited to shocks of low Mach number. For a steady-state process the conservation of the number of particles implies that

$$n_j v_{pj} = n_{j0} v_{pj0} = \text{constant} \quad (3-4)$$

With this restriction the radius of the particles depends only on the mass flow rate:

$$\frac{r_j}{r_{j0}} = \left( \frac{\dot{m}_{pj}}{\dot{m}_{pj0}} \right)^{1/3} = \left( \frac{\dot{m}_{pj}}{\alpha_j \dot{m}_{p0}} \right)^{1/3} \quad (3-5)$$

Each size group of particles is transferring mass from the particles to the gas at a rate  $\Psi_j/A_x$  per unit volume of mixture. The mass conservation principle for steady-state flow requires that the derivative of the mass flow rate is equal to the negative of the volumetric "sink"  $\Psi_j/A_x$ . This is the steady-state form of equation (1-81) of Chapter I:

$$\frac{d}{dx} (\dot{m}_{pj}) = - \frac{\Psi_j}{A_x} \quad (3-6)$$

Next consider the gas phase. The average velocity will be denoted by  $v_g$  and the density of gas per unit volume of two phase mixture by  $\sigma_g$ . The overall conservation of mass requires that the gas mass flow rate plus the total particle mass flow rates be a constant:

$$\dot{m}_g + \dot{m}_p = \dot{m}_0 = \text{constant} \quad (3-7)$$

The constant  $\dot{m}_0$  is evaluated from initial conditions.

The particles undergo changes in velocity because of the drag force exerted by the gas phase ( $F_j/A_x$  force on size  $j$  per unit volume). External body forces and momentum transfers by physical collisions between the particles will be neglected:

$$\dot{m}_{pj} \frac{dv_{pj}}{dx} = \frac{F_j}{A_x} \quad (3-8)$$

This corresponds to equation (1-82) of Chapter I (reduced by using equation (3-6)). The terms accounting for the gas phase and particle phase Reynolds stresses have been neglected. We will, in fact, ignore all terms with property fluctuations. This is a matter which deserves further study. No experimental information on fluctuations is available for the shock wave

case. The present knowledge of drag and heat transfer coefficients is actually so unreliable and meager that the analysis of fluctuations might be a futile refinement at this time.

The overall gas and particle momentum equation assumes that the overall momentum is a constant. Thus any viscous effects in the bulk of the gas phase are neglected:

$$\sum_j \dot{m}_{pj} v_{pj} + \dot{m}_g v_g + p = i = \text{constant} \quad (3-9)$$

In this equation,  $p$  is the gas phase pressure. The volume of the particles has been assumed negligible compared with that of the gas. Rudinger [23] has recently investigated the overall effect of this assumption.

The "thermal" energy equation for the particles shows that changes in the particle temperature are the result of heat transfer to the gas and heat required for the liquid-to-gas phase transition:

$$\dot{m}_{pj} \frac{dh_{pj}}{dx} = - \frac{\psi_j}{A_x} h_{fg} + \frac{Q_j}{A_x} \quad (3-10)$$

The temperature of the particle is assumed to be uniform. This assumption is usually good for metallic solids because of their high thermal diffusivity and also for liquids because of circulation within the drop. This has been verified experimentally for large drops [24].

Let  $h_g$  denote the specific enthalpy of the gas. The gas-plus-particle mixture will be assumed to be adiabatic; thus the energy equation reads:

$$\dot{m}_g \left( h_g + \frac{1}{2} v_g^2 \right) + \sum_j \dot{m}_{pj} \left( h_{pj} + \frac{1}{2} v_{pj}^2 \right) = j = \text{constant} \quad (3-11)$$

Conduction and diffusional transport of energy in the gas phase have been neglected. The enthalpies may be measured relative to a reference datum as long as the enthalpy of species B in the gas phase and the enthalpy of species B in the particles have the same reference.

The equations above contain the terms  $\dot{m}_{ij}$ ,  $F_{ij}$ , and  $Q_{ij}$ , representing the interchange of mass, momentum, and heat between the particles of size  $j$  and the gas. We divide these by the number density to get

$$\begin{aligned} (\omega_B m_B)_{ij} &= \Psi_j / (A_x n_j) \\ f_{ij} &= F_{ij} / (A_x n_j) \\ q_{ij} &= Q_j / (A_x n_j) \end{aligned} \quad (3-12)$$

where  $(\omega_B m_B)_{ij}$ ,  $f_{ij}$ , and  $q_{ij}$  refer to the mass, momentum, and heat transfer for a single representative particle  $i$  of size  $j$ .

The mass transfer from the particles to the gas will be assumed as a diffusion-controlled process. The gas in the immediate neighborhood of the particle surface is assumed to

be saturated with species B in an amount determined by the particle temperatures. This determines the mole fraction of species B at the surface of the particle  $\chi_{BS}$ . When there is a net flux of species B to or from the particle it is because the mole fraction of species B in the bulk of the gas phase has a value different from the equilibrium value. For a diffusion process of species B through a stagnant film of species A, the mass transfer coefficient is defined by the equation relating the total molar flow rate  $\mathcal{W}_B$  and the driving concentration gradient (see Bird, et al. [21], Chapter 21):

$$\mathcal{W}_{Bij} = k_{xj} A_{j\text{sur}} \frac{\chi_{BSj} - \chi_{Bq}}{1 - \chi_{BSj}} \quad (3-13)$$

In a similar manner, the drag and heat transfer coefficients are defined by the relations

$$f_{ij} = C_{Dj} A_{j\text{sur}} \frac{1}{2} \rho_g (v_g - v_{rj})^2 \quad (3-14)$$

$$q_{ij} = h_{qj} A_{j\text{sur}} (T_{rj} - T_g) \quad (3-15)$$

Experimental correlations for the transfer coefficients are expressed in terms of dimensionless numbers. These are the



Reynolds number, the Nusselt number for heat transfer, the Nusselt number for diffusion, the Schmidt number, and the Prandtl number:

$$\begin{aligned}
 Re_{y_j} &= \frac{\rho_g 2r_j |v_g - v_{rj}|}{\mu} \\
 Nu &= h_{gj} 2r_j / k \\
 Nu_D &= k_{xj} 2r_j / (c D_{AB}) \\
 Sc &= \mu / (\rho D_{AB}) \\
 Pr &= \mu c_p / k
 \end{aligned}
 \tag{3-16}$$

In these equations  $k$  is the thermal conductivity of the gas,  $c$  is the concentration of the gas (moles/cc),  $D_{AB}$  is the binary diffusion coefficient,  $\mu$  is the viscosity, and  $c_p$  is the heat capacity.

Combining all the preceding equations beginning with equation (3-12) (and noting that  $n_j$  may be eliminated by eq. (3-4) and the particle mass flow rate definition) will yield

$$\Psi_j / A_x = \frac{3}{2} \frac{\dot{m}_{rj}}{Q_{adj}} \frac{m_B}{m_A} \frac{Nu_{Dj} \mu}{Sc \rho_g r_j v_{rj}} \frac{\chi_{Bs_j} - \chi_{Bg}}{1 - \chi_{Bs_j}} \tag{3-17}$$

$$F_j / A_x = \frac{3}{8} \frac{\dot{m}_{rj}}{Q_{adj}} C_{Dj} \frac{\dot{m}_g}{r_o \rho_g} \frac{|v_g - v_{rj}| (v_g - v_{rj})}{v_g v_{rj}} \tag{3-18}$$

$$\frac{Q_j}{A_r} = \frac{3}{2} \frac{m_{pi}}{R_{adj}^2} \frac{Nu_j}{Pr} \frac{\mu C_p}{\rho_e r_o^2 v_{pj}} (T_{pj} - T_g) \quad (3-19)$$

In these equations  $R_{adj}$  is the nondimensional radius formed by dividing the actual radius by a reference  $r_o$ . The thermodynamic properties should be evaluated at a mean value for the gas film around the particle instead of the "free stream values." However, this choice has not been tested experimentally [21, p. 409] and this refinement will not be made here.

The transfer coefficients are the primary source of uncertainty in the formulation of the problem. For the shock relaxation problem one needs the drag of a particle in an accelerating flow influenced by the presence of other particles and undergoing heat and mass transfer. Torobin and Gauvin [25, 26, 27] have reviewed the drag coefficient experiments for accelerated motion. They were unable to explain the large decrease in drag coefficient found in some acceleration experiments. The steady-flow drag coefficient for low  $Re_y$  is the well-known formula of Stokes:

$$C_D = 24 / Re_y \quad (3-20)$$

At higher Reynolds numbers the experimental data is approximated by the relation

$$C_D = .48 + 28 Re_y^{-.85} \quad (3-21)$$

Ingebo [28] performed unsteady drag measurements on both solid and vaporizing particles and reported the following law which is considerably lower than the steady flow value:

$$C_D = 27 Re_y^{-.84} \quad (3-22)$$

Rudinger [29] measured the drag coefficient for solid particles by performing shock-tube experiments and he obtained still another value:

$$C_D = 6000 Re_y^{-1.7} \quad (3-23)$$

Rudinger considers this formula tentative and feels that extraneous factors may have been influential. In most of the calculations the steady flow equation will be used simply because more accurate information is lacking.

The heat transfer coefficient for spheres in steady flow is given by Ranz and Marshall [30]:

$$Nu = 2 + .6 Re_y^{1/2} Pr^{1/3} \quad (3-24)$$

When there is no flow the equation gives  $Nu = 2$  which corresponds to the theoretical value for the conduction of heat through the stagnant inert gas surrounding a sphere. The mass transfer coefficient is found by replacing  $Nu$  by  $Nu_D$  and  $Pr$  by  $Sc$ . This analogy depends upon the assumption of small heat and mass transfer rates such that the mass transfer does not affect the temperature profile:

$$Nu_D = 2 + 0.6 Re_D^{1/2} Sc^{1/3} \quad (3-25)$$

When  $Re_D = 0$  this equation gives the theoretical value for the diffusion of a species through a stagnant spherical film.

This concludes the dynamical analysis of the problem. In the next section the thermodynamic equations will be described. In these equations it will be assumed that the liquid drops have a constant density and uniform temperature. The gas phase is considered as a mixture of perfect gases. Also, it must be remembered that the volume occupied by the particles is small compared with the mixture volume so that the gas density based upon the mixture volume is nearly the same as that based upon the actual volume.

Under these assumptions the perfect gas law is written

$$p_g = \rho_g RT_g = \frac{m_g}{V_g} RT_g = \frac{m_g RT_g}{V_g} \quad (3-26)$$

$$p_g = p_a + p_b$$

$$p_a = x_a p \quad ; \quad p_b = x_b p$$

The partial pressures of species A and B are denoted by  $p_A$  and  $p_B$ . The molecular weight of the gas mixture is the sum of the mole fractions times the molecular weight of each species:

$$\begin{aligned} m_g &= x_A m_A + x_B m_B \\ &= [x_A (1 - \xi) + \xi] m_A \end{aligned} \quad (3-27)$$

where

$$\xi = m_B / m_A$$

The mass fraction of a species will be denoted  $\omega$  (mass of a species per mass of gas mixture). It is related to the mole fraction through the molecular weights; for instance,

$$\omega_A = x_A \frac{m_A}{m_g} \quad (3-28)$$

Combining the two preceding equations gives

$$\chi_A = \frac{\xi \omega_A}{1 + \omega_A (\xi - 1)} \quad (3-29)$$

The mass fraction can also be expressed in terms of the mass flow rates:

$$\omega_A = \frac{\rho_A}{\rho_g} = \frac{\rho_A v_g^*}{\rho_g v_g} = \frac{\dot{m}_A}{\dot{m}_g} \frac{\dot{m}_{g0}}{\dot{m}_g} \quad (3-30)$$

The subscript  $0$  designates the initial state. Because species A is the diluent it is conserved and  $\dot{m}_A$  is a constant. Hence

$$\omega_A = \omega_{A0} \frac{\dot{m}_{g0}}{\dot{m}_g} \quad (3-31)$$

The specific enthalpy of the gas mixture is the sum of the component enthalpies:

$$h_g = \omega_A h_A + \omega_B h_B \quad (3-32)$$

Constant specific heats will be assumed for the species and the particles:

$$\begin{aligned} h_A &= c_{pA} (T_g - T_0) \\ h_B &= c_{pB} (T_g - T_0) + h_{fg}^0 \\ h_{pi} &= c_{pi} (T_{pi} - T_0) \end{aligned} \quad (3-33)$$

The heat of vaporization at the reference temperature  $T_0$  is  $h_{fg}^0$ . The heat of vaporization at any temperature  $\hat{T}_B$  differs from  $h_{fg}^0$  because of difference between the specific heats of the liquid and the vapor:

$$\begin{aligned} h_{fg}(\hat{T}_B) &= h_B - h_L \\ &= (C_{PB} - C_{PL})(\hat{T}_B - T_0) + h_{fg}^0 \end{aligned} \quad (3-34)$$

The final equation for the statement of the problem is supplied by the Clausius-Clapeyron relation. The slope of the vapor pressure curve for equilibrium of pure species B liquid and vapor is related to the heat of vaporization:

$$\frac{d\hat{p}_B}{d\hat{T}_B} = \frac{\hat{p}_B}{R_B \hat{T}_B^2} h_{fg}(\hat{T}_B) \quad (3-35)$$

$\hat{p}_B$  is chosen to distinguish from  $p_B$  previously defined. The vapor is assumed to be a perfect gas; hence this equation is not valid near the critical point. Substitution of equation (3-34) gives

$$d \ln \hat{p}_B = \left[ h_{fg}^0 / R_B \hat{T}_B^2 + (C_{PB} - C_{PL}) \frac{\hat{T}_B - T_0}{R_B \hat{T}_B^2} \right] d \hat{T}_B \quad (3-36)$$

Integration yields the vapor pressure as a function of the liquid temperature. In the problem at hand the partial pressure of the

vaporizing species B at the particle surface is assumed to be the equilibrium value corresponding to the particle temperature, i.e.,

$\hat{p}_B = p_{Bs_j}$  and  $\hat{T}_B = T_{p_j}$ . The final equation is

$$\frac{p_{Bs_j}}{p_{B0}} = \left(\frac{T_{p_j}}{T_0}\right)^{\frac{C_{pB} - C_{pL}}{R_B}} \cdot \exp\left\{-\frac{(C_{pB} - C_{pL})}{R_B}\left(1 - \frac{T_0}{T_{p_j}}\right)\right\} \quad (3-37)$$

$$\cdot \exp\left\{\frac{h_{fg}^0}{R_B T_0}\left(1 - \frac{T_0}{T_{p_j}}\right)\right\}$$

The first two terms can be seen to represent a correction for the case when  $h_{fg}$  is constant. Empirically the relation

$$\frac{p_{Bs_j}}{p_{B0}} = \exp\left\{\eta\left(1 - \frac{T_0}{T_{p_j}}\right)\right\} \quad (3-38)$$

is sometimes used. In this instance  $\eta$  is determined from experiment but should be approximately

$$\eta = \frac{h_{fg}^0}{R_B T_0} \quad (3-39)$$

A graph of vapor pressure-temperature relationship is given as Figure 3-2.

The preceding equations give all the necessary relations to solve the problem. Before this is done it is convenient to nondimensionalize the variables as follows:



$$\dot{M}_{pj} = \dot{m}_{pj} / a_0 \rho_{g0} \quad ; \quad \dot{M}_g = \dot{m}_g / a_0 \rho_{g0}$$

$$V_g = v_g / a_0 \quad ; \quad V_{pj} = v_{pj} / a_0$$

$$P = p / a_0^2 \rho_{g0} \quad ; \quad H = h / a_0^2$$

$$\Theta_g = T / T_0 \quad ; \quad \Theta_{pj} = T_{pj} / T_0$$

$$C_p^* = c_p / r_0 R_0 \quad ; \quad \mu^* = \mu / r_0 a_0 \rho_{g0}$$

$$\delta = \sigma_r / \rho_{g0} \quad ; \quad \mathcal{R} = R / R_0 = m_{g0} / m_g$$

$$R_{adj} = r_j / r_{0j} \quad ; \quad R_{efj} = r_{0j} / r_0 \quad (3-40)$$

$$\Psi_j = \frac{\psi}{A_x} \frac{\rho_2 r_0}{a_0 \rho_{g0}^2} \quad ; \quad \hat{F}_j = \frac{F_j}{A_x} \frac{\rho_2 r_0}{(a_0 \rho_{g0})^2}$$

$$Q_j = \frac{Q_j}{A_x} \frac{\rho_2 r_0}{a_0^3 \rho_{g0}^2} \quad ; \quad \Sigma = \frac{\lambda}{r_0} \frac{\rho_{g0}}{\rho_2}$$

In terms of these variables the equations to be solved reduce to

$$\dot{M}_g + \sum_j \dot{M}_{pj} = V_{r0} (\delta + 1) \quad (3-41)$$

$$\dot{M}_g V_g + \sum_j \dot{M}_{pj} V_{pj} + P = I \quad (3-42)$$

$$\dot{M}_g \left( H_g + \frac{1}{2} V_g^2 \right) + \sum_j \dot{M}_{pj} \left( H_{pj} + \frac{1}{2} V_{pj}^2 \right) = J \quad (3-43)$$

$$\frac{d \dot{M}_{pj}}{d X} = \Psi_j \quad (3-44)$$

$$\dot{M}_{pj} \frac{d V_{pj}}{d X} = F_j \quad (3-45)$$

$$\dot{M}_{pj} \frac{dH_{pj}}{dX} = - \Psi_j H_{Tj} + q_j \quad (3-46)$$

$$Rad_j = (\dot{M}_{pj} / \alpha_j M_{po})^{1/3} \quad (3-47)$$

$$\Psi_j = \frac{3}{2} \frac{\dot{M}_{pj}}{Rad_j^2} \frac{m_B}{m_f} \frac{Nu_D}{Sc} \frac{\mu^*}{V_{pj}} \frac{x_{Bsj} - x_{Bg}}{1 - x_{Bsj}} \quad (3-48)$$

$$F_j = \frac{3}{8} \frac{\dot{M}_{pj}}{Rad_j} \dot{M}_g C_{oj} \frac{|V_g - V_{pj}| (V_g - V_{pj})}{V V_{pj}} \quad (3-49)$$

$$q_j = \frac{3}{2} \frac{\dot{M}_{pj}}{Rad_j^2} \frac{Nu}{Pr} \mu^* C_{pj}^* (\Theta_{pj} - \Theta_g) \quad (3-50)$$

$$P = \frac{\dot{M}_g R \Theta_g}{\gamma_0 V_g} \quad (3-51)$$

$$H = \omega_A H_A + \omega_B H_B$$

$$H_{ij} = C_{PL}^* (\Theta_{ij} - 1)$$

$$H_A = C_{PA}^* (\Theta_g - 1)$$

$$H_B = C_{PB}^* (\Theta_g - 1) + H_{fg}^0$$

(3-52)

$$H_{fg} = H_{fg}^0 + (C_{PB}^* - C_{PL}^*) (\Theta_g - 1)$$

(3-53)

$$\frac{P_{gsj}}{P_{g0}} = \Theta_{ij}^{\gamma_0 \frac{m_B}{m_{g0}}} C_{Pfg}^* \exp \left\{ -\gamma_0 \frac{m_B}{m_{g0}} C_{Pfg}^* \left( 1 - \frac{1}{\Theta_{ij}} \right) \right\}$$

$$\cdot \exp \left\{ H_{fg}^0 \gamma_0 \frac{m_B}{m_{g0}} \left( 1 - \frac{1}{\Theta_{ij}} \right) \right\}$$

(3-54)

The specification of the thermodynamic properties of the mixture will require that one assign values for the following:

$$P_r, S_c, C_{PA}^*, C_{PB}^*, C_{PL}^*, H_{fg}^{\circ}, \xi, \chi_{B_0}, \delta \quad (3-55)$$

The drop sizes and the amount of liquid in each size is specified by the constants

$r_0 =$  reference radius

$$R_{efj} = r_{j_0} / r_0$$

$$\alpha_j = \sigma_{pj} / \sigma_{p_0} \quad (3-56)$$

$$\mu^* = \frac{\mu}{r_0 a_0 \rho_{g_0}}$$

The reference radius  $r_0$  does not actually enter into the non-dimensional problem except through the parameter  $\mu^*$  which, for fixed initial gas phase state, must be considered as the primary drop size parameter.

The initial conditions for the dependent variables can be given arbitrarily, as previously noted. Here the initial conditions are assumed to be produced by a shock wave in the gas phase (subscript  $l$ ). For this situation the Mach number of the shock (and  $r_0$ ) and the shock tables provide the initial data. The initial gas temperature is simply the temperature ratio across the shock, while the particle temperature is unity according to the assumption that the particles are initially unaffected by the shock:

$$\Theta_{g1} = T_1 / T_0 ; \Theta_{p1} = 1 \quad (3-57)$$

The initial particle velocity is unchanged across the shock and hence it is the shock Mach number. The initial gas velocity is the velocity ratio of the shock times the Mach number:

$$V_{p1} = V_{p0} = M_0 \quad (3-58)$$

$$V_{g1} = v_{g1} / a_0 = (v_{g1} / v_{g0}) M_0$$

Finally, the nondimensional mass flow rates at the initial state are also related to the shock Mach number and the loading factor:

$$\dot{M}_{g1} = \dot{M}_{g0} = \frac{\dot{m}_{g0}}{a_0 \rho_{g0}} = \frac{v_{g0} \rho_{g0}}{a_0 \rho_{g0}} = M_0 \quad (3-59)$$

$$\dot{M}_{p1} = \dot{M}_{p0} = \frac{\dot{m}_{p0}}{a_0 \rho_{g0}} = \frac{v_{p0} \rho_{p0}}{a_0 \rho_{g0}} = M_0 \delta$$

The mass flow rate for a particular particle size is formed, employing the definition of  $\alpha_j$  and noting that all particles have the same velocity at the initial point.

The problem is now to solve equations (3-41) through (3-54) (plus a few additional thermodynamic relations for the gas mixture), when the properties of the mixture are specified by

equations (3-55) and (3-56) and the initial values of the dependent variables are specified according to equations (3-57), (3-58), and (3-59). The numerical solution was accomplished on a computer as the next section will describe.

### C. Description of Computer Solution

The solution begins at Station 1 just downstream of the gas shock where the independent variable  $X$  is set equal to zero. The main dependent variables are the mass flow rates, the velocities, and the temperatures ( $\dot{M}_g, \dot{M}_{Pj}, V_g, V_{Pj}, \theta_g,$  and  $\theta_{Pj}$ ). The equations which are to be integrated refer to the particle properties and are given by equations (3-44), (3-45), and (3-46). When the initial data are substituted into these equations, the right-hand side of each equation is known and may be integrated one step,  $DX$ . This will furnish new values of the particle properties  $V_{Pj}, \dot{M}_{Pj},$  and  $\theta_{Pj}$  at  $X + DX$ . This integration is performed for all the particle size groups.

With the state of the particles at  $X = 0 + DX$  known, it remains to solve for the gas properties. Equation (3-41) yields the gas-phase mass flow rate  $\dot{M}_g$ , since all the  $\dot{M}_{Pj}$  are known. With  $\dot{M}_g$  known, the mass fraction  $\omega_A$  (and hence  $\omega_B$ ) is found from equation (3-31). This leaves the gas velocity and temperature as the only major unknown variables. These variables will be found by iterating on two equations, using the Newton-Raphson method to estimate the increments to change the variables at each step in the iteration. From the energy equation [equation (3-43)], a function  $F_1(\dot{V}_g, \theta_g)$  is formed:

$$F_1(\hat{V}_g, \hat{\Theta}_g) = H_g(\hat{\Theta}_g) + \frac{1}{2} \hat{V}_g^2 + \frac{1}{\hat{M}_g} \sum_j \dot{M}_{rj} (H_{rj} + \frac{1}{2} V_{rj}^2) - \frac{J}{\hat{M}_g} \quad (3-60)$$

$H_g$  is an explicit function of  $\hat{\Theta}_g$  through equation (3-52). When the proper values of the gas properties are found,  $V_g = \hat{V}_g$  and  $\Theta_g = \hat{\Theta}_g$ , the energy equation is satisfied, and  $F_1(V_g, \Theta_g) = 0$ . Next, the pressure is eliminated from the momentum equation [equation (3-42)] by equation (3-51) and another function is formed:

$$F_2(\hat{V}_g, \hat{\Theta}_g) = \frac{Q}{r_0} \hat{\Theta}_g + \frac{1}{2} \hat{V}_g^2 + \frac{V_g}{\hat{M}_g} \left\{ \sum_j \dot{M}_{rj} V_{rj} - I \right\} \quad (3-61)$$

This equation is also zero when the proper values of  $\hat{V}_g$  and  $\hat{\Theta}_g$  are found.

A choice is made for the values  $\hat{V}_g$  and  $\hat{\Theta}_g$ . Then Taylor's series are written about that point to the point  $(V_g, \Theta_g)$ :

$$0 = F_1(\Theta_g, V_g) = F_1(\hat{V}_g, \hat{\Theta}_g) + \frac{\partial F_1}{\partial \hat{V}_g} \bigg|_{\hat{V}_g, \hat{\Theta}_g} (V_g - \hat{V}_g) + \frac{\partial F_1}{\partial \hat{\Theta}_g} \bigg|_{\hat{V}_g, \hat{\Theta}_g} (\Theta_g - \hat{\Theta}_g) + \dots \quad (3-62)$$



$$0 = F_2(V_g, \Theta_g) = F_2(\hat{V}_g, \hat{\Theta}_g) + \frac{\partial F_2}{\partial \hat{V}_g} \bigg|_{\hat{V}_g, \hat{\Theta}_g} (V_g - \hat{V}_g) + \frac{\partial F_2}{\partial \hat{\Theta}_g} \bigg|_{\hat{V}_g, \hat{\Theta}_g} (\Theta_g - \hat{\Theta}_g) + \dots \quad (3-63)$$

If only first-order terms are retained, then the above is a linear system for unknowns  $(V_g - \hat{V}_g)$  and  $(\Theta_g - \hat{\Theta}_g)$  once  $\hat{V}_g, \hat{\Theta}_g$  are specified. Solving for these increments gives corrections for new estimates of  $\hat{V}_g$  and  $\hat{\Theta}_g$ :

$$\hat{V}_{g \text{ new}} = \hat{V}_{g \text{ old}} + (V_g - \hat{V}_g)$$

$$\hat{\Theta}_{g \text{ new}} = \hat{\Theta}_{g \text{ old}} + (\Theta_g - \hat{\Theta}_g) \quad (3-64)$$

The process is continued until the correction is as small as desired.

When the gas properties are found, the solution is complete at  $\mathbf{X} = \mathbf{O} + D\mathbf{X}$  and another step in the integration may be taken. This describes the essential aspects of the computational scheme. A flow diagram is shown in Appendix D, a dictionary of FORTRAN symbols is given in Appendix E, and the program listing comprises Appendix F.

#### D. Asymptotic Theory of Two-Phase Shock Structure

The preceding discussion of the two-phase shock was presented as a typical relaxation process for two-phase dispersed flow. The

gas-phase shock was viewed as a mechanism to provide the initial disequilibrium state, and the particles were assumed to penetrate the shock without change. Likewise, the shock was assumed to be unaffected by the particles passing through it.

At low density a gas-phase shock has a thickness of range of a centimeter. Physically, one would not expect the assumption above to be valid for small particles whose density was of comparable order of magnitude to the gas density. Therefore, it is of interest to look at the problem in a more general light and to see how the assumed problem, gas shock plus relaxation zone, fits into the general equations for two-phase, one-dimensional flow.

The problem is stated in a way similar to the formulation of the theory of gas-phase shock waves. What are the solutions to the one-dimensional, dispersed, two-phase flow equations which allow the passage from a uniform upstream state to a different uniform downstream state?

The upstream state is taken as given and it is possible to find the downstream state by solving the conservation equations for a jump in a two-phase flow. This provides the upstream and downstream boundary conditions for the structure problem. The differential equations for the structure of the jump will appear too complicated to solve directly and so an asymptotic solution will be proposed. As indicated in the previous physical arguments, the problem can be separated into two problems if the parameter  $\epsilon = \rho_s / \rho_g \rightarrow \infty$ ; hence this is the proper perturbation parameter.

Formally, the equations and boundary conditions (up- and downstream states) to be solved are considered, and the equations are nondimensionalized so that the variables are of order unity as the parameter  $\epsilon \rightarrow \infty$ . The equations and boundary conditions which result from this limit constitute the zero-order problem in an asymptotic expansion in  $\epsilon$ . It will be found that the zero-order solution will not satisfy both the upstream and downstream boundary conditions; hence, one must be ignored. The downstream boundary condition is the proper one to ignore. Since the zero-order solution does not satisfy both boundary conditions, it is not a uniformly valid solution, i.e., it is "singular" as  $x \rightarrow \infty$ . The solution is usually called the "outer" solution and is actually the solution to the structure of a gas-phase shock wave.

The next task is to find a solution which is valid as  $x \rightarrow \infty$ . To do this, one rescales the  $x$  variable (call it  $X$ ) so that the terms which were neglected and caused the singularity in the outer problem, will be of order unity as the parameter  $\epsilon \rightarrow \infty$ . Carrying out this process results in the differential equations for the relaxation zone, as given in the first part of this chapter. This constitutes the "inner" problem. The inner equations require only one set of boundary conditions, whereas the solution must actually satisfy two sets. At one boundary the equilibrium downstream conditions must be satisfied ( $X \rightarrow \infty$ ). At the other boundary ( $X \rightarrow 0$ ) the inner solution must match the outer solution as the outer variable  $x \rightarrow \infty$ , that is, the outer solution must satisfy the boundary conditions downstream of a gas shock. It turns out that if the conditions behind the gas shock

are prescribed, then the equilibrium conditions at will also be satisfied.

The previous discussion indicates that the solutions for a gas shock plus a relaxation zone are actually the first terms in two matched asymptotic expansions in the density parameter  $\epsilon$  as  $\epsilon \rightarrow \infty$ . This will be demonstrated in the next few pages by using the actual equations.

The one-dimensional equations for the gas phase are written in dimensional form:

Continuity:

$$\frac{d}{dx} \rho_g v_g = \frac{\Psi}{A_x} \quad (3-65)$$

Momentum:

$$\rho_g v_g \frac{dv_g}{dx} + \frac{dp}{dx} = \frac{d}{dx} [(2\mu + \lambda) \frac{dv_g}{dx}] - \frac{F_x}{A_x} - \frac{\Psi}{A_x} (v_g - v_p) \quad (3-66)$$

Energy:

$$\begin{aligned} \frac{d}{dx} \left[ \rho_g v_g \left( h_g + \frac{1}{2} v_g^2 \right) \right] = & \frac{d}{dx} \left[ \kappa \frac{dT}{dx} + v_g (\lambda + 2\mu) \frac{dv_g}{dx} + \sum_k \rho_k h_k (v_k - v_g) \right] \\ & - \frac{F_x}{A_x} v_p - \frac{Q}{A_x} + \frac{\Psi}{A_x} \left( h_{BS} + \frac{1}{2} v_p^2 \right) \quad (3-67) \end{aligned}$$

The equation for the particles are:

Continuity:

$$\frac{d}{dx} \sigma_p v_p = - \frac{\Psi}{A_x} \quad (3-68)$$

Momentum:

$$\sigma_p v_p \frac{dv_p}{dx} = \frac{F_x}{A_x} \quad (3-69)$$

Thermal Energy:

$$\sigma_p v_p \frac{dh_p}{dx} = - \frac{\Psi}{A_x} h_{fg} + \frac{Q}{A_x} \quad (3-70)$$

In the equations above, the volumetric source terms are given in dimensional form by equations (3-18), (3-19), and (3-20), and will not be repeated here. The thermodynamic equations for the gas and the particles complete the set of equations. The boundary conditions are two uniform equilibrium states which satisfy the two-phase jump equations.

The initial state is characterized by the velocity, gas thermodynamic properties, particle loading, particle radius, and

liquid density. One can imagine a sequence of problems where all the initial data are held constant except the liquid density, which is increased; i.e.,  $\rho_l / \rho_{g0} \rightarrow \infty$ . Thus, if  $T_0$ ,  $a_0$ ,  $\rho_{g0}$  and  $r_0$  are used as reference quantities, one would expect the nondimensional variables to be of order unity as  $\epsilon \rightarrow 0$ . These nondimensional variables were used previously in the first part of this chapter and are given by equations (3-40). A few new variables will also be used:

$$\begin{aligned}
 \hat{\rho}_g &= \frac{\rho_g}{\rho_{g0}} & \hat{\mu} &= \frac{2\mu + \lambda}{r_0 a_0 \rho_{g0}} \\
 \hat{k} &= \frac{k T_0}{r_0 a_0^3} & \hat{q}_r &= \frac{q_r}{\rho_{g0}} \\
 \hat{A} &= \frac{x}{r_0} & \hat{\epsilon} &= \frac{\rho_l}{\rho_{g0}}
 \end{aligned} \tag{3-71}$$

Introducing the nondimensional variables gives the following set of equations:

Gas Continuity:

$$\frac{d}{dt} \hat{\rho}_g V_g = \left( \frac{\Psi}{A_x} \frac{r_0}{\rho_{g0} a_0} \right) = \frac{1}{\hat{\epsilon}} \Psi \tag{3-72}$$

Gas Momentum

$$\begin{aligned} \hat{\rho}_g V_g \frac{dV_g}{ds} + \frac{dP}{ds} &= \frac{d}{ds} \left( \hat{\mu} \frac{dV_g}{ds} \right) - \left( \frac{F}{A_r \hat{\rho}_g a_r} \right) - \left( \frac{\Psi}{A_r \hat{\rho}_g a_r} \right) (V_g - V_r) \\ &= \frac{d}{ds} \left( \hat{\mu} \frac{dV_g}{ds} \right) - \frac{1}{\epsilon} \mathcal{F} - \frac{1}{\epsilon} \Psi (V_g - V_r) \end{aligned} \quad (3-73)$$

Gas Energy:

$$\begin{aligned} \frac{d}{ds} \left[ \hat{\rho}_g V_g \left( H_g + \frac{1}{2} V_g^2 \right) \right] &= \frac{d}{ds} \left[ \hat{k} \frac{d\theta_g}{ds} + \hat{\mu} V_g \frac{dV_g}{ds} + \sum_k H_k \hat{\rho}_k (V_k - V_g) \right] \\ &\quad - \frac{1}{\epsilon} \left[ V_r \mathcal{F} + \mathcal{Q} - \Psi \left( H_{B_s} + \frac{1}{2} V_r^2 \right) \right] \end{aligned} \quad (3-74)$$

Particle Continuity:

$$\frac{d}{ds} \hat{\sigma}_r V_r = -\frac{1}{\epsilon} \Psi$$

Particle Momentum:

$$\hat{\sigma}_r V_r \frac{dV_r}{ds} = \frac{1}{\epsilon} \mathcal{F} \quad (3-75)$$

Particle Thermal Energy:

$$\hat{\sigma}_r V_r \frac{dH_r}{ds} = -\frac{1}{\epsilon} \Psi H_{T_g} + \frac{1}{\epsilon} \mathcal{Q}$$

Before taking the limit  $\epsilon \rightarrow \infty$  in the equations above, the detailed expressions for  $\Psi$ ,  $\mathcal{F}$ , and  $q$  given by equations (3-49), (3-50), and (3-51) should be checked to verify that these quantities are actually independent of  $\epsilon$ . Performing the limit on the gas phase equations gives a set of equations in which no interphase transport terms appear. This set is identical with the Navier-Stokes formulation of the problem of a gas-phase shock wave. The limiting equations for the particles have trivial solutions:

$$\begin{aligned} \frac{d}{ds} (\dot{M}_p) &= 0 & ; & \quad \dot{M}_p = \text{constant} \\ \frac{d}{ds} (V_p) &= 0 & ; & \quad V_p = \text{constant} \\ \frac{d}{ds} (H_p) &= 0 & ; & \quad H_p = \text{constant} \end{aligned} \quad (3-76)$$

Thus, the zero-order equations give constant values for the particle flow and produce the pure gas-shock structure problem for the gas phase. There are two sets of boundary conditions to satisfy: the equilibrium conditions across a two-phase jump; however, the particle properties are constant and can obviously satisfy the boundary conditions only at one end. Likewise, the gas shock will not satisfy the end conditions for a two-phase shock but can be made to coincide with the conditions at one end. It is appropriate to let these problems satisfy the upstream boundary conditions and allow the solutions to be "singular" at  $x = \infty$ . To correct this situation an "inner" or "boundary layer" solution is required.



The inner solution should satisfy the proper downstream boundary condition at one end and match the outer solution at the other. To find the proper differential equations the distance variable  $\Delta$  is magnified by introducing a new independent variable:

$$\Sigma = \frac{\Delta}{\epsilon} \quad (3-77)$$

There is no need to rescale the dependent variables.

The new distance variable  $\Sigma$  is introduced into the full set of two-phase equations (3-72), (3-73), (3-74), and (3-75). Then the limit  $\epsilon \rightarrow \infty$  taken and the equations previously given for the relaxation zone result:

Gas:

$$\frac{d}{d\Sigma} \dot{M}_g = \Psi$$

$$\dot{M}_g \frac{dV_g}{d\Sigma} + \frac{dP}{d\Sigma} = -\mathcal{F} - \Psi (V_g - V_r)$$

$$\begin{aligned} \frac{d}{d\Sigma} \left[ \dot{M}_g \left( H_g + \frac{1}{2} V_g^2 \right) \right] &= -\mathcal{F} V_r - q \\ &+ \Psi \left( H_{gs} + \frac{1}{2} V_r^2 \right) \end{aligned} \quad (3-78)$$

Particles:

$$\frac{d\dot{M}_p}{dX} = -\Psi$$

$$\dot{M}_p \frac{dV_p}{dX} = \bar{f}_r \quad (3-79)$$

$$M_p \frac{dH_p}{dX} = -\Psi H_{fg} + q$$

By performing a little algebra and adding the gas and particle equations, it is possible to reproduce the overall equations (3-41), (3-42), and (3-43). The particle equations (3-45), (3-46), and (3-47) are identical with the equations above. The equations above will admit only one set of boundary conditions; however, if the boundary conditions are chosen to match the outer solution, the solution will also satisfy the downstream equilibrium conditions. In fact, specification of any set of initial conditions will determine a final equilibrium state.

To summarize, it has been found that the problem of the structure of a two-phase discontinuity can be split into two problems. The first problem is the pure gas-phase structure problem, while the particles remain unaffected. The second problem is the relaxation zone and is matched to the solution of the first problem. The solutions to these problems constitute the zero-order terms in two matched asymptotic expansions in the density parameter  $\epsilon = \rho_p / \rho_{g0} \rightarrow \infty$ . In this

connection it is noted that all of the solutions are independent of  $\epsilon$ , as they should be.

#### E. Discussion of Related Problems

The equations which describe the structure of a two phase relaxation zone require boundary conditions at only one point. Then the solution for all downstream points is determined. Therefore, the nature of the process which produced the disequilibrium is arbitrary and the equations can be applied to any problem by specifying the proper initial conditions.

One physical phenomenon which was not accounted for in the analysis was the addition of particles to the flow. This extension would be of great practical importance since large droplets are known to break up or shed small particles until the surface forces can retain the particle shape.

Additional improvements to make the computer solutions more realistic must include better equations for the drag coefficient. This is primarily an experimental problem but theory must supply the equations by which the results are analyzed. Along these same lines is the problem of the Reynolds stresses. Experimental determinations of particle and gas fluctuations would be extremely useful in formulating these terms. Simple estimates of the fluctuations might be arrived at by considering the present knowledge about vortex shedding (size, frequency, dissipation, etc.) from spheres. By taking the aggregate of all the particle wakes, one might produce an estimate of the velocity fluctuations.

The shock wave plus a relaxation zone is only one type of two-phase discontinuity. There are also solutions for which the initial velocity of the mixtures is subsonic. In these solutions the gas and particles change state over an extended region similar to the relaxation zone without any initial gas shock. The jump states for these weak solutions have been discussed by Soo [14], and the structure has been analyzed by Kriebel [11]. Both of these papers considered solid particles.

The mass transfer mechanism assumed throughout this chapter has been the diffusion-controlled process from the drop surface to the gas phase. If only a single chemical species is present, the composition gradient is nonexistent and this assumption is inappropriate. For this situation, the evaporation and condensation rate for a pure liquid-gas system should be used to find the mass transfer rate. The assumption of isothermal particles would probably also be invalid because the evaporation rates are extremely high compared with diffusional rates.

Another modification of the problem is possible by changing the droplet-gas interaction to describe burning droplets. The theoretical model of a burning particle has been reviewed in a book by Williams [31]. The burning rate for a droplet is essentially a diffusion-controlled process with slightly different boundary conditions. The heat and momentum interchanges should also be modified to describe this special situation.

The asymptotic theory of two-phase discontinuities given in the previous section implicitly assumed that there was no gas-phase chemical reaction. If one takes an even more general

attitude and considers the gas mixture as combustible, then the asymptotic theory would separate the two-phase combustion wave into a gas-phase wave and a "relaxing" two-phase combustion region. The gas-phase waves would be the usual detonation and deflagration waves. The jump conditions for the two-phase detonation has been studied by Williams [32]. He has also formulated an analysis of two-phase deflagration and investigated the burning velocity for "heterogeneous" combustion [3, 33]. This model assumes no gas-phase combustion wave and in this respect Williams' heterogeneous combustion is analogous to the weak shock wave described above. The structure of a heterogeneous detonation wave was discussed in Williams [34].

It is interesting to note that the shock and detonation waves are relatively thin and one can easily imagine a decoupling between the gas-phase wave and the relaxation region. The gas-phase deflagration wave, on the other hand, is somewhat thicker and the coupling between the gas wave and the relaxation zone could be significant. This would imply that first-order terms (anyway, the second term) in the asymptotic expansions would be significant.

## CHAPTER IV

## DISCUSSION OF COMPUTER SOLUTIONS

A. Introduction

The system of equations for the description of the relaxation zone of a two-phase shock was formulated in the preceding chapters. In this chapter the results of several computer solutions to these equations will be discussed. Various aspects of the relaxation zone have been investigated previously by Carrier [1], Rudinger [10], and Kriebel [11]. In all of these papers the particles were considered to be solid and there was no mass transfer between the two phases. The inclusion of mass transfer is the primary difference between this work and the previous solutions. In the subsequent discussion this effect will be emphasized, and the conclusions of the other workers will be quoted only when they pertain directly to this purpose.

In formulating the problem in Chapter III, it was necessary to assume an expression for the drag coefficient. The "steady flow" law was chosen because of a lack of reliable and consistent experimental results for the actual situation. Rudinger [10] has pointed out that the structure of the relaxation zone depends strongly upon the choice of the drag law. He has also performed experiments [29] where the results differ substantially from any previous correlation. Primarily because of these facts, one should have little confidence in the quantitative values of the results of the computer solution. Thus one must view the importance of the calculations as a study of the relative effects of changing the various parameters.

## B. Parametric Study

The formulation of the nondimensional system of equations requires eleven independent nondimensional parameters to be specified before a solution can be obtained. These are listed below:

$$Pr = \frac{\mu C_p}{k}$$

$$Sc = \frac{\mu}{\rho_g D_{AB}}$$

$$C_{pA}^* = \frac{C_{pA}}{\gamma_0 R_0}$$

$$C_{pB}^* = \frac{C_{pB}}{\gamma_0 R_0}$$

$$C_{pL}^* = \frac{C_{pL}}{\gamma_0 R_0}$$

$$\bar{M} = \frac{m_B}{m_A}$$

$$M_0 = \frac{\mu_0}{a_0}$$

$$\mu^* = \frac{\mu}{\rho_{g0} a_0 r_0}$$

$$\delta = \frac{\sigma r_0}{\rho_{g0}}$$

$$\chi_{B0} = \frac{P_{B0}}{P_0} = \frac{P_{B0} \gamma_0}{\rho_{g0} a_0^2}$$

$$H_{fg}^0 = \frac{h_{fg}}{a_0^2}$$

The immediate object is to perform a parametric study emphasizing the mass transfer process. A sequence of solutions will be computed using various values of the parameters which exert the most influence upon the mass transfer. All other parameters will be held constant.

Species B is present in both the liquid and the gaseous phases. The driving force for the mass transfer is the concentration gradient, and at the droplet surface the concentration of species B is determined by the vapor pressure curve or the

pure substance. This curve is characterized by two parameters:  $x_{B0}$ , the initial mole fraction of species B, and  $H_{fg}^{\circ}$ , the latent heat of vaporization (see Fig. 3-2). In addition to these parameters the loading factor  $\delta$  and the viscosity radius parameter  $\mu^*$  will be varied. Delta is chosen because it has a strong influence upon the solutions, and  $\mu^*$  because the droplet radius is an important variable from an experimental standpoint.

All the other parameters will be fixed with following values. The Mach number of the gas shock is taken as 1.3. The inert species A and the vapor of species B are assumed to have specific heat ratios of 1.4. This implies that  $C_{pA}^*$  and  $C_{pB}^*$  are both equal to 2.5. The liquid specific heat is taken as twice that of its vapor, i.e.,  $C_{pL}^* = 5.0$ . The molecular weight ratio is set equal to one. This ratio is not believed to have a strong influence upon the solution.

The four parameters under investigation were assigned a range of values which was thought appropriate to cover most substances and situations. The viscosity-radius parameter was computed using the viscosity of oxygen at normal pressure and temperature and allowing for particle sizes of 4 to 100 microns in diameter:

$$\mu^* = .025 \quad (4 \text{ microns dia})$$

$$\mu^* = .005 \quad (100 \text{ microns dia})$$

The loading parameter represents the mass of liquid per unit volume of mixture divided by the mass of gas per unit volume of mixture. Lightly and heavily loaded mixtures were considered to be



$$\delta = .2$$

$$\delta = 1.5$$

The mole fraction parameter depends upon the vapor pressure of species B and the total gas-phase pressure. Theoretically could range between zero and unity. The values chosen for computation were

$$\chi_{B_0} = .1$$

$$\chi_{B_0} = .7$$

$$\chi_{B_0} = .9$$

The intermediate value was included because the value .9 gave results significantly different than .1 for some cases. Some typical values of  $\chi_{B_0}$  for several substances are given below:

Hydrazine	.02 (68°F),	.2 (160°F)
Ethyl Alcohol	.06 (68°F),	.83 (160°F)
n-Hexadecane	.01 (300°F)	
n-Dodecane	.01 (200°F)	
Octane	.03 (88°F)	
F 11	.6 (50°F),	1.0 (75°F)
F 113	.23 (50°F),	.47 (80°F)

These values are for a total pressure of 1 atmosphere and temperatures as noted. For some substances there is a large change in the vapor pressure for only a small change in the temperature. This is a result of the large heat of vaporization. The heat of vaporization plays a dual role: it indicates the slope of the vapor pressure curve and it indicates the heat given up when the gas condenses upon the drop. Typical values of  $H_{fg}^{\circ}$  are shown below:

Hydrazine	13
Water	10.5
Methyl Alcohol	5.4
Ethyl Alcohol	3.9
n-Hexadecane; n-Dodecane	3.3
Octane; F11	1.5
F 113	1.7

The range chosen for study was 2 to 16.

The four parameters can be considered as independent variables in a four-dimensional space. The range chosen for each parameter constitutes the side of a four-dimensional cube and the solutions corresponding to the interior points are of interest here. To investigate the cube with the minimum of effort, only the center point and the corner points are calculated. With these results it is easy to determine where intermediate calculations should be performed.

The center point corresponds to values of the parameters of

$$\mu^* = .002$$

$$H_{fg}^0 = 9.$$

$$x_{B_0} = .5$$

$$\delta = 1.$$

The results for this case are plotted on Figure 4-1 as functions of the nondimensional distance. The actual distance is obtained only if one specifies explicitly the particle radius and the ratio of the particle material density to the gas density. For

a typical liquid slightly lighter than water, one unit on the distance scale is about .9 cm. The distance scale changes as the viscosity-radius parameter changes; however, curves with different real distance scales have purposely not been plotted on the same graph.

As one interprets the symbols on the figures, it is well to recall that the subscript  $p$  refers to the particles, and  $g$  to the gas. One new variable which was not defined in Chapter III has been introduced:  $W_g$ . This is the ratio of the mass flow rate of gas divided by the initial value upstream of the gas-phase shock. It indicates the amount of mass interchanged between the two phases. In Figure 4-1,  $W_g$  first decreases indicating condensation from the gas into the particle. This initial behavior was anticipated in the discussion in Chapter III. The condensation soon stops as the particle temperature rises and hence the partial pressure at the particle surface has been increased to equal the partial pressure of species B in the gas phase. The particles increase their temperature by two mechanisms: heat transfer from the gas, and heat given up by the condensing vapor. As the particle temperature continues to increase, the partial pressure at the surface exceeds that in the main gas stream and diffusion of the vapor away from the particles occurs. The partial pressure at the surface is maintained at the equilibrium value corresponding to the particle temperature by evaporation. At equilibrium for downstream the net effect for the center point conditions was vaporization of a small portion of the liquid.

The velocity of both the particles and the gas decreases behind the shock. Viewed from a shock wave coordinate system, the particles approach with a supersonic velocity and are initially unaffected by the gas shock. The gas velocity is reduced to a subsonic value as it passes through the shock and the two phases ultimately move with the same velocity as they approach mechanical equilibrium. The gas temperature begins at a high value because of the compression of the shock; it increases to a maximum, and then decreases to a value lower than the starting value. Both of these effects have been noted by Rudinger [23] for solid particles also. A more detailed discussion of the gas temperature curves will be given later.

Figure 4-1 gives an overall view of the relaxation zone. From now on, attention is focused upon one variable at a time and the differences caused by changing the parameters are thereby emphasized. The graphs are organized in the following manner: all curves for the different values of  $\mu^*$ , the radius-viscosity parameter, are on separate sheets; then, if need be, all curves for the same value of the loading parameter are grouped together on the same sheet. Thus on one sheet the primary comparison is for various values of the heat of vaporization and the initial mole fraction. Each curve is designated by two numbers separated by a comma; the first number is the value of  $H_{fg}^\circ$  and the second is the value of  $\chi_{B0}$ . Sometimes three numbers are used, the third is then the loading factor  $\delta$ .

The nondimensional mass flow rate of gas is plotted on Figure 4-2 for  $\mu^* = .025$  (4-micron diameter). The corresponding set of curves for  $\mu^* = .005$  was not plotted since the results

have the same character. All the curves initially decrease, indicating condensation. Curves for  $H_{fg}^{\circ} = 16$  all reach a minimum and ultimately show a small amount of net vaporization.

It is concluded that  $H_{fg}^{\circ} = 16$  represents a case where the mass transferred between the phases is not significant, irrespective of the values of other parameters. The situations which result in a large net interchange of mass occur when  $\chi_{Bo}$  has a low value and  $\chi_{Bg}$  a high value. The net effect is condensation of the gas phase which can lose 80 to 90% of its mass in severe cases ( $H_{fg}^{\circ} = 2$ ,  $H_{fg}^{\circ} = .9$ ). The region where mass transfer effects are most dramatic has been located, and, to complete the picture, computations were made at intermediate values of  $H_{fg}^{\circ}$  and  $\chi_{Bo}$ . Before leaving Figure 4-2 it should be noted that the thickness of the relaxation zone increases appreciably as the loading factor  $\delta$  is increased.

Both the gas and particle velocities are given on Figures 4-3 and 4-4. The first figure is for the loading factor  $\delta = .2$  and the second for  $\delta = 1.5$ . The major difference between the two graphs is that the relaxation zone is shorter for the higher loading factors. Another difference is that the final equilibrium velocities are much lower for  $\delta = 1.5$ . The trends with  $H_{fg}^{\circ}$  and  $\chi_{Bo}$  are consistent with the previous results that low  $H_{fg}^{\circ}$  and high  $\chi_{Bo}$  give appreciable effects on the relaxation. The curves for  $H_{fg}^{\circ} = 16$  lie on top of each other along with the curve for  $H_{fg}^{\circ} = 2$ ,  $\chi_{Bo} = .1$ . The final equilibrium states differ by about .1; hence it appears that the interaction process out to  $X' = 3$  has been largely mechanical and that a very slow

vaporization process will moderate the curve over an extremely long distance.

The pressure variable plotted on Figure 4-5 is not the one used in the basic equations. This pressure ratio is non-dimensionalized by the pressure upstream of the gas shock. The curves for  $\delta = 1.5$  rise more steeply and have much higher final values than those for  $\delta = .2$ . Again curves for high  $X_{g_0}$  and low  $H_{f_0}^{\circ}$  give distinctive behavior.

The temperature variables show the most interesting and varied behavior. For this reason the computer runs for both  $\mu^* = .025$  (4-micron diameter) and  $\mu^* = .005$  (100-micron diameter) were plotted. The negligible effect of varying  $\mu^*$  is demonstrated when one compares Figures 4-6 and 4-8 and Figures 4-7 and 4-9. The effect of changing  $\delta$  is to shorten the relaxation zone, as noted for the case of all the other variables. Delta also has a pronounced effect on the shape of the gas-phase temperature curve. The increase in  $\delta$  has produced pronounced peaking of the curves and generally lowered the final equilibrium value. When  $H_{f_0}^{\circ}$  has a high value the particle temperatures rise to a plateau which slopes upward slightly as  $X'$  increases. This indicates an equilibrium between the rate of heating the particle by convection from the gas and the rate of cooling the particle by evaporation. These curves are seen to approach the thermal equilibrium between particles on gas very slowly. For low values of  $H_{f_0}^{\circ}$  the particle temperature rises in a smooth arc to the equilibrium value without establishing this balance.

In order to verify the gas temperature curves and gain an insight into the wavy behavior, a separate calculation of the gas temperature was made. In the computer solution the gas temperature is found by solving several algebraic equations after the differential equations for the particle properties have been integrated. An alternate method is to integrate a differential equation for the gas temperature. In this way one can observe directly what terms are causing the gas temperature to change. To obtain this equation, the overall energy equation [equation (3-43)] is differentiated. Then substituting various other equations and definitions, the following result may be obtained:

$$\frac{dT_g}{dX} = \frac{\Psi}{C} \left\{ C_{p0}^* (T_L - T_g) + \frac{1}{2} (V_g - V_p)^2 \right\} + \frac{q}{C} + \frac{d\hat{h}}{C} (V_g - V_p) + \frac{V}{C} \frac{dP}{dX} \quad (4-1)$$

where

$$C = \dot{M}_g (\omega_A C_{pA} + \omega_B C_{pB})$$

The first three terms represent the direct influence of the gas-particle interaction: the vaporization, the heat transfer, and the drag. The last term represents the effect of compression of the gas phase. This equation was integrated term by term and the results are shown as Figures 4-10 through 4-13. The accumulative effect of each term is depicted on a separate graph. The three curves on each graph are for various different

initial conditions. One case corresponds to the wavy pattern for low  $H_{fg}^{\circ}$  and high  $\chi_{B_0}$ , another to the sluggish curves for high  $H_{fg}^{\circ}$  (irrespective of  $\chi_{B_0}$ ), and the third to the amplified behavior of a high loading factor.

The integral of the first term on the right-hand side of equation (4-1) is the direct effect of the difference in energy between the main gas stream and the gas which is changing phase. In all cases the contribution of this term is very small. The second term is the contribution by heat transfer. Note that this term is so large that the scale on the graph (Fig. 4-11) is one half of those of the other figures. The heat transfer is always tending to an overall negative effect. Figure 4-12 shows the drag of the particles upon the gas. For the high case this term is negligible; however, for both the other cases it is significant. The last graph in this series shows the effect of compression of the main gas. All three cases are greatly influenced by this term.

In general, the effect of increasing the loading factor is to intensify the gas-particle interaction. In the early portion of the relaxation zone the drag work on the gas and the compression of the gas dominate and increase the gas temperature in spite of the heat transfer to the particles. The heat transfer increases and finally depresses the temperature in the latter stages of the process. When the mixture contains only a small mass of particles the balance between the mechanical effects and the heat transfer is more delicate.



Let us discuss the case of small loading and high latent heat  $H_{fg}^{\circ}$ . The high latent heat means that a small change in the liquid temperature results in a large change in the vapor pressure (see Fig. 3-2). When the particles first pass through the shock, condensation occurs and heat is given up to the particles. Only a little condensation is required to increase the particle temperature substantially. But the increased particle temperature results in a very large increase in partial pressure at the particle surface. The condensation changes to evaporation as the partial pressure of the surface exceeds that in the gas stream. The heat transfer to the particle soon determines the rate of vaporization as the droplet temperature stabilizes (a wet bulb temperature is established in this case). All of this can occur in a short distance behind the shock wave, as indicated by the particle temperature curves. In the case shown here, mechanical effects tend to increase the gas temperature as the vapor is slowly added to the gas, and the heat transfer to the particles slowly decreases the temperature. The approach to equilibrium is very sluggish.

Now when  $H_{fg}^{\circ}$  is low and the loading still small, a completely different temperature curve is observed. The condensation process occurs throughout the relaxation region and the particles do not approach a quasi-steady temperature. Since  $H_{fg}^{\circ}$  is small the partial pressure does not rise rapidly as the particle temperature increases, so that the diffusion of vapor to the surface continues even for relatively large temperatures. The particle temperature rises as more condensation occurs and the difference

between the gas and particle temperature decreases to zero. Thus the heat transfer changes sign and begins to aid in increasing the gas temperature. It is interesting that there exists a situation of heat transfer away from the drop and simultaneous condensation upon the particle. The heat transfer plays a moderating role as the mechanical effects produce the final equilibrium gas temperature.

Several solutions have been discussed where  $H_{fg}^0$ ,  $\chi_{g0}$ , and  $S$  were altered, and the changes produced in the temperature curves have been noted. Rudinger [10] presented results for solid particles when he changed the Mach number, the drag law, and the specific heat ratio. He noted that the gas temperature curve can have almost any shape. Thus it seems that a wide variety of effects compete to influence the gas temperature, and the final curve is sensitive to changes in a large number of parameters.

### C. Two Particle Sizes

In this section the results of computations where two particle sizes were present in the mixture are shown. This problem is of interest because spray-producing equipment frequently produces particles of two separate size groups. The reader is referred to Kriebel's work [11] for examples with three sizes. The initial conditions and constants were chosen to be the same as the ones used in the parametric study of Section B. The parameters which were varied in Section B were fixed in the two particle size problem. The latent heat  $H_{fg}^0$  was taken as 5,  $\chi_{g0}$  as .5, and the loading factor as unity. There are now two

viscosity-radius parameters and these were computed for 4- and 50-micron-diameter particles in oxygen at NPT. This means that the ratio of diameters of the two size groups is 12.5. Another parameter is introduced when the analysis is extended to two particle sizes, the fraction of mass in particle size group one, say. The loading factor  $\mathcal{S}$  is still the ratio of the total mass of condensed phase to the mass of gas phase. The "group loading factor,"  $\alpha_1$ , is the ratio of the mass of condensed phase in size group one to the total mass of condensed phase. An  $\alpha_2$  could be defined also; however, it would be superfluous since  $\alpha_1 + \alpha_2$  must equal one.

Three cases were computed in which  $\alpha_1$  was changed while everything else was held constant as described above. The results for  $\alpha_1 = .9, .5, \text{ and } .1$  are shown as Figures 4-14 through 4-22. Each case consists of a set of three figures, one each for velocities, temperatures, and mass flow rates. The first set is for  $\alpha_1 = .9$ ; that is, .9 of the liquid mass is in the form of a 4-micron particle. As seen on Figure 4-14, the small particles and the gas interact strongly and in a short distance reach the same velocity. The large particles change their velocity over a much longer distance. Since there is only a small amount of large particles (.1 of the liquid mass) they produce little change in the gas velocity as they approach equilibrium. Figure 4-15 depicts the temperatures. Again, the small particles and the gas interact strongly and the large particles approach equilibrium without affecting the gas temperature. The last figure in this set is Figure 4-16. It shows the mass flow rates of the gas and both particle groups. They have been

normalized by the initial values so that all curves begin at one. At first, the particles gain mass as condensation occurs. The small particles grow at a much faster rate and soon reach a peak and evaporation begins. Only a small amount of vaporization occurs and the small particles reach equilibrium with a slight net increase in size. The large particles grow throughout the relaxation zone. However this has little effect upon the gas mass flow rate which is, more or less, just the opposite of the small particles.

The case when the liquid mass is equally distributed between the two size groups is shown in Figures 4-17 through 4-19. Figure 4-17 shows that the small particles interact over a slightly longer region than they did in the first case. This corresponds to the observation made in the single-particle study that increasing the loading factor shortens the relaxation zone. The stronger interaction of the large particles and the gas is also evident in this figure as we note that the gas velocity changes more smoothly over the entire relaxation zone. The graph of the temperatures is similar to the first case with the same effects as noted in the velocity plots. The mass flow rate graph is given in Figure 4-18. The trends are again similar to the first case. There is, however, a net loss in mass from the small particles.

The last case, Figures 4-20 through 4-22, is for .9 of the liquid mass in the form of large particles. The gas velocity reflects this situation as it changes almost entirely because of the interaction with the large particles. The temperature

curves also show little influence from the small particles. The gas temperature no longer has a peak in the early portion of the relaxation zone. It rises continually and has a low shallow peak caused by the large particle interaction. The large particles slowly increase their temperature in an unspectacular manner. An unusual aspect is that the temperature of the small particles does not equilibrate rapidly to the gas temperature. The velocity of the small particles was essentially the gas velocity throughout a major portion of the relaxation process.

The particle temperature rises rapidly at first but then takes a more moderate rate in spite of the mechanical equilibrium. To explain this, consider Figure 4-22, which shows the mass flow rates. The large particles grow because of condensation throughout the relaxation zone. The mass transfer is moderate and the gas mass flow rate shows no significant change. The small particles show a large decrease in mass which occurs throughout the relaxation zone. For all practical purposes the small particles have completely vaporized (they only comprised .1 of the liquid mass to start with). Now it is possible to piece together the following picture about the temperature of the small particles. The temperature levels off once the vaporization starts because of the cooling effect of the phase change. The heat transferred from the gas is sufficient to raise the particle temperature (and thus increase the vapor pressure at the surfaces) and supply energy for the phase change. The gas temperature is maintained and increased by the strong mechanical interaction with the large particles. A similar case was not found in the single particle size work; all the cases

where a large change in mass flow rate occurred were for condensation, not evaporation. Even in this case it is noted that although most (if not all) of the mass of the small particles changed to gas, there was not much mass to start with.

#### D. n-Dodecane-Oxygen System

A special computation was performed using the properties which correspond to a mixture of liquid n-dodecane in oxygen at NPT. There is a large difference in the molecular weights of these two species,  $\xi = 5.33$ .

For mixtures of such dissimilar molecules there are highly nonlinear variations in the transport properties as the composition of the mixture changes. In view of this it was decided to allow the viscosity and thermal conductivity of the mixture change with composition but still ignore the temperature dependence. The viscosity of a mixture can be computed from Wilkie's formula (see Bird, et al. [21], p. 24):

$$\mu_{AB} = \frac{\chi_A \mu_A}{\chi_A + \chi_B \phi_{AB}} + \frac{\chi_B \mu_B}{\chi_B + \chi_A \phi_{BA}}$$

where

$$\phi_{ij} = \left[ 1 + \left( \frac{m_j}{m_i} \right)^{\frac{1}{4}} \left( \frac{\mu_i}{\mu_j} \right)^{\frac{1}{2}} \right]^2 \cdot \left[ 8 + 8 \frac{m_i}{m_j} \right]^{-\frac{1}{2}}$$

An analogous formula is valid for the conductivity where  $\mu_{AB}$ ,  $\mu_A$ , and  $\mu_B$  are replaced by the proper conductivity and the  $\phi_{ij}$  are unaltered.

The properties of n-dodecane were estimated from various formula from kinetic theory. The viscosity was computed from equation 1.4-18 in Bird, et al. [21], p. 23:

$$\mu = 2.67 \cdot 10^{-5} \frac{\sqrt{M T}}{\sigma^2 \Omega_k}$$

where  $\mu$  [ $g\ cm^{-1}\ sec^{-1}$ ],  $T$  [ $^{\circ}K$ ],  $\sigma$  [ $\text{\AA}$ ]; and  $\Omega_k$  is a function of  $T/(\epsilon/k)$ . The constants  $\sigma$  and  $\epsilon/k$  were estimated from a knowledge of the critical temperature and molar volume of the substance (Bird, et al. [21], p. 22).

The binary diffusion coefficient was estimated by the following formula (Bird, et al. [21], p. 511):

$$D_{AB} = .00186 \frac{\sqrt{T^3 \left( \frac{1}{M_A} + \frac{1}{M_B} \right)}}{\rho \sigma_{AB}^2 \Omega_{DAB}}$$

where  $\rho$  is in atmospheres. A nondimensional diffusion coefficient is formed so that the Schmidt number is

$$S_c = \frac{\mu^*}{(\rho D_{AB})^*}$$

In the calculations the variation in the Schmidt number with density was ignored.

The thermal conductivity of polyatomic molecules can be estimated by Eucken's formula:

$$k = \left( c_p + \frac{5}{4} R \right) \mu$$

To apply this formula the specific heat is obtained from experimental data and the viscosity is calculated as above.

Computations were performed for a shock with a Mach number of 1.3 and particles of 25-micron radius. The vapor pressure of n-dodecane is extremely small at room temperature and the initial gas mixture has nearly the same properties as oxygen. Thus the initial state is still given by a shock wave in a gas with gamma equal to 1.4 as in the previous computations. The nondimensional constants have the following values:

$$C_{pA}^* = 2.5$$

$$\chi_{B_0} = .0001$$

$$C_{pD}^* = 4.49$$

$$r_{REP} = .0025 \text{ cm}$$

$$C_{pL}^* = 5.69$$

$$\mu_A^* = .00192$$

$$H_{fg} = 3.33$$

$$\mu_B^* = .00042$$

$$\xi = 5.33$$

$$\rho_L / \rho_{g_0} = 570$$

$$\gamma_0 = 1.4$$

$$(\rho_{g_0} D_{AB})^* = .00047$$

$$\delta = 1.0$$

Normal dodecane has a low value of  $H_{fg}^0$  and an extremely low value of  $\chi_{B_0}$ . This combination did not show significant mass transfer in the parametric study of Section B.



The curves for this case are shown in Figure 4-23. Only the velocity and temperature curves are plotted since the mass flow rate variable gave no significant change from its initial value of one. In view of this the calculations were repeated with the program modified to exclude vaporization. The results of this run show only slight differences from the original computations, and would be imperceptible on the scale of Figure 4-23. Since the amount of mass transfer between the phases was not significant the expressions for the transport coefficients as functions of the mixture composition were an unnecessary refinement.

The results of this section indicate that mass transfer can be ignored in systems of n-dodecane at room temperatures. In fact, the generalization might be made that when the vapor pressure of the liquid is a small fraction of the total gas pressure for the temperature range of the problem, then mass transfer may be ignored. A similar conclusion was proposed by Busch, et al. [35], based upon the computation of several equilibrium end states.

## CHAPTER V

## SUMMARY

Two fairly distinct topics are covered in this work: a derivation of the basic equations for dispersed two-phase flow, and the numerical solution for the relaxation zone behind a shock wave. Two chapters are devoted to each topic. In the first chapter the continuity and momentum equations are discussed, while the energy and state equations are the subject of the second. The shock wave relaxation problem is formulated in the third chapter, and in the fourth, the numerical results are analyzed.

The derivation in this study takes an essentially different approach from those of previous authors. This work starts with the conservation equations of continuum mechanics and proceeds from the local flow to an average description of the two-phase flow. This is accomplished by integrating the locally valid equations over a control volume and interpreting the integrals as average properties of a dispersed two-phase flow. Limiting the control volume to zero size results in differential equations for the average two-phase properties. Because the detailed flow field is unsteady it is also necessary to time-average the equations. This process introduces the fluctuations of the local flow, and the final two-phase equations contain terms similar to the Reynolds stresses of turbulent flow theory.

In formulating the particle-phase momentum equation, a particle-phase pressure term arises naturally. This term depends

upon the pressure within the particle, which in turn is dependent upon the gas-phase pressure. The exact dependence involves the nature of the detailed flow around a particle. Whatever the actual case is, an assumption is required in order to eliminate the particle-phase pressure from the momentum equation. This assumption plays the role of an equation of state for the particle phase.

The thermal energy equation for the particle phase is also derived from basic equations. Instead of deriving an energy or thermal energy equation for the gas phase, the simpler task of deriving an overall gas-plus-particle energy equation has been chosen here. The two-phase conservation equations are not a complete set without a description of the thermodynamics of the phases. The proper thermodynamics equations are found in a straightforward manner by time- and area-averaging the equations of state which are valid locally.

By defining average properties for the particles and for the gas, the variables and equations have been constructed to describe two coexistent continua which interact. The interaction is manifested in the heat transfer, mass transfer, and drag functions which appear in the equations. These functions will usually be evaluated from experimental data. The process of averaging local variables allows many of the details of the complex local flow field to be ignored. However, they cannot be completely disregarded. For example, the unsteady flow was time-averaged but this introduced the Reynolds stresses as new variables. Thus additional information is required which really depends upon the

local flow. The area-averaging process produced several "new" average velocities, each weighted with a different property, i.e., density, mass flux, or momentum flux. These various average velocities could be related to each other if the local flow is known. In practice, then, one must make assumptions about the Reynolds stresses and the various averages in order to apply the two-phase equations. The appropriate assumptions depend upon the particular problem being considered. It has been customary in most papers on two-phase flow to ignore this problem or assume that these effects are negligible. The latter has been done in this work for solution of the relaxation zone behind a shock wave.

The shock relaxation problem, as it is formulated here, is a straightforward extension of previous papers which dealt with solid particles. Neglecting Reynolds stresses and the distinction between the various area averages casts some doubt upon the exactness of the results presented in this work. Another area of even greater uncertainty is the drag coefficient for this situation. Nevertheless some useful information might be obtained by performing a parametric study emphasizing those parameters which most directly affect the mass transfer process.

The shock relaxation zone problem is proposed on the basis of physical arguments. A gas-phase shock, which is very thin, exists unaffected by the presence of particles. Likewise, the particles are unaffected by the gas shock. This establishes the initial conditions for a relaxation zone in which the gas and particles interact. In the last part of Chapter III the artificial separation of these two regions, i.e., gas shock and

relaxation zone, is formalized. The differential equations and boundary conditions for two-phase flow are examined and solutions which will pass from one uniform equilibrium state to a different equilibrium state are sought. The density parameter  $\epsilon = \rho_l / \rho_g$  appears to be of fundamental importance in two-phase flow and the problem is solved as an asymptotic expansion in  $\epsilon$  as  $\epsilon \rightarrow \infty$ . It turns out that the problem is singular, and two matched expansions are required. The first term in one expansion is the solution to the gas-phase shock wave, while the particles are unaffected. The first term in the second expansion is the solution to the relaxation zone problems, as previously formulated on physical grounds.

By including the possibility of gas-phase reactions it is possible to develop an asymptotic theory of two-phase waves. The outer solution would be the gas-phase shock wave, deflagration wave, or detonation wave. The matching inner solutions would be either a simple relaxation zone or one with combustion around the individual particles (sometimes called heterogeneous combustion).

The results of the computer calculations are discussed in Chapter IV. A parametric study was made in which the following were systematically changed:  $\mu^*$ , the viscosity-radius parameter;  $\mathcal{S}$ , the loading factor;  $H_{fg}^\circ$ , the heat of vaporization; and  $X_{g0}$ , the initial vapor pressure of the liquid. The first two parameters,  $\mu^*$  and  $\mathcal{S}$ , are important from an experimental standpoint. The viscosity-radius parameter does not affect the equilibrium end states and has only a slight effect on the shape

of the curves through the relaxation zone. The actual length of the relaxation zone varies considerably as this parameter is changed. The loading factor  $\mathfrak{S}$  is the ratio of the initial mass flow rate of particles to the mass flow rate of gas. The final equilibrium state changes as this parameter is altered. As  $\mathfrak{S}$  is increased the interaction between the particles and the gas is stronger, i.e., the presence of the particles modifies the gas-phase variables to a greater extent. There is also a slight shortening of the relaxation zone and a pronounced peaking of the gas temperature curves. All in all, the structure of the relaxation zone is amplified as the loading factor increases.

The latent heat of vaporization  $H_{fg}^{\circ}$  and the initial mole fraction  $\chi_{g0}$  characterize the vapor pressure curve of a substance. Since the vapor pressure is a boundary condition for the mass transfer process, these parameters have pronounced effect upon this aspect of the solutions. By examination of the mass transfer rate equations and physical arguments, it can be concluded that condensation will occur in the initial portion of the relaxation zone. Condensation does not always continue, however. When  $H_{fg}^{\circ}$  has a high value the amount of mass transferred between the phases is small and the net effect is a vaporization of some liquid. In this case a balance is established between the heat transfer to the particle and the heat required for vaporization. The droplet temperature stabilizes at a wet bulb temperature and the gas temperature slowly decreases to the equilibrium value.

The cases where  $\chi_{g0}$  has a low value also result in a negligible amount of mass transfer between the phases. A study

was made using the actual properties of n-dodecane, which has an extremely low vapor pressure at room temperature ( $\chi_{D_0} = .0001$ ). In this instance two calculations were performed: one with mass transfer and another where the mass transfer was arbitrarily zero. There was negligible difference between the results.

The most prominent mass transfer effects occur for the combination of high  $\chi_{D_0}$  and low  $W_{f_2}$ . The condensation process continues throughout the relaxation zone and a large portion of the gas phase may be lost. The velocities of both the gas and particles are decreased as substantial condensation occurs. The gas temperature curve is the result of many competing effects and has varied behavior. In severe cases, where mass transfer was significant, the gas temperature oscillated about the particle temperature curve.

In addition to the n-dodecane and parametric studies, several runs were made with two particle sizes. The ratio of the particle sizes was fixed at 12.5 and the total loading factor was held constant. The mass of particles in each size group was varied from one run to the next. If most of the liquid mass is in the form of small particles, they interact with the gas in a short distance to reach a semiequilibrium state. Then the large particles relax to this state without affecting the gas phase. For the opposite case, where most of the liquid occurs in large drops, more complicated behavior may result. The large drops may grow by condensation while the small drops are completely vaporized.

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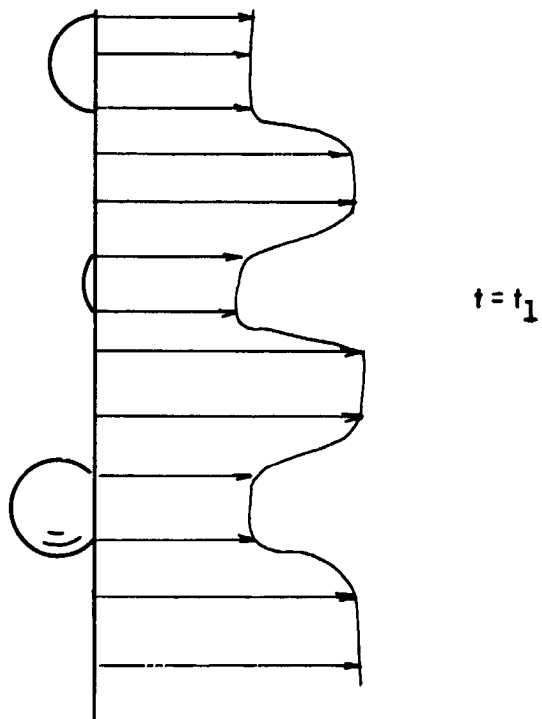
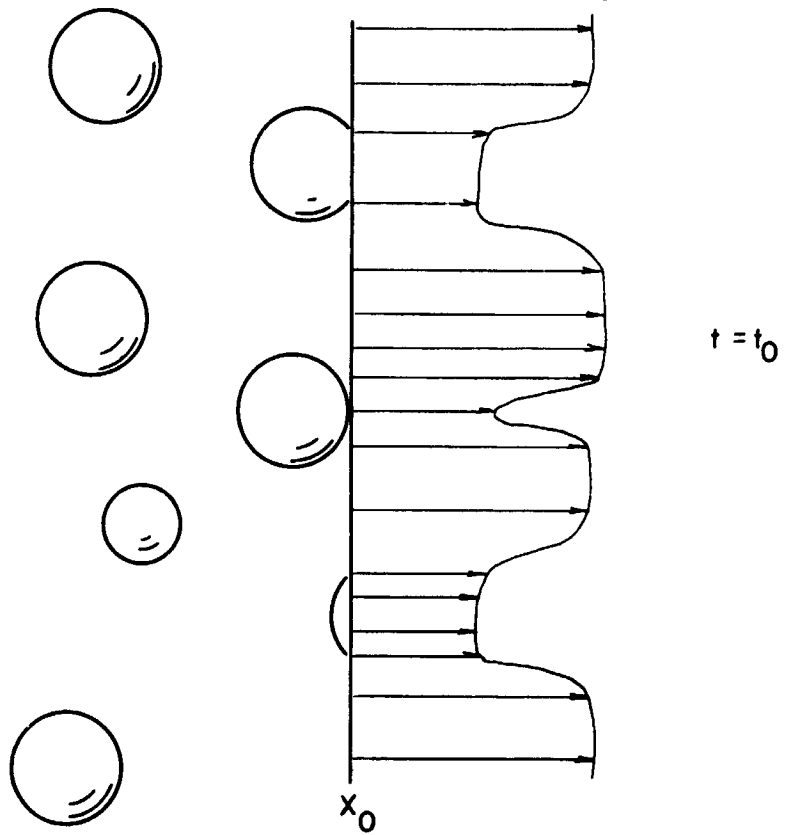


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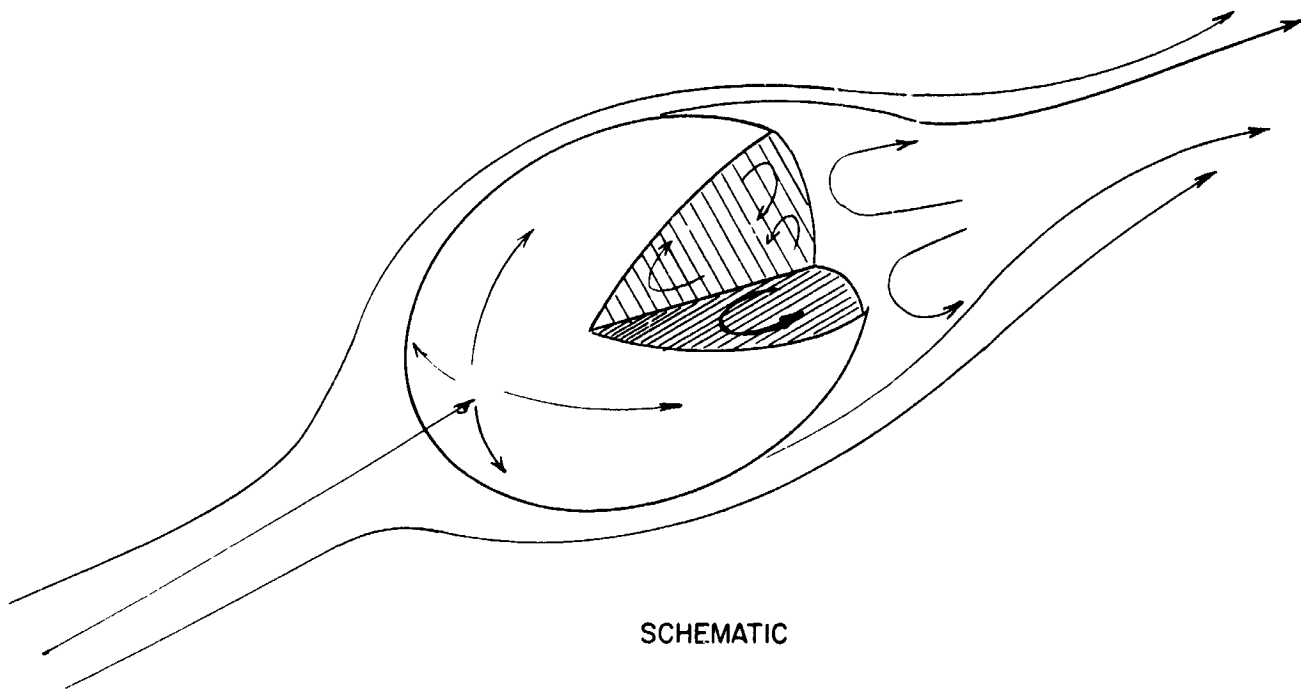
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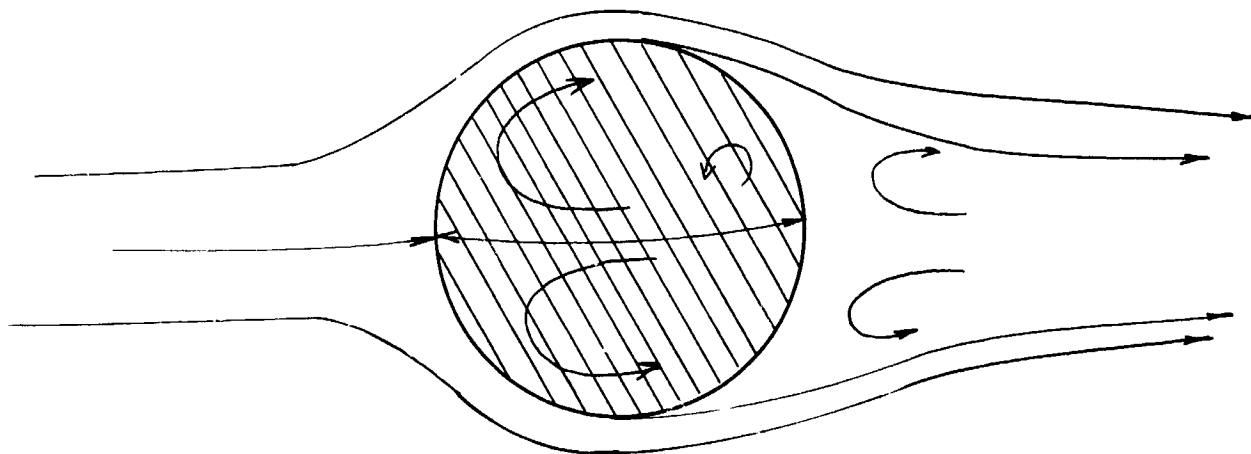
X-DIRECTION VELOCITY PATTERN  
AT ONE LOCATION



# FLOW AROUND A PARTICLE



SCHEMATIC

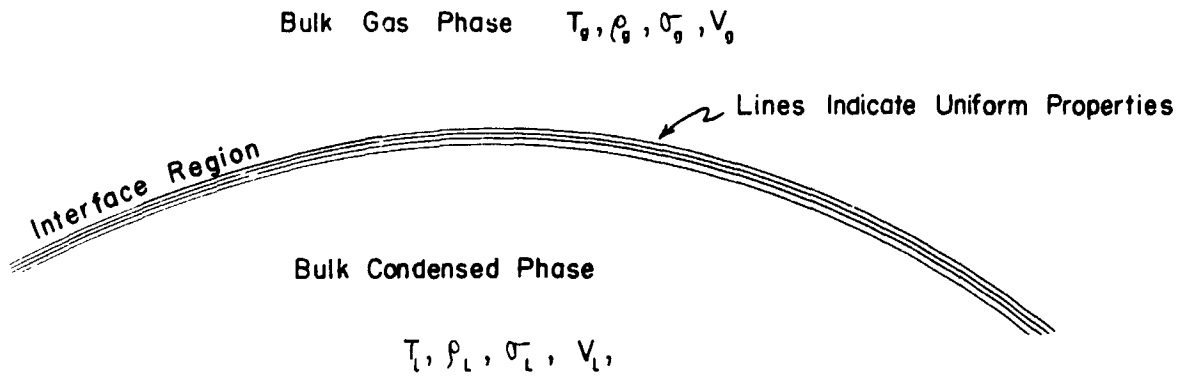


CROSS - SECTION VIEW

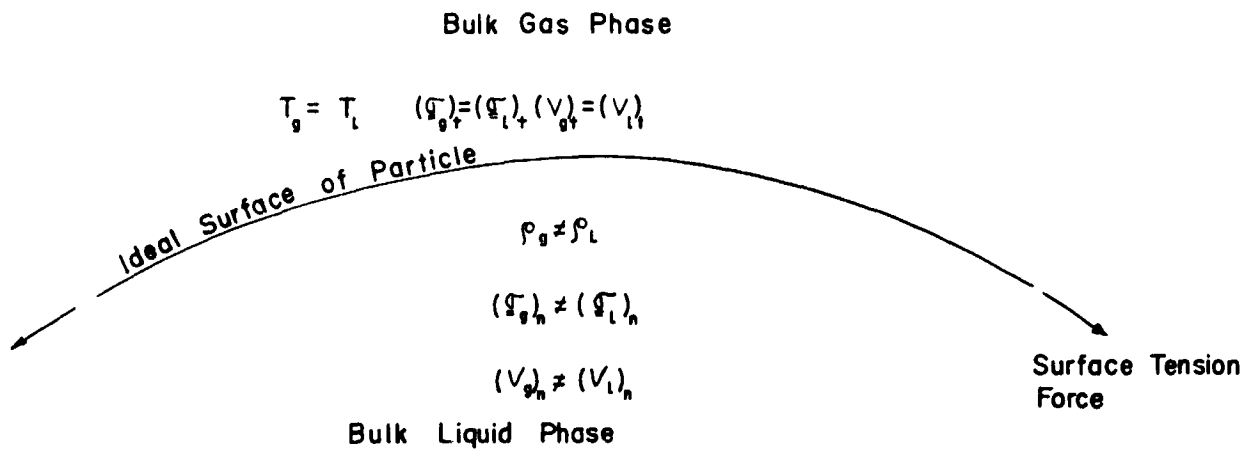
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# INTERFACE BETWEEN PHASES



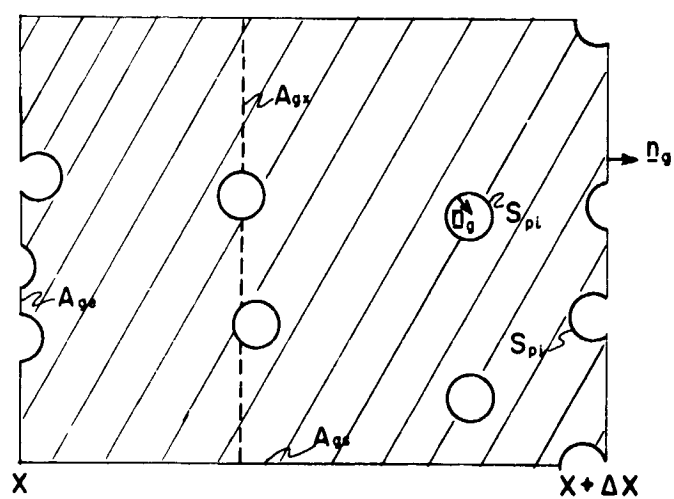
# SURFACE MODEL



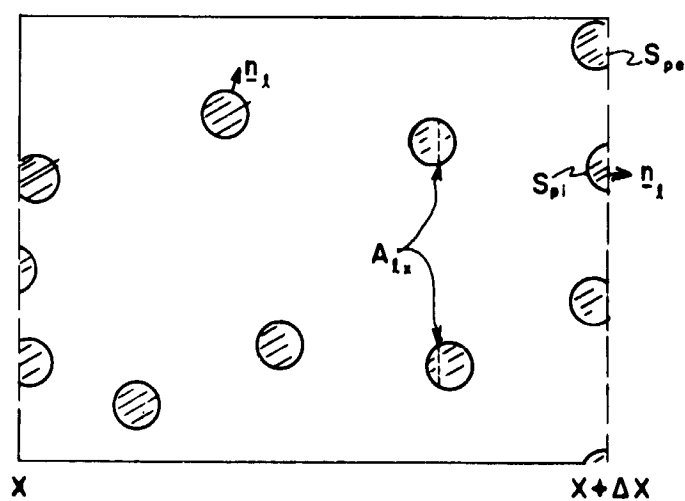
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## CONTROL VOLUMES



GAS PHASE

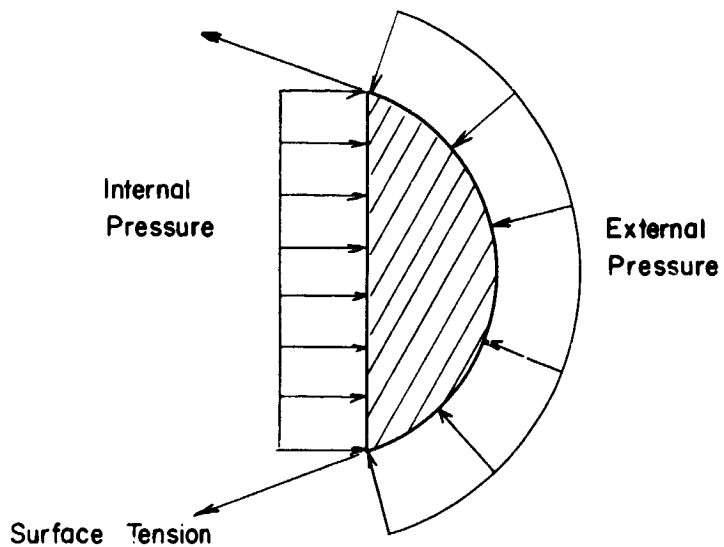


PARTICLE PHASE

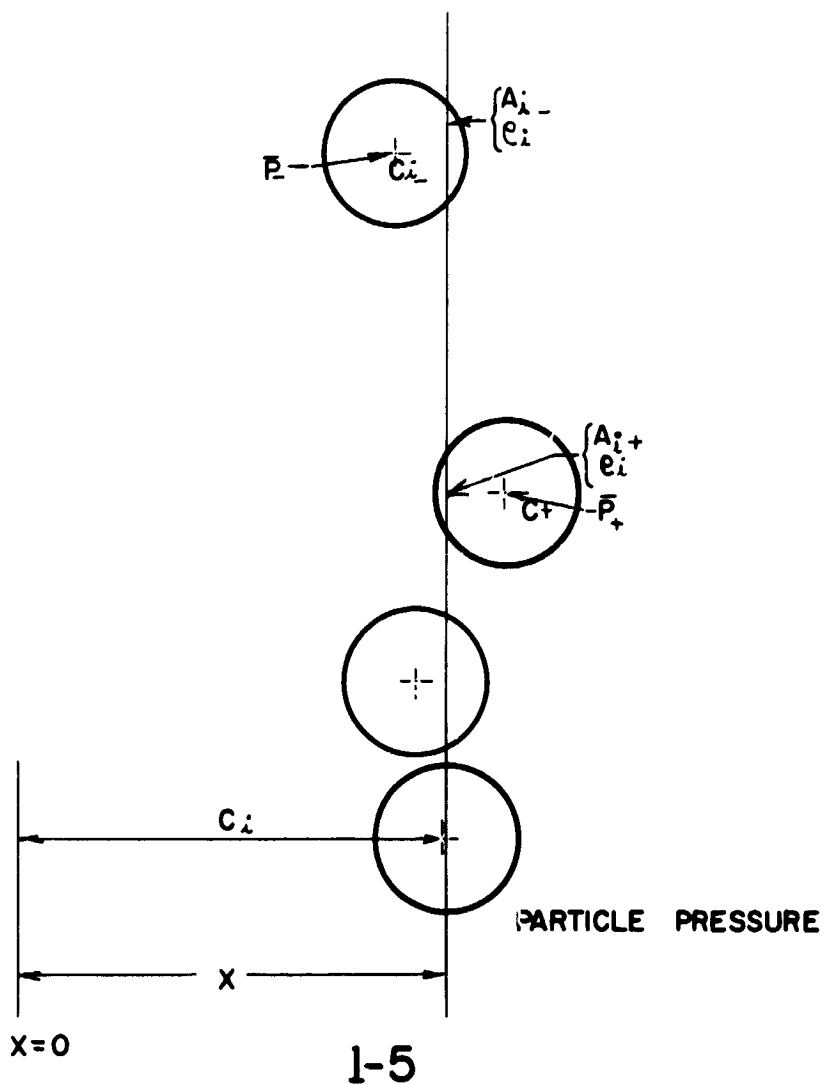
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# PARTICLE PHASE PRESSURE

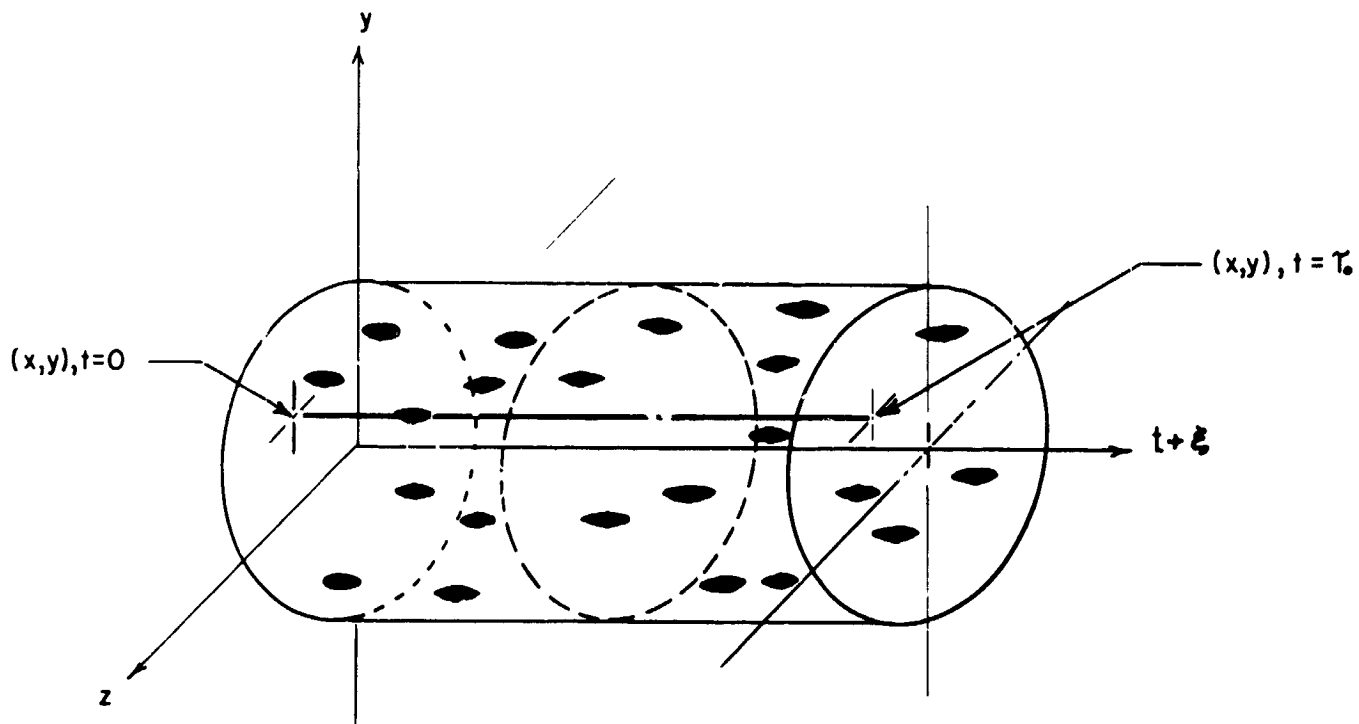
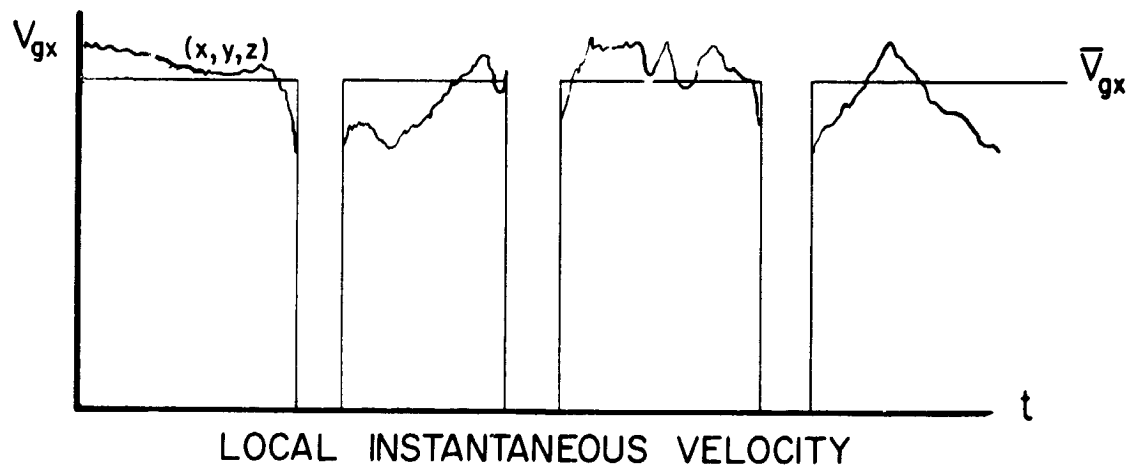


FORCES ON STATIC PARTICLE



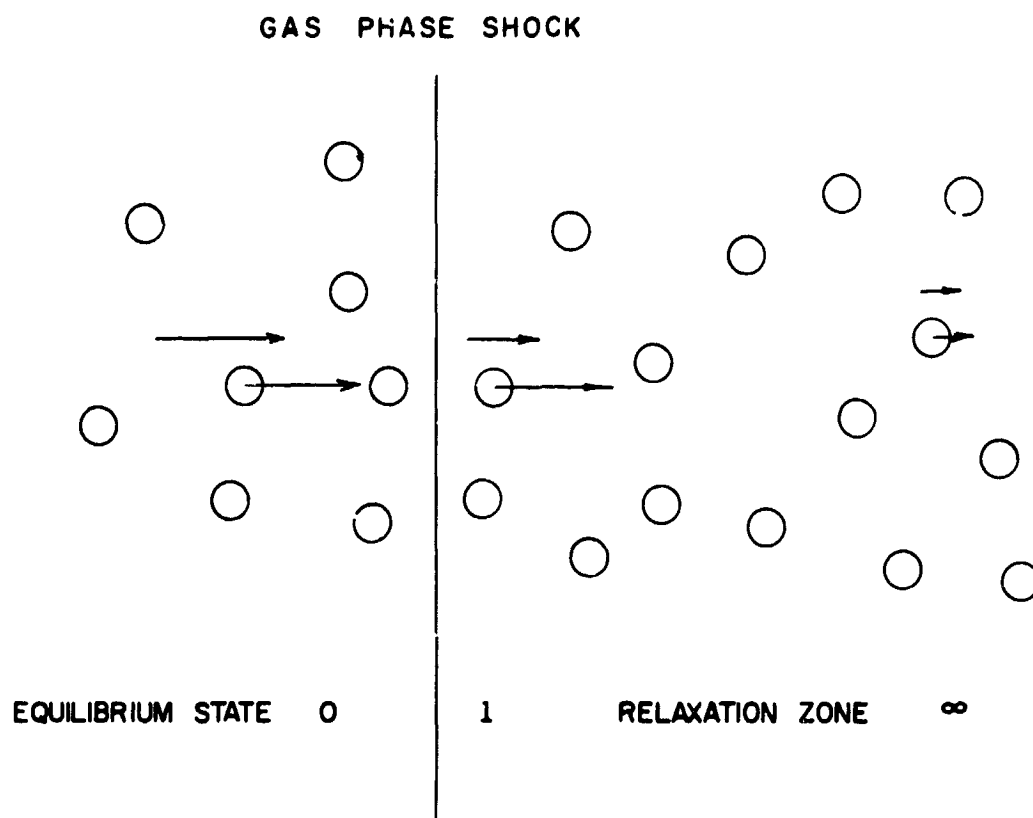


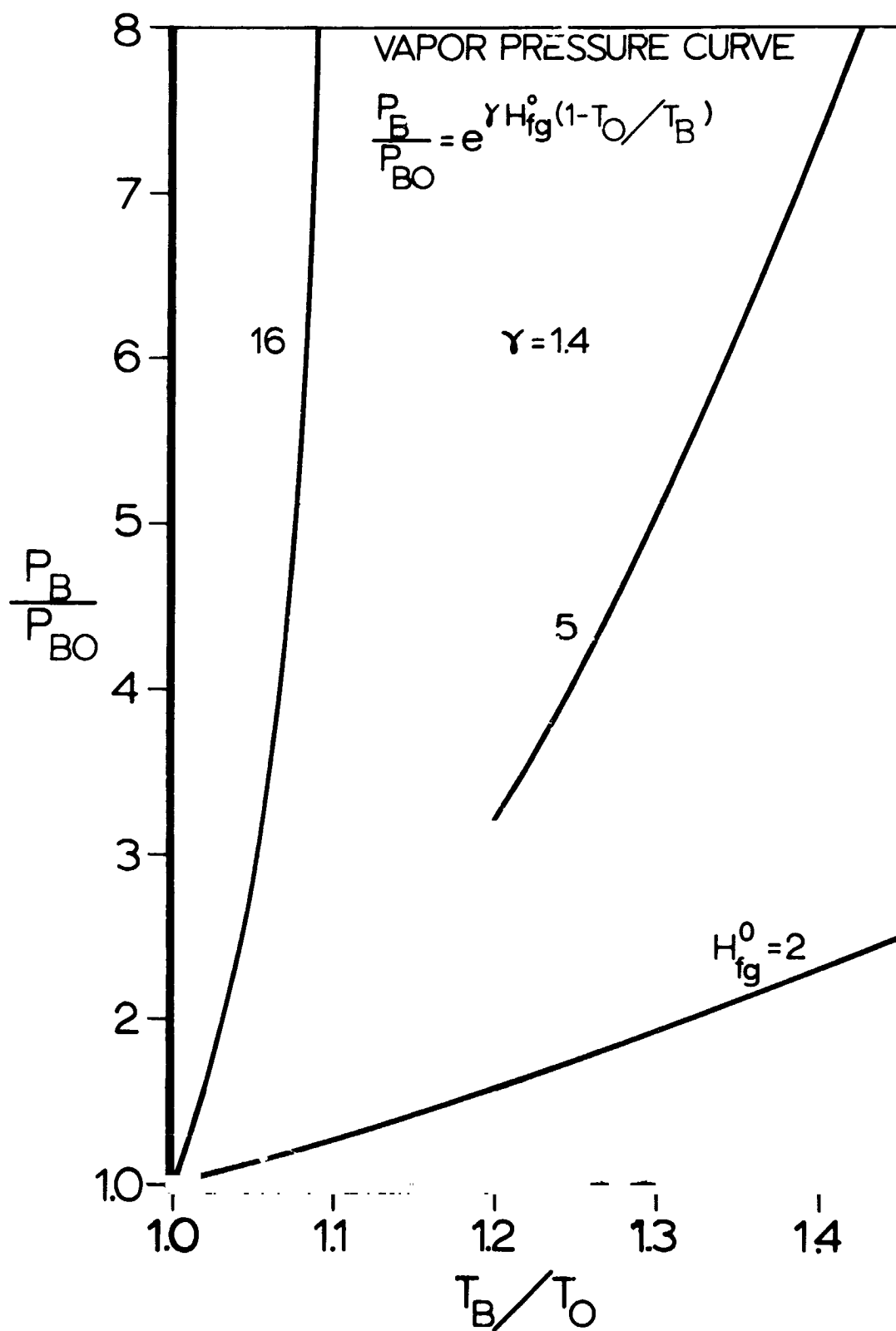
## TIME AVERAGES

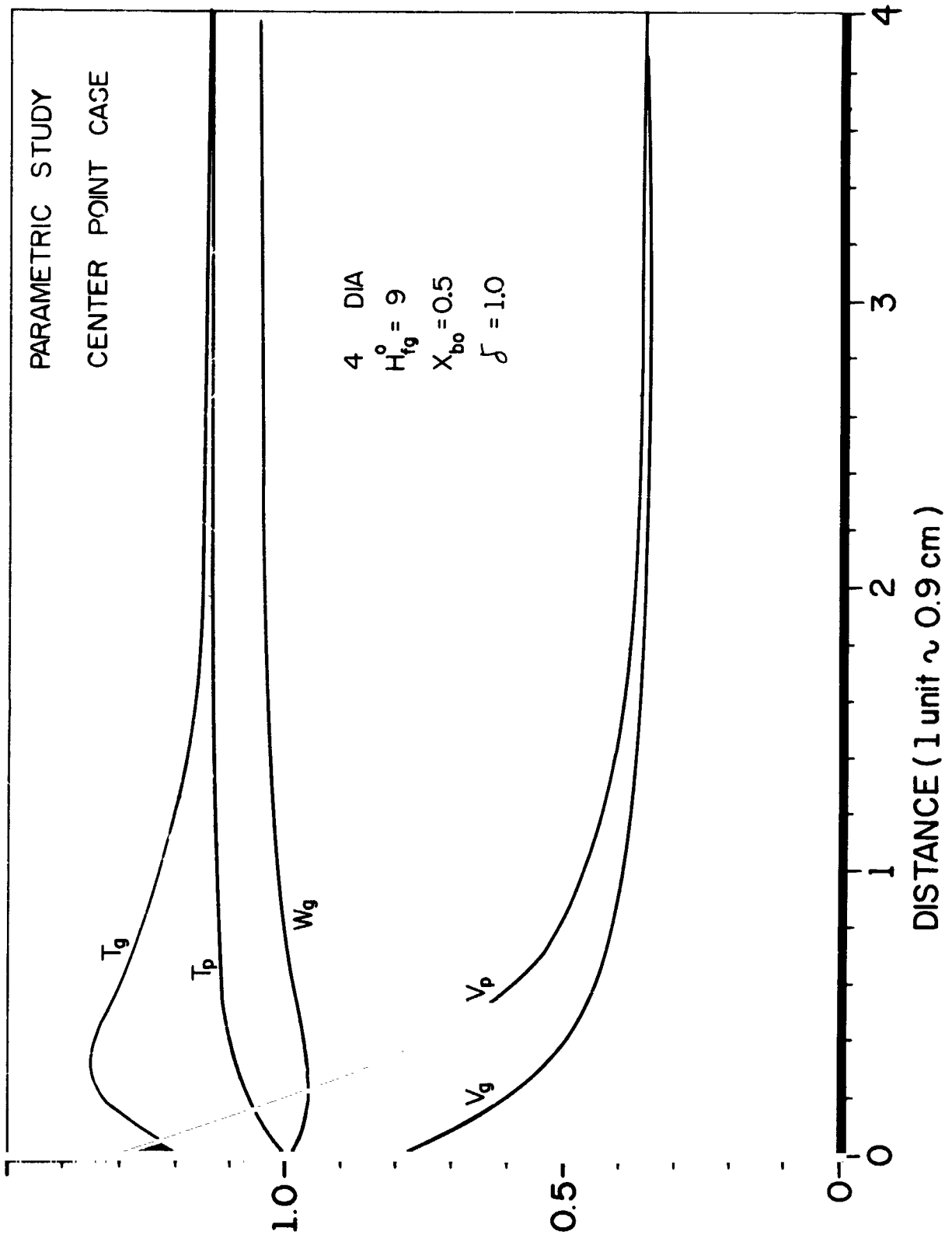


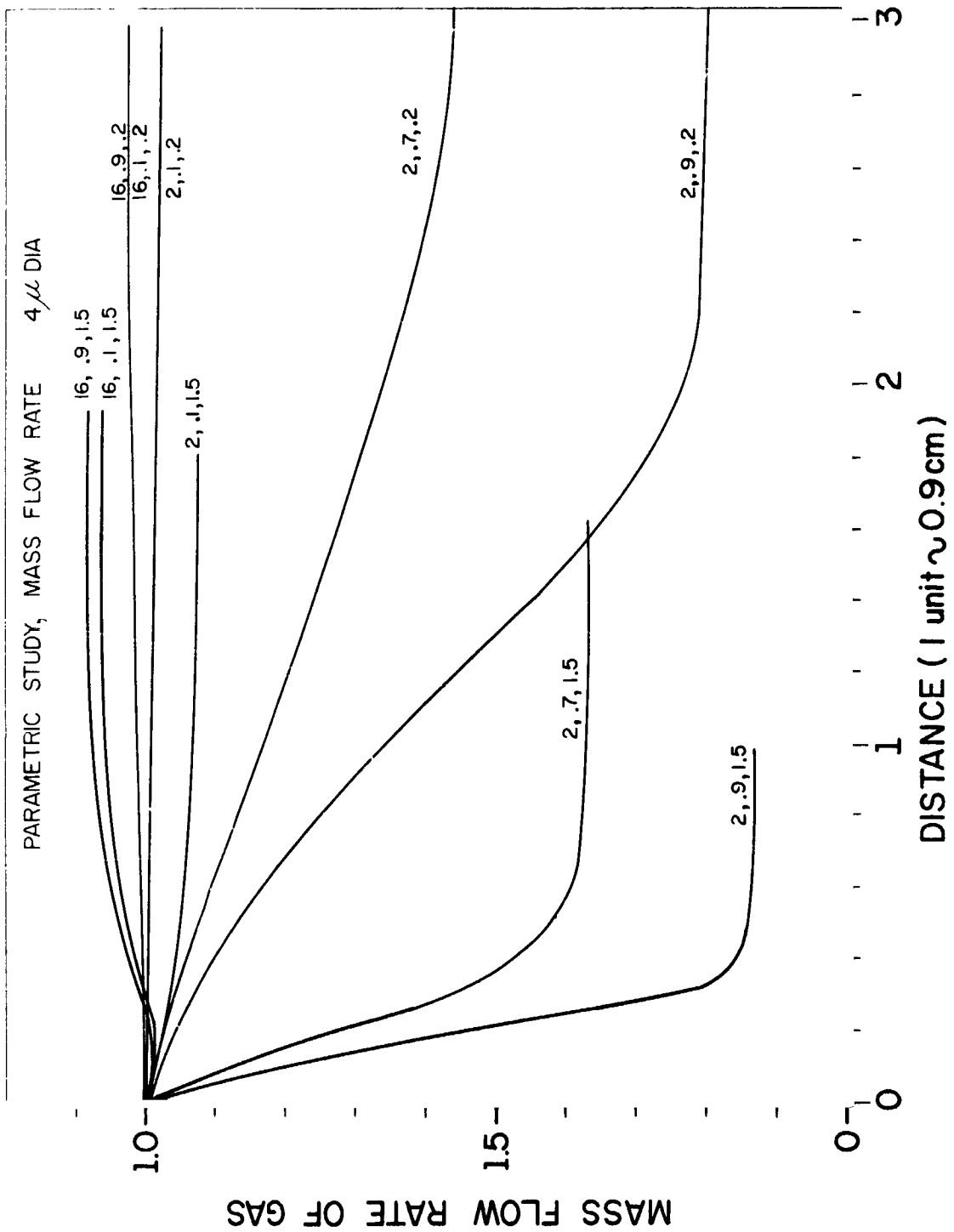
PARTICLE HISTORY AT A CROSS-SECTION

## TWO PHASE SHOCK STRUCTURE

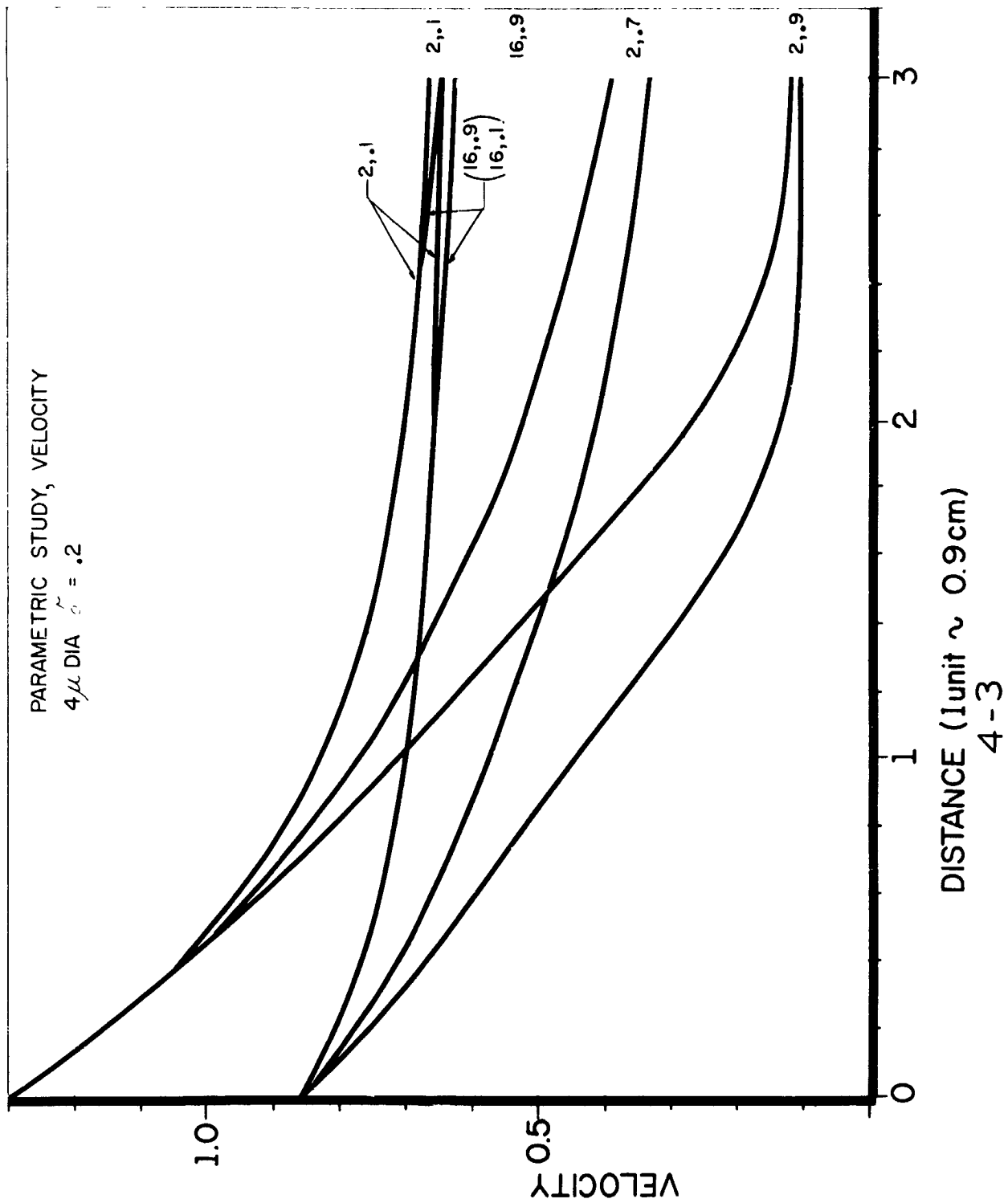


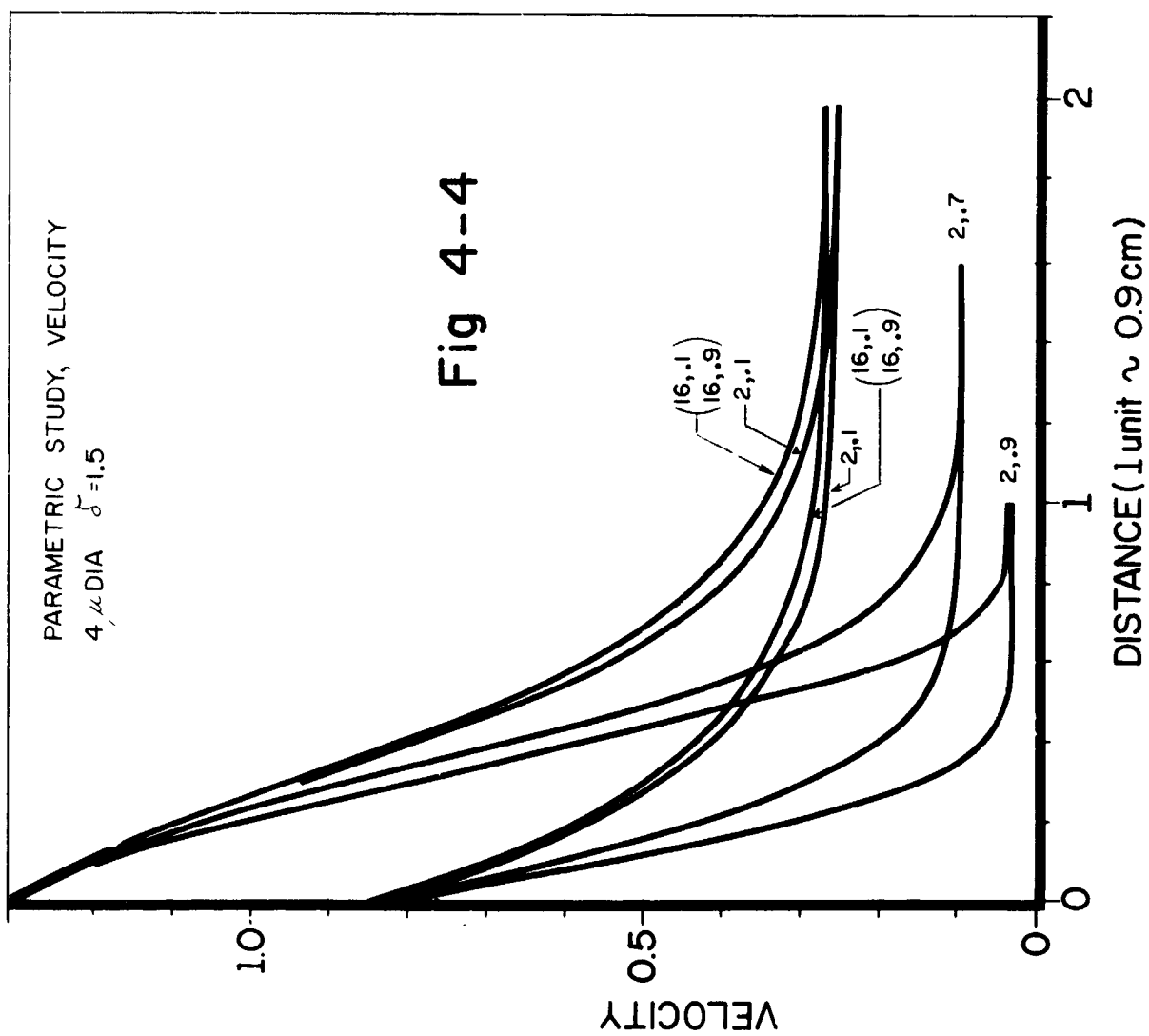




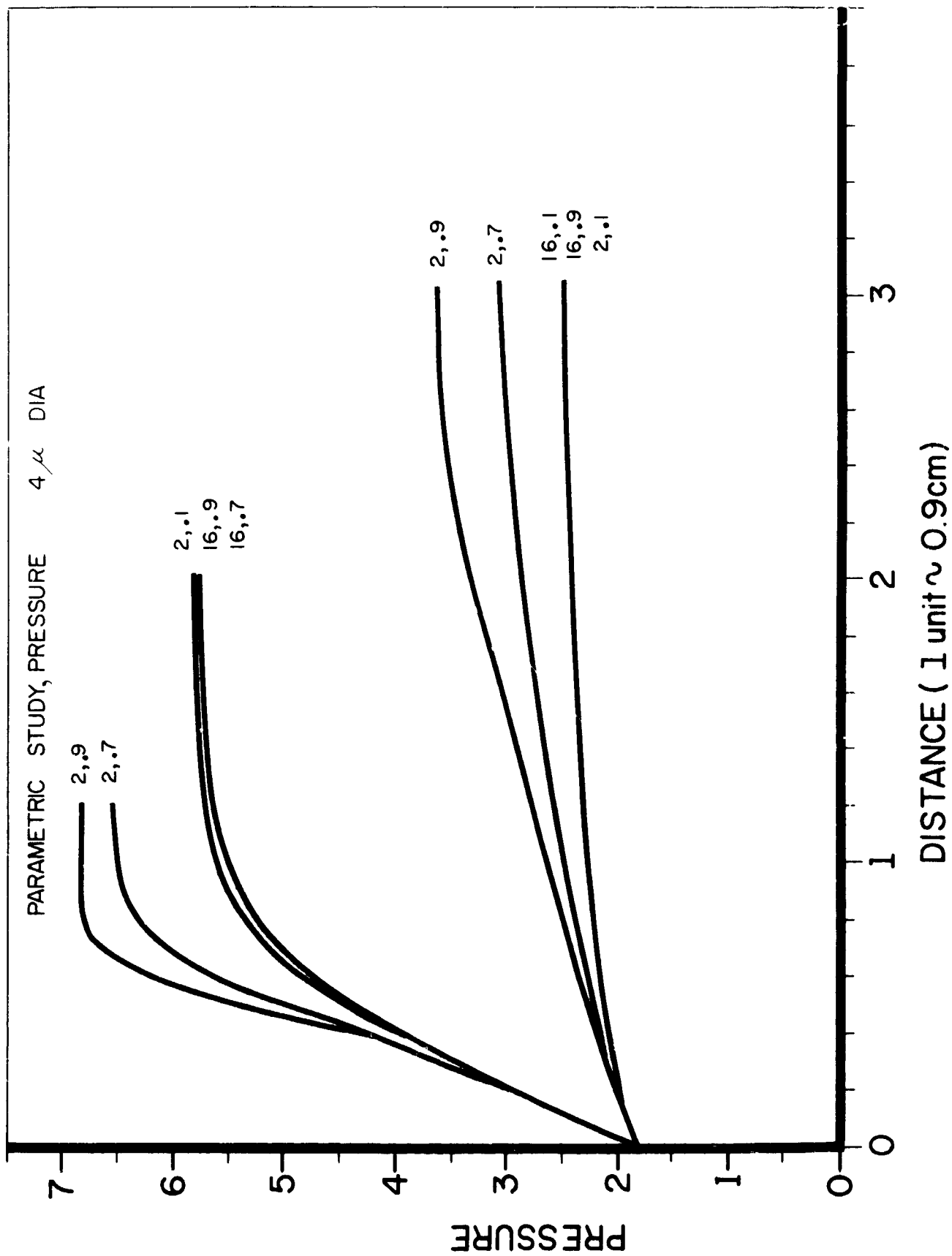


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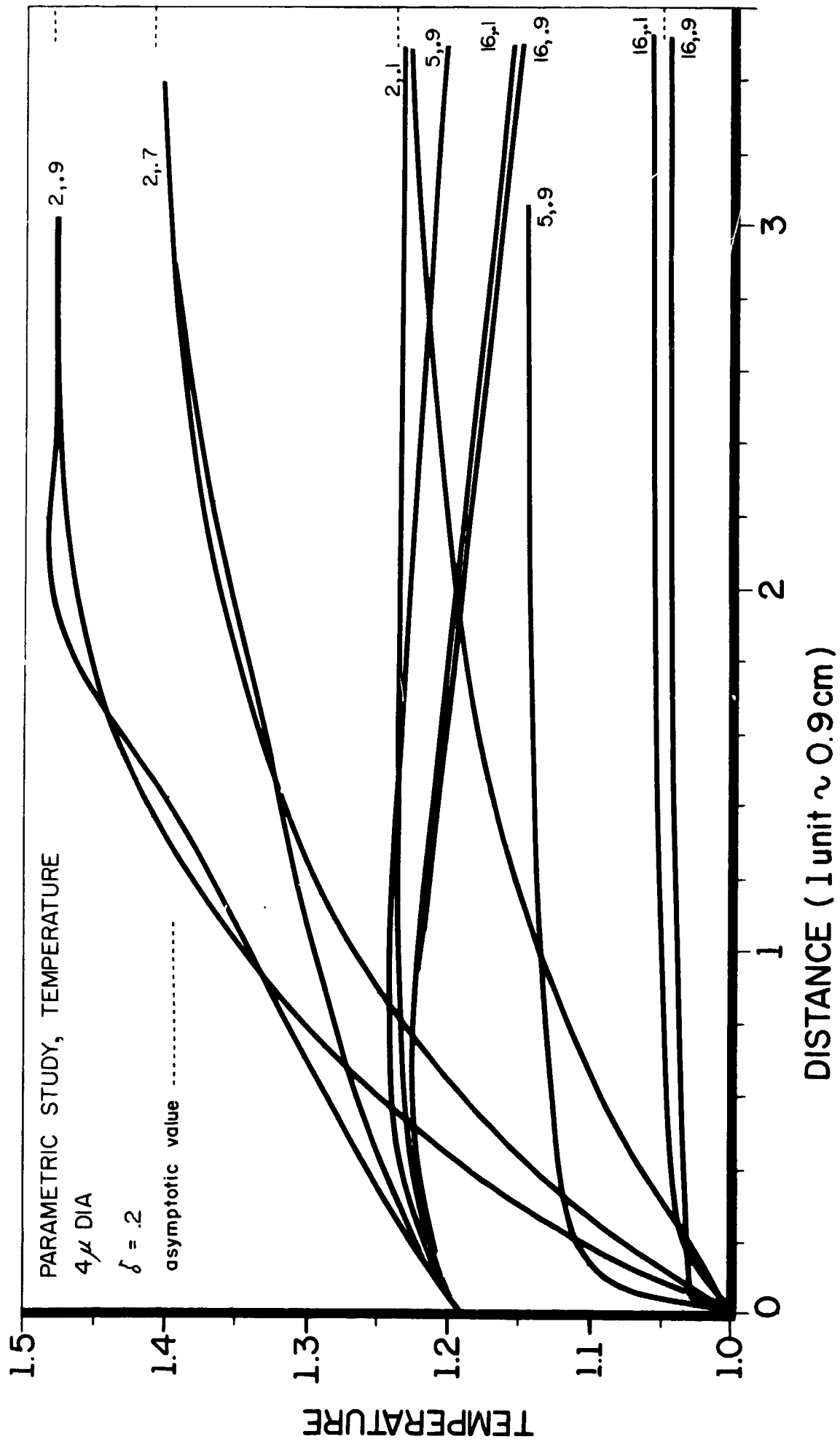


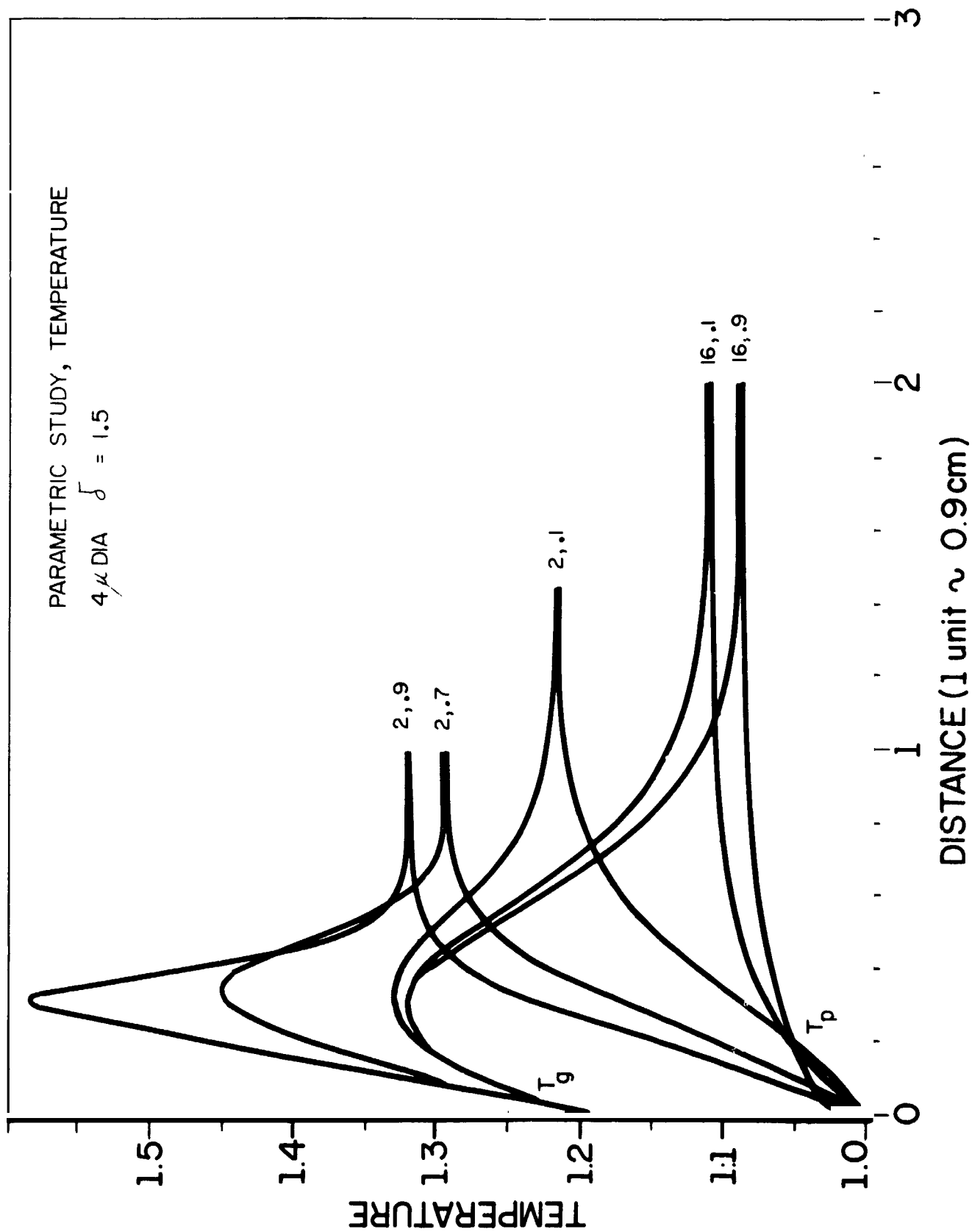


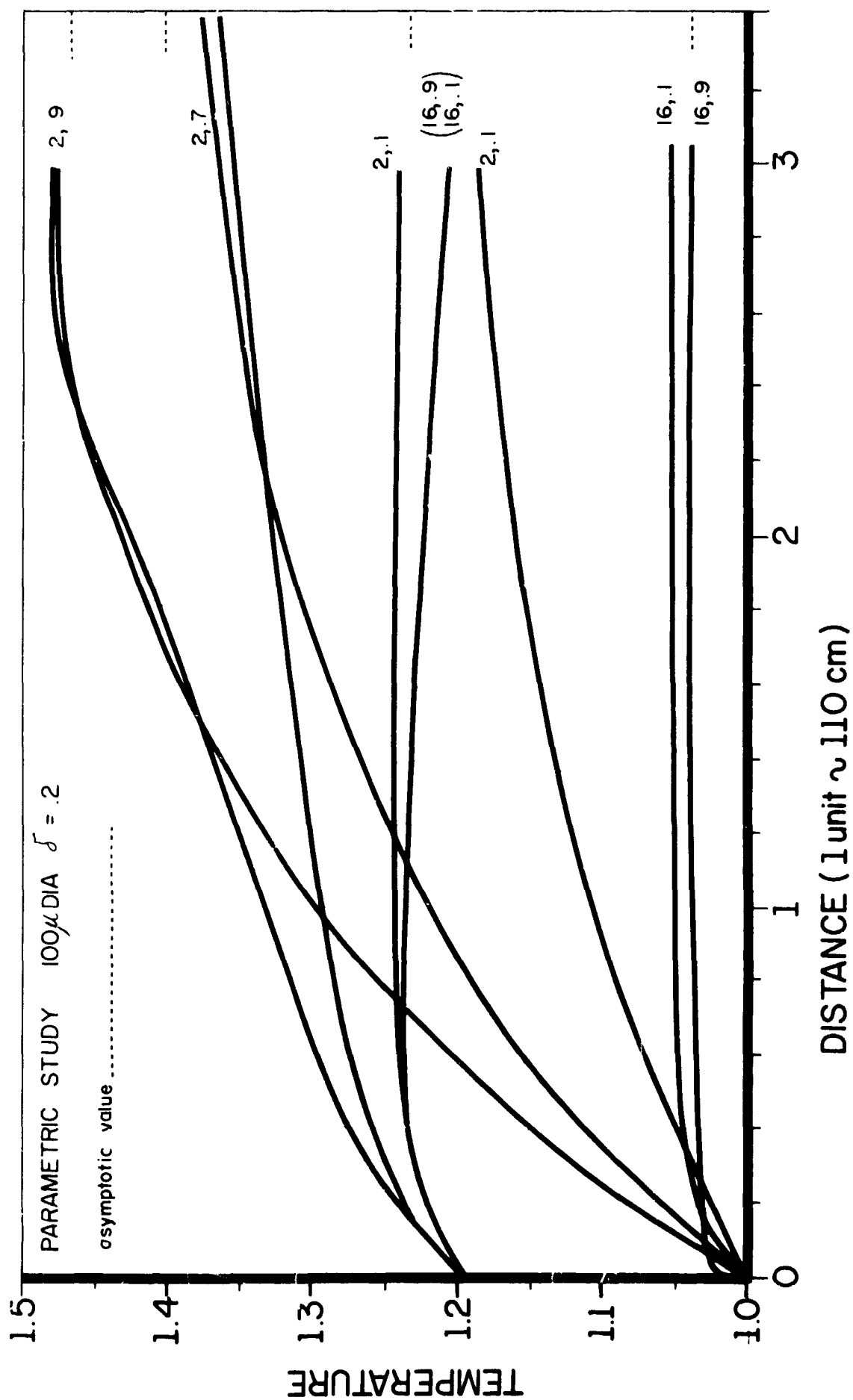
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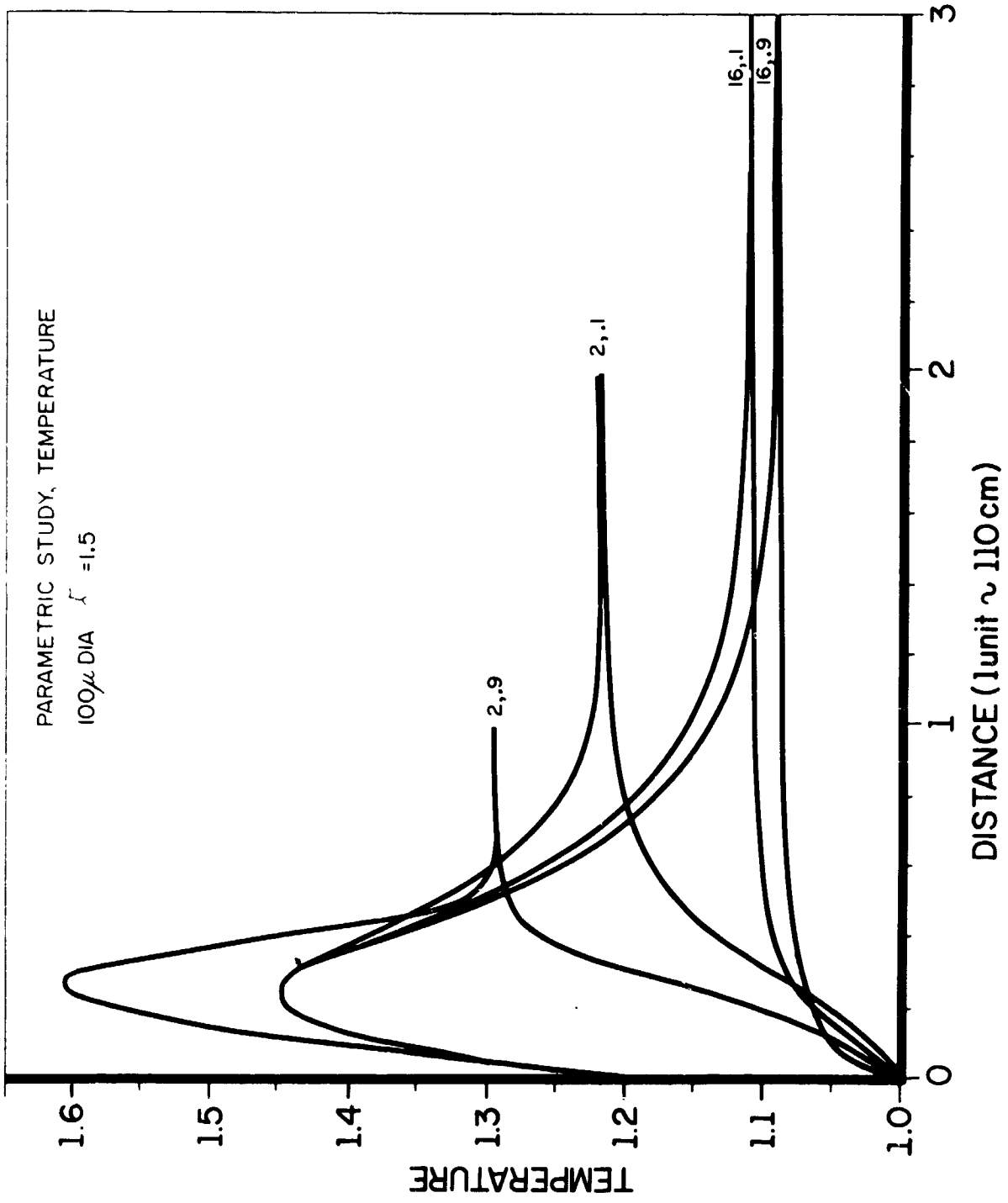


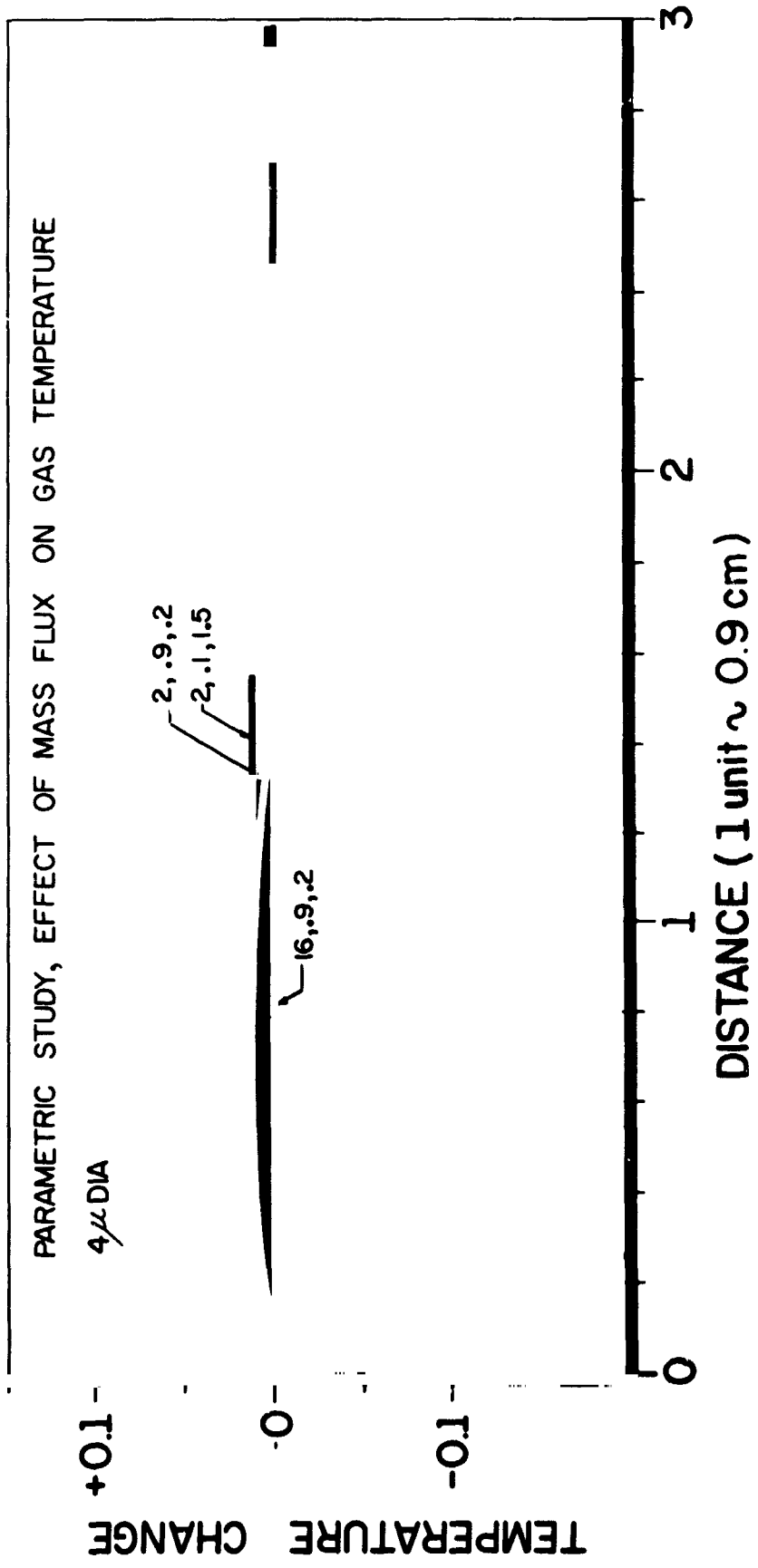




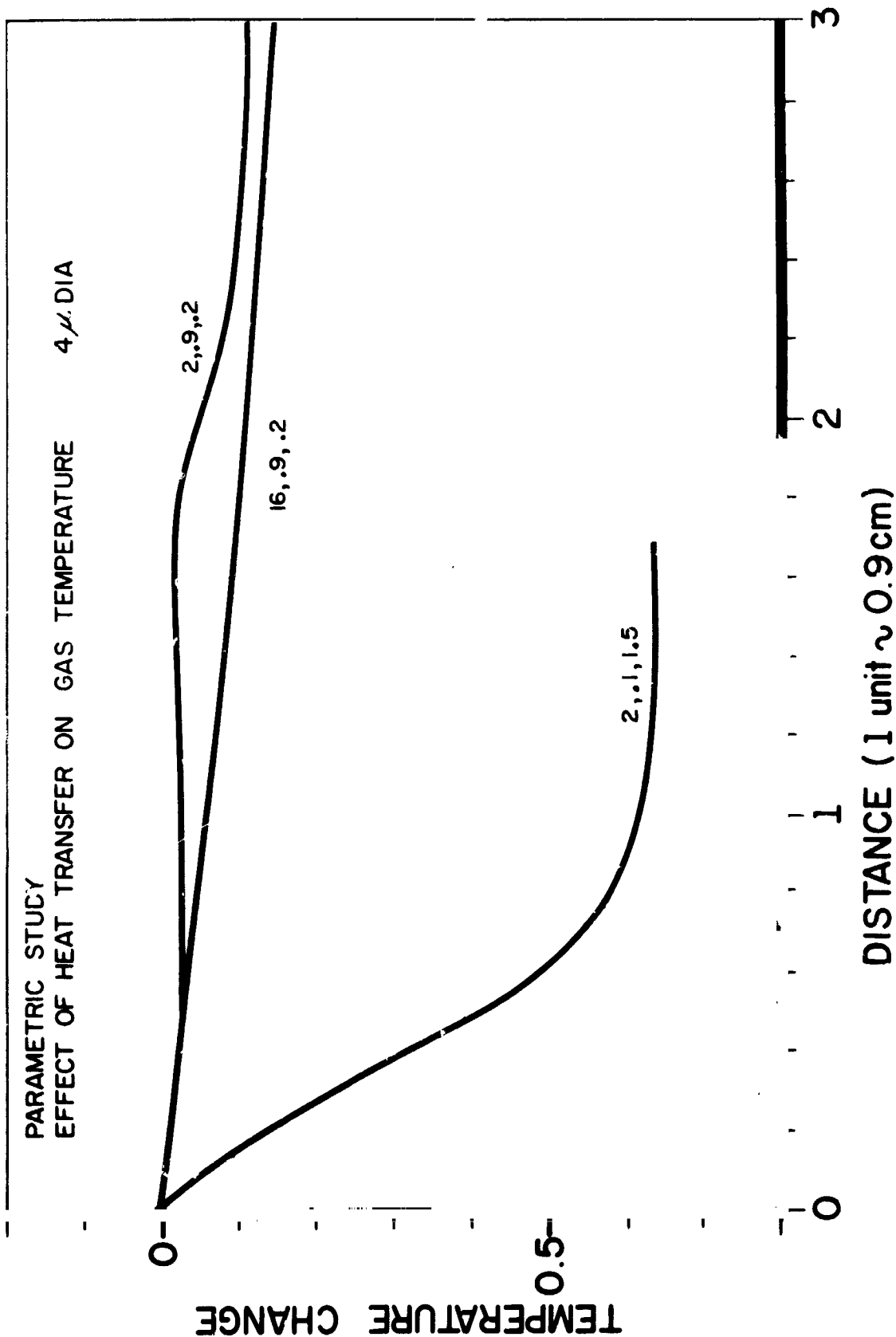


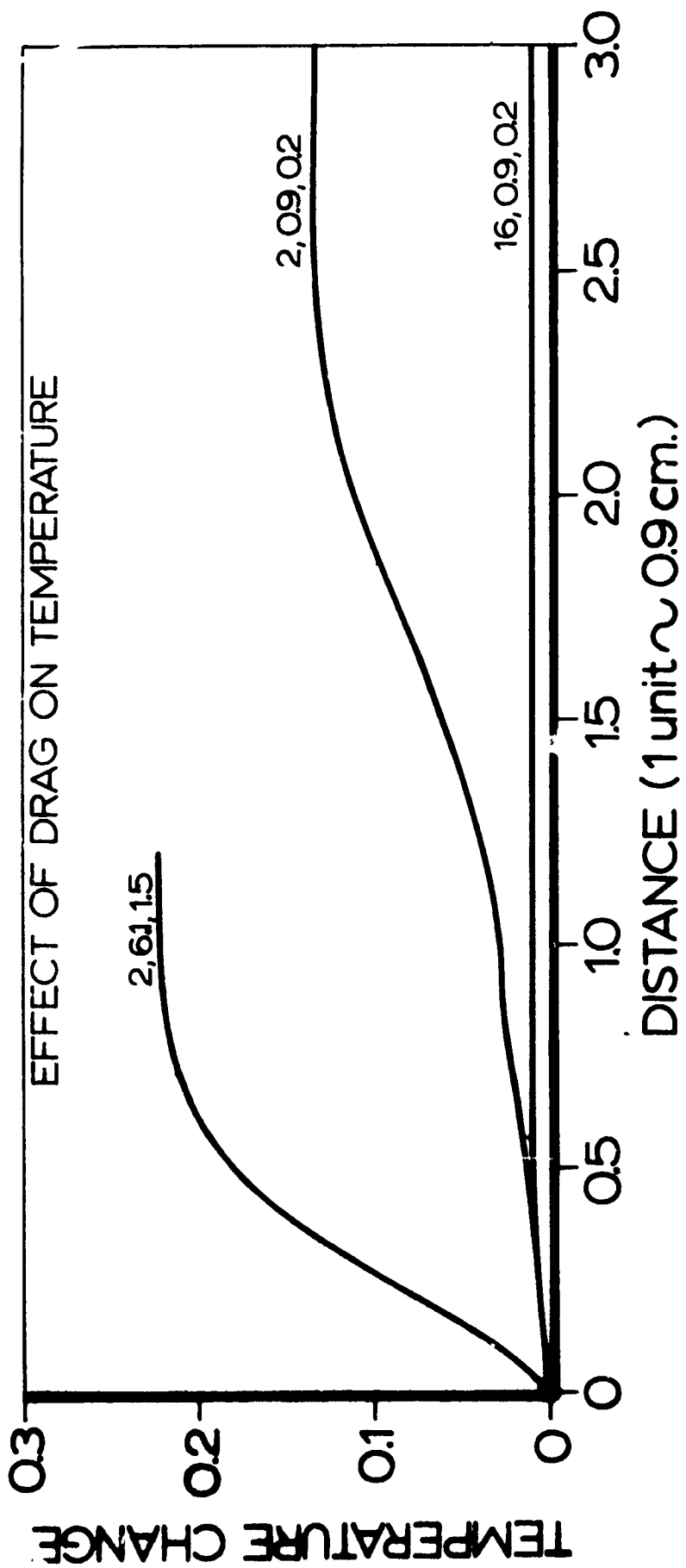




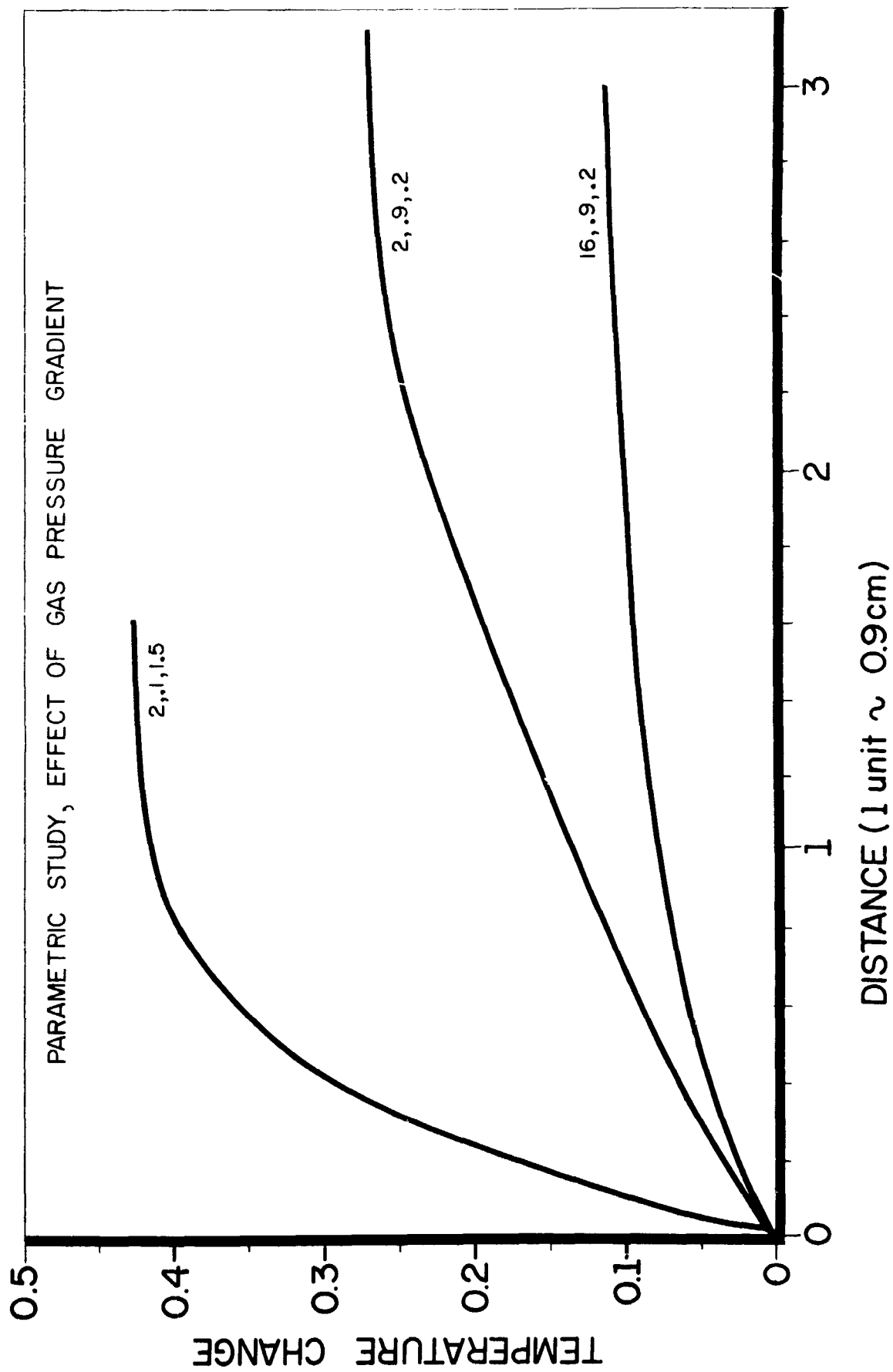


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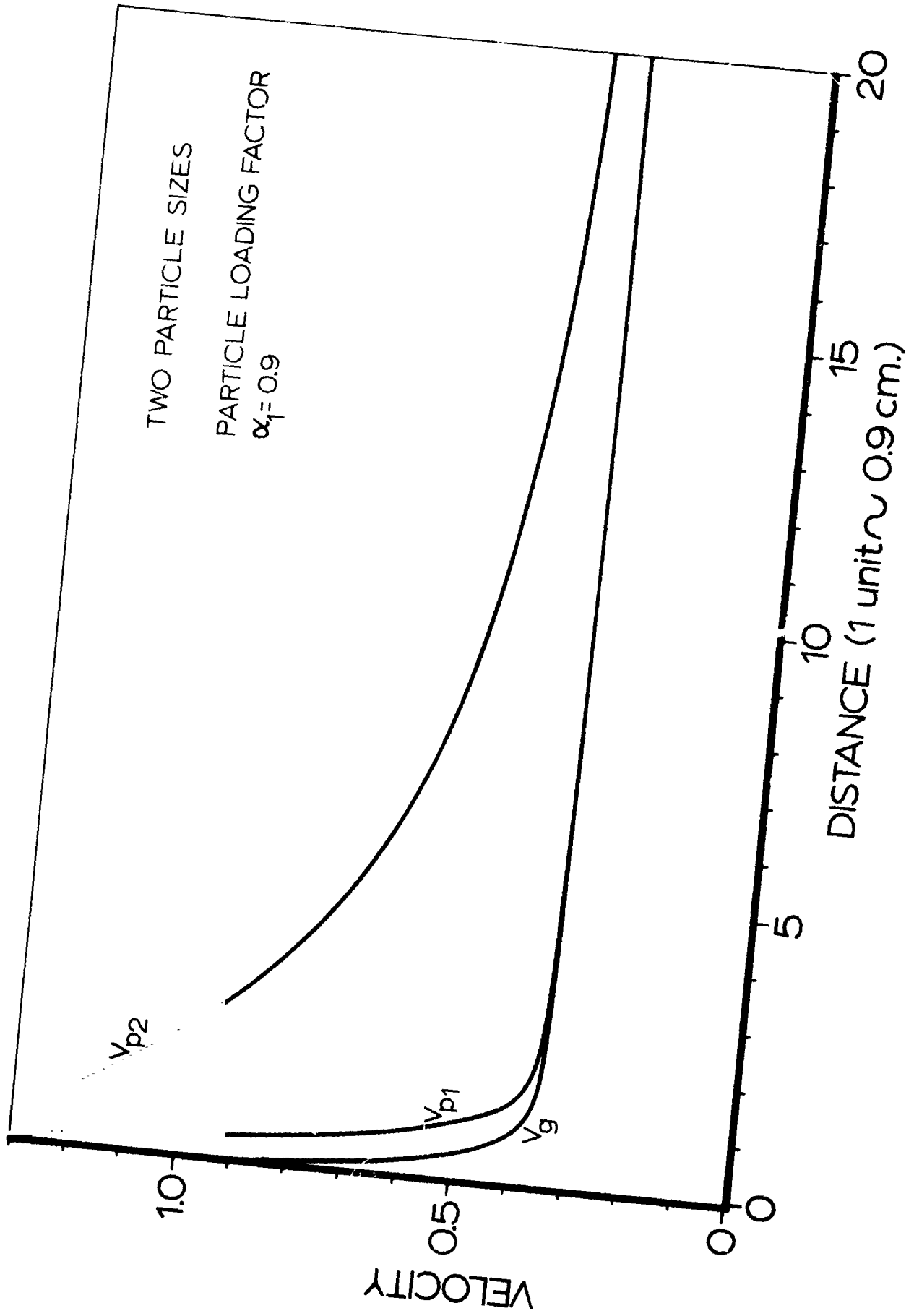




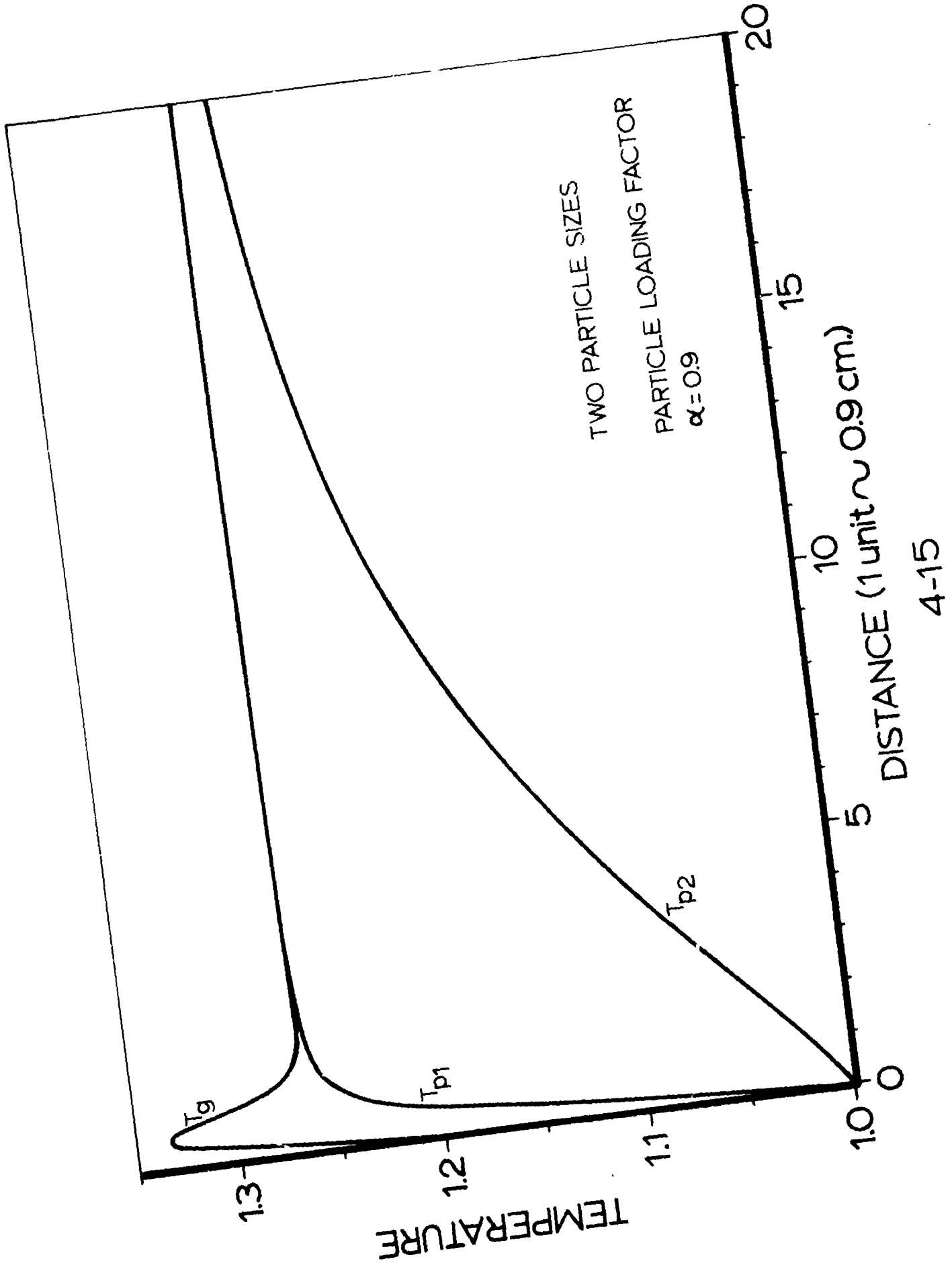
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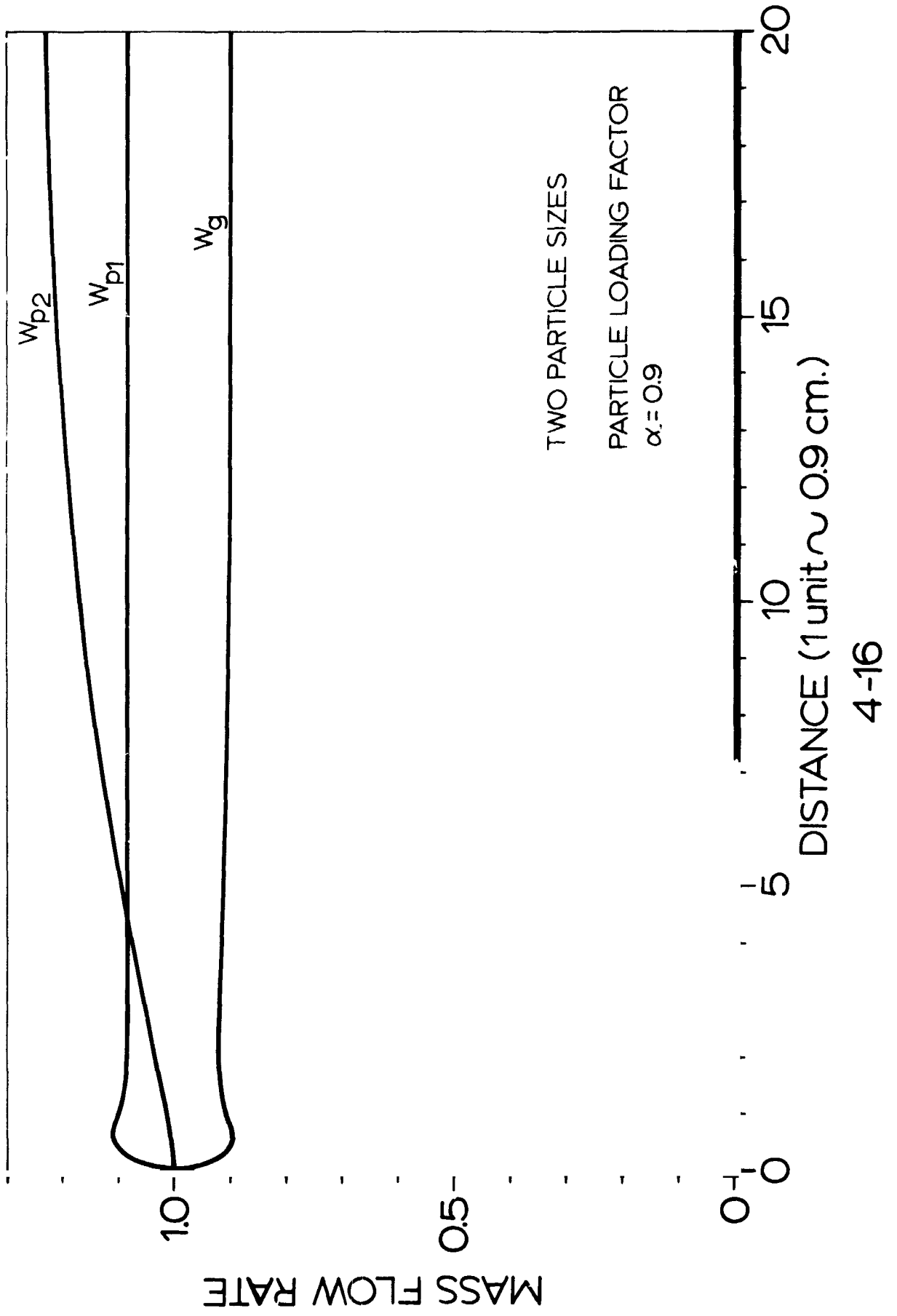


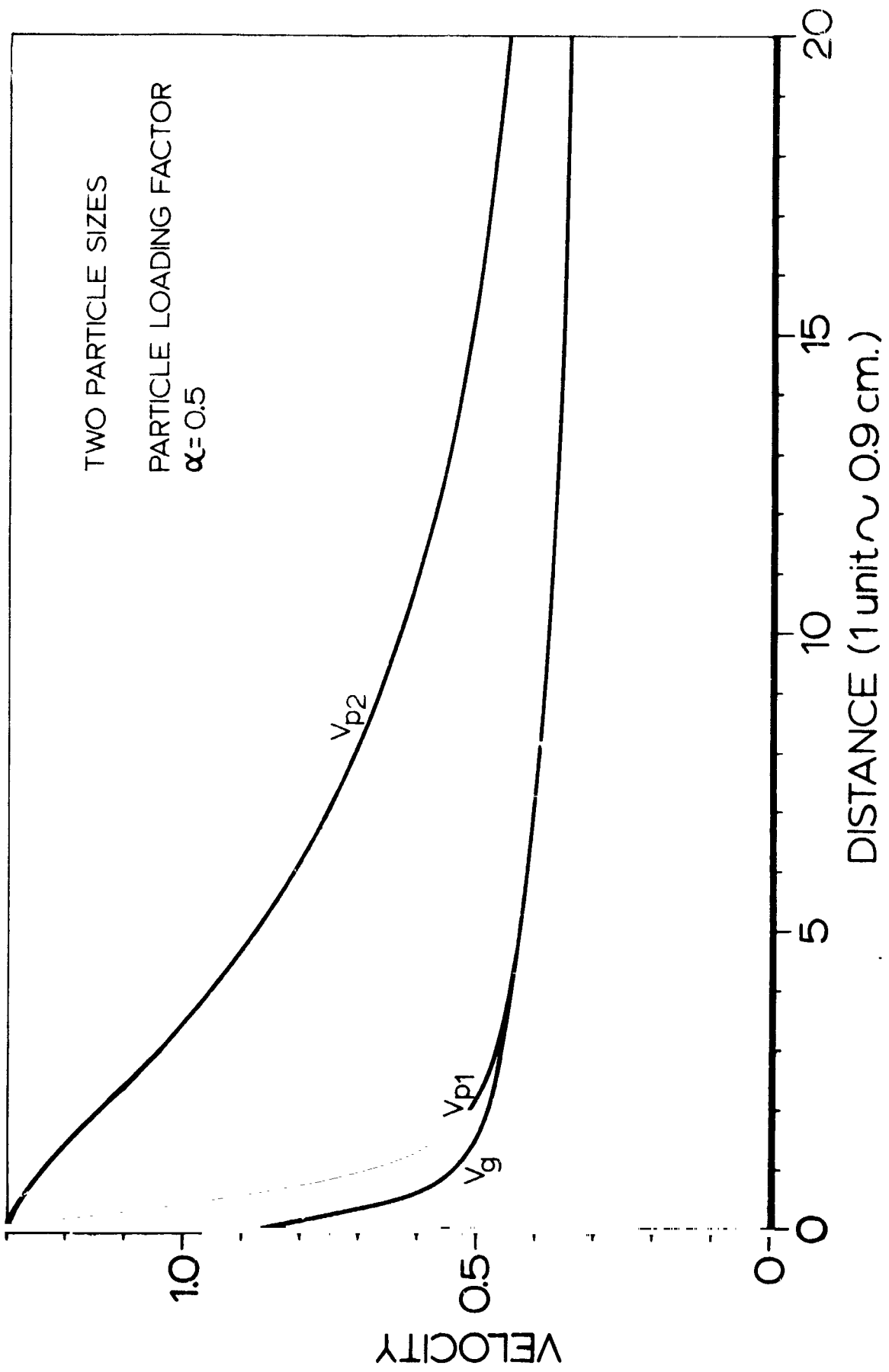


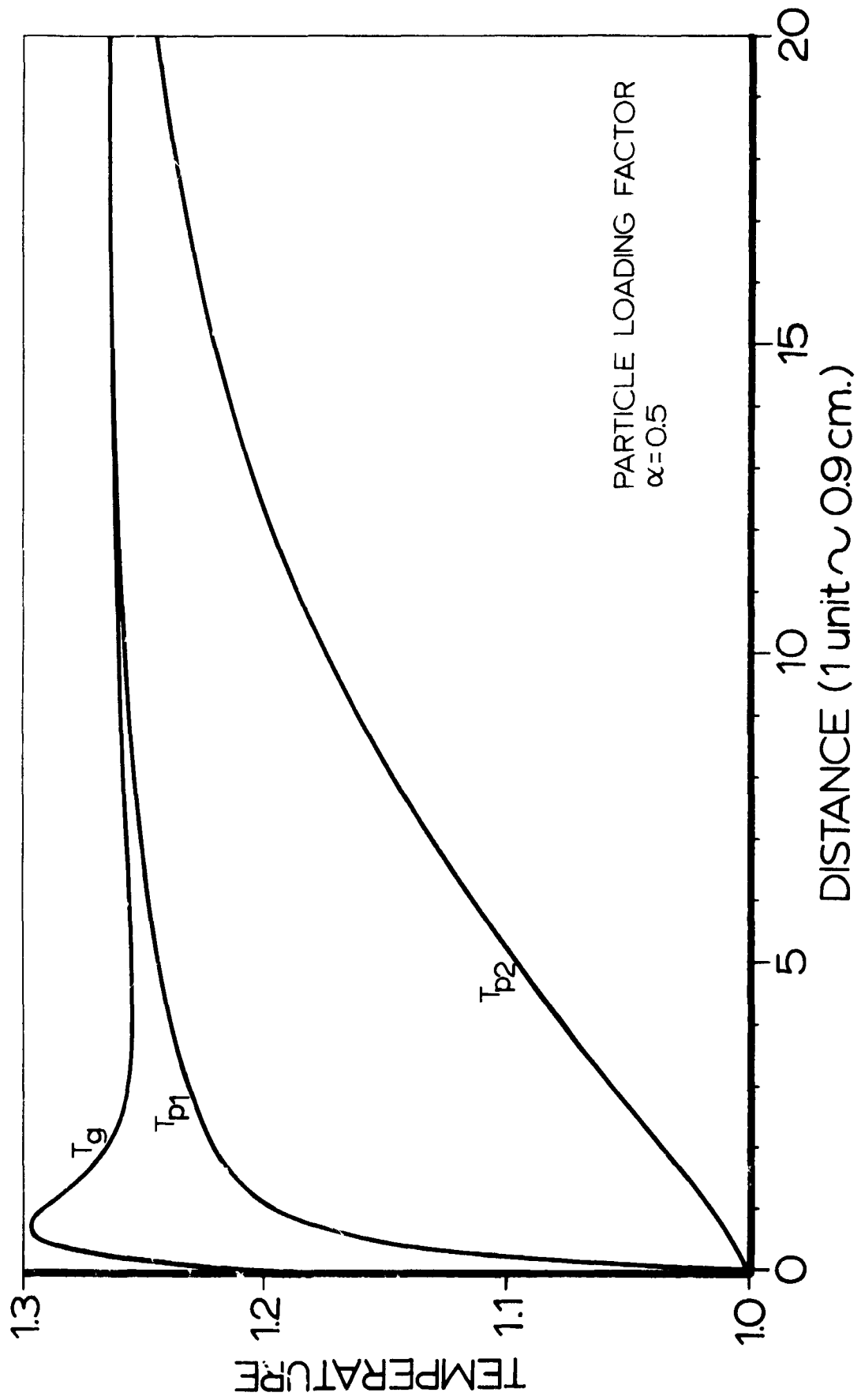


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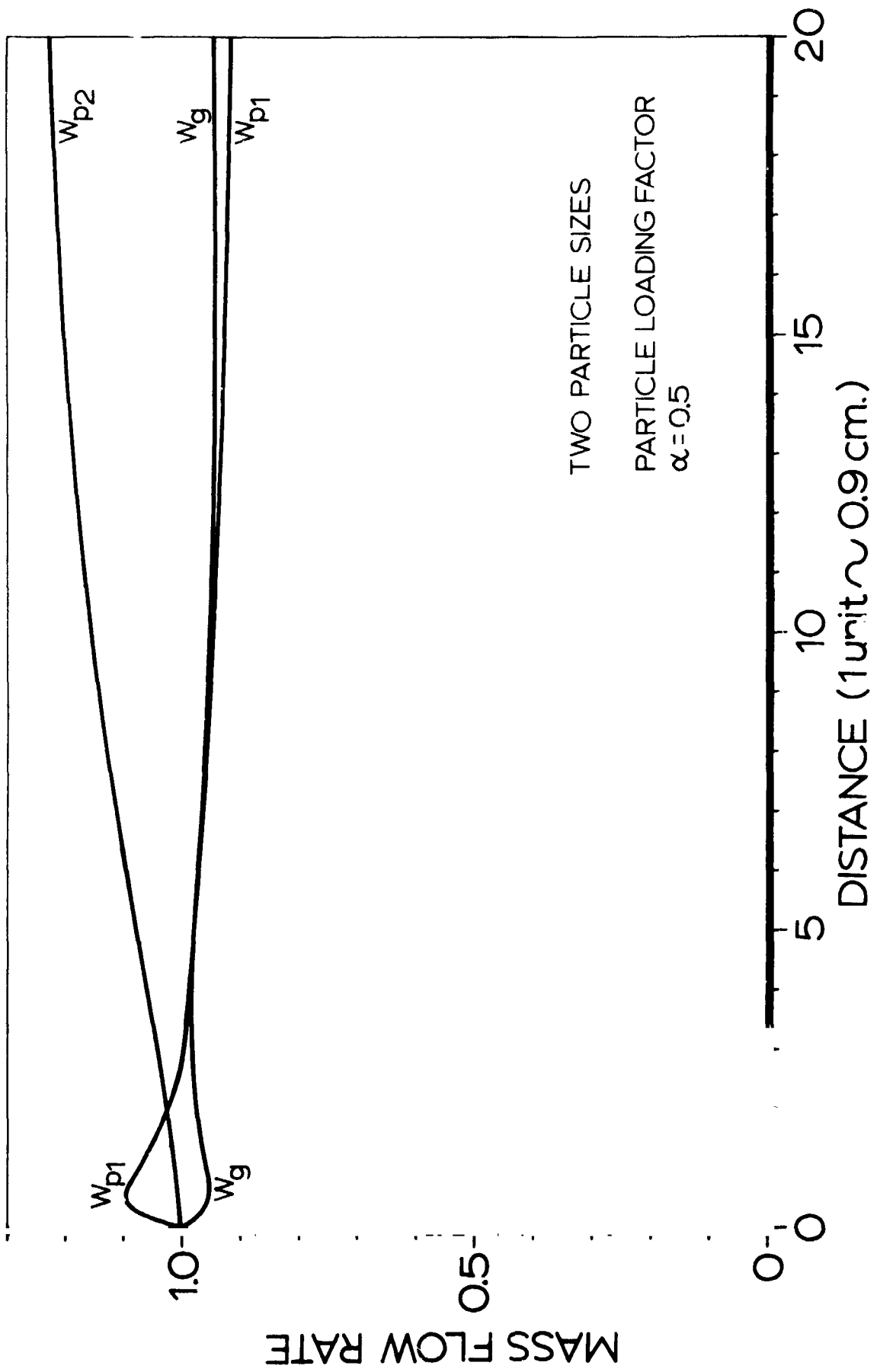




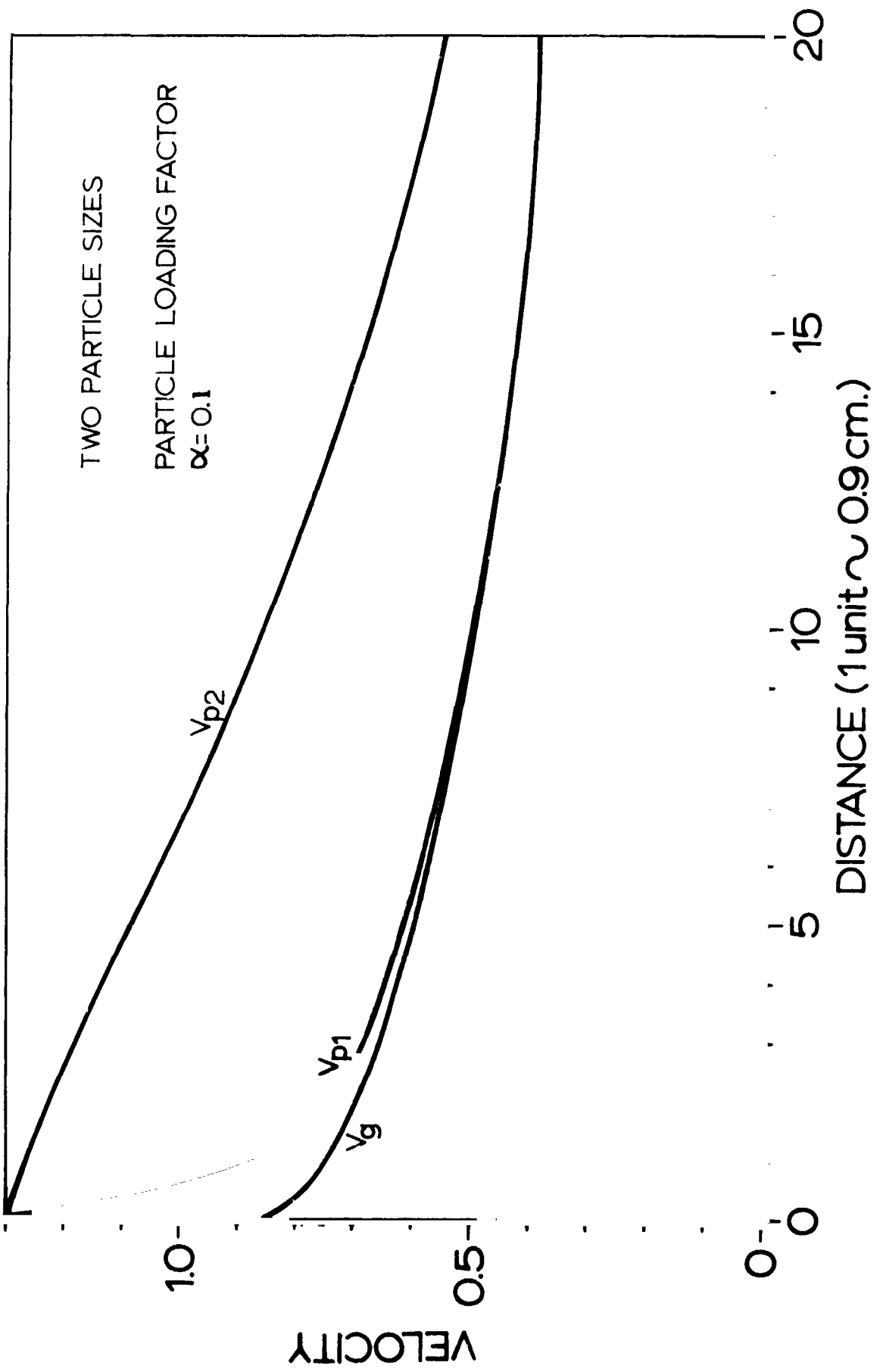


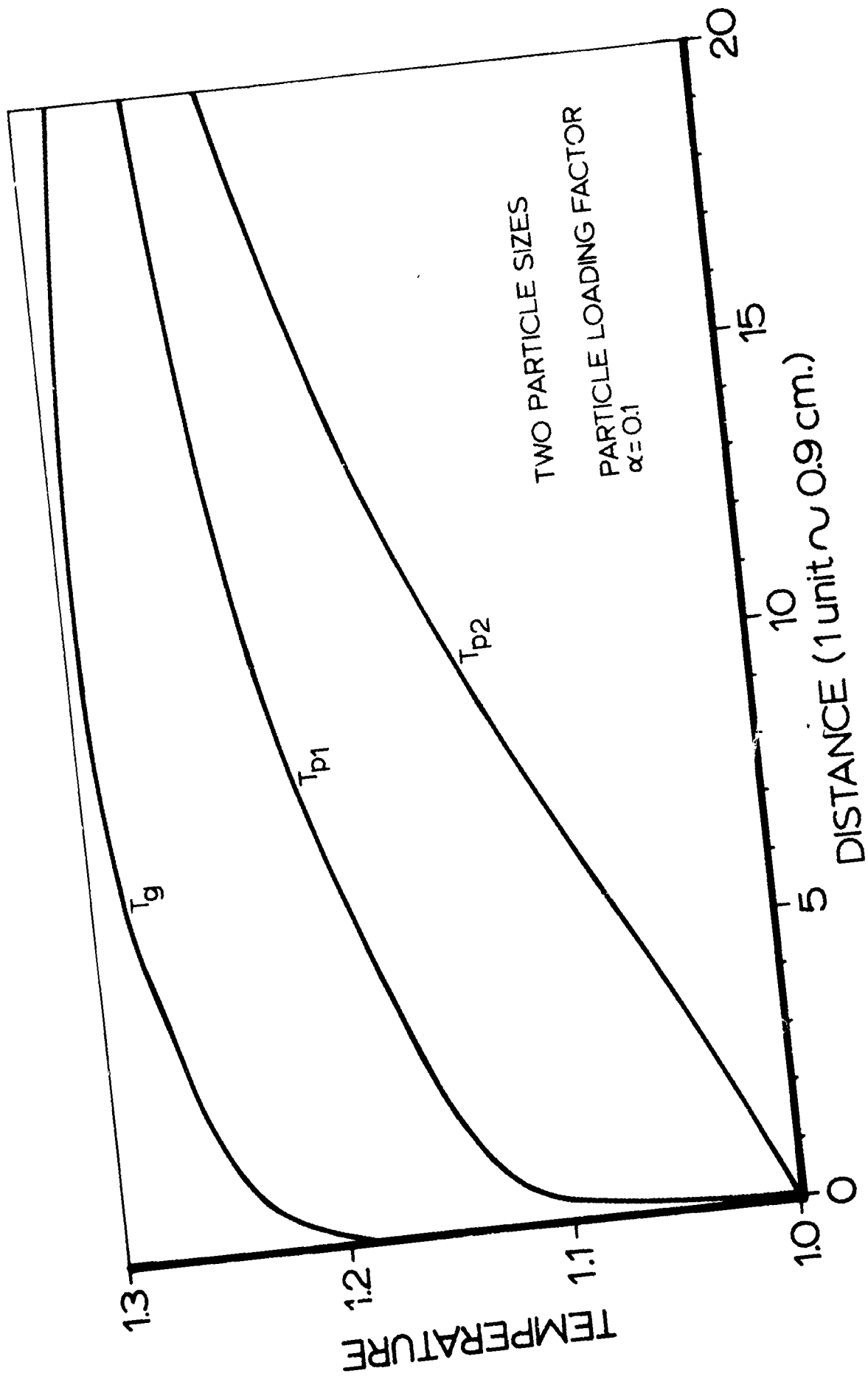


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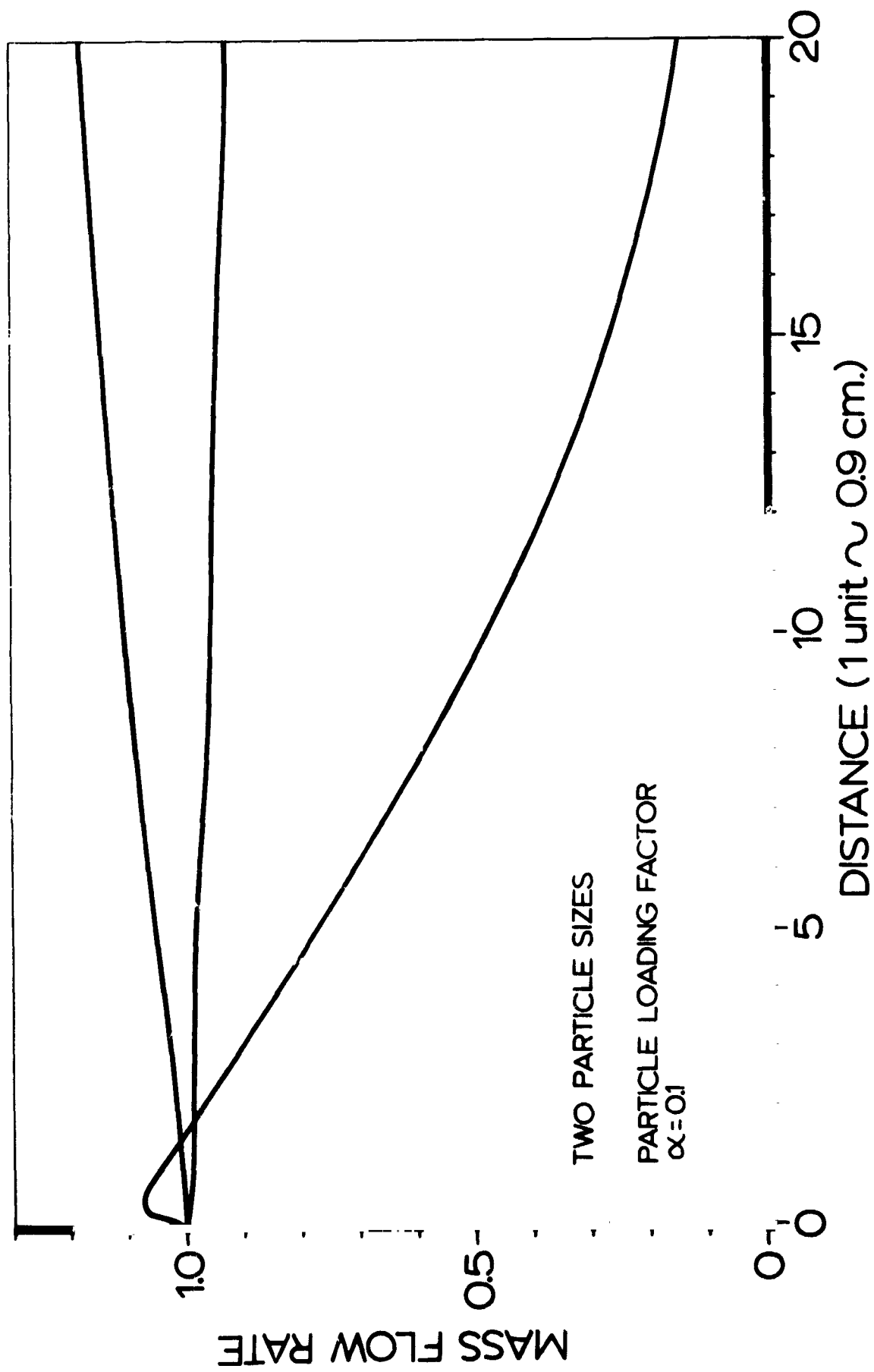


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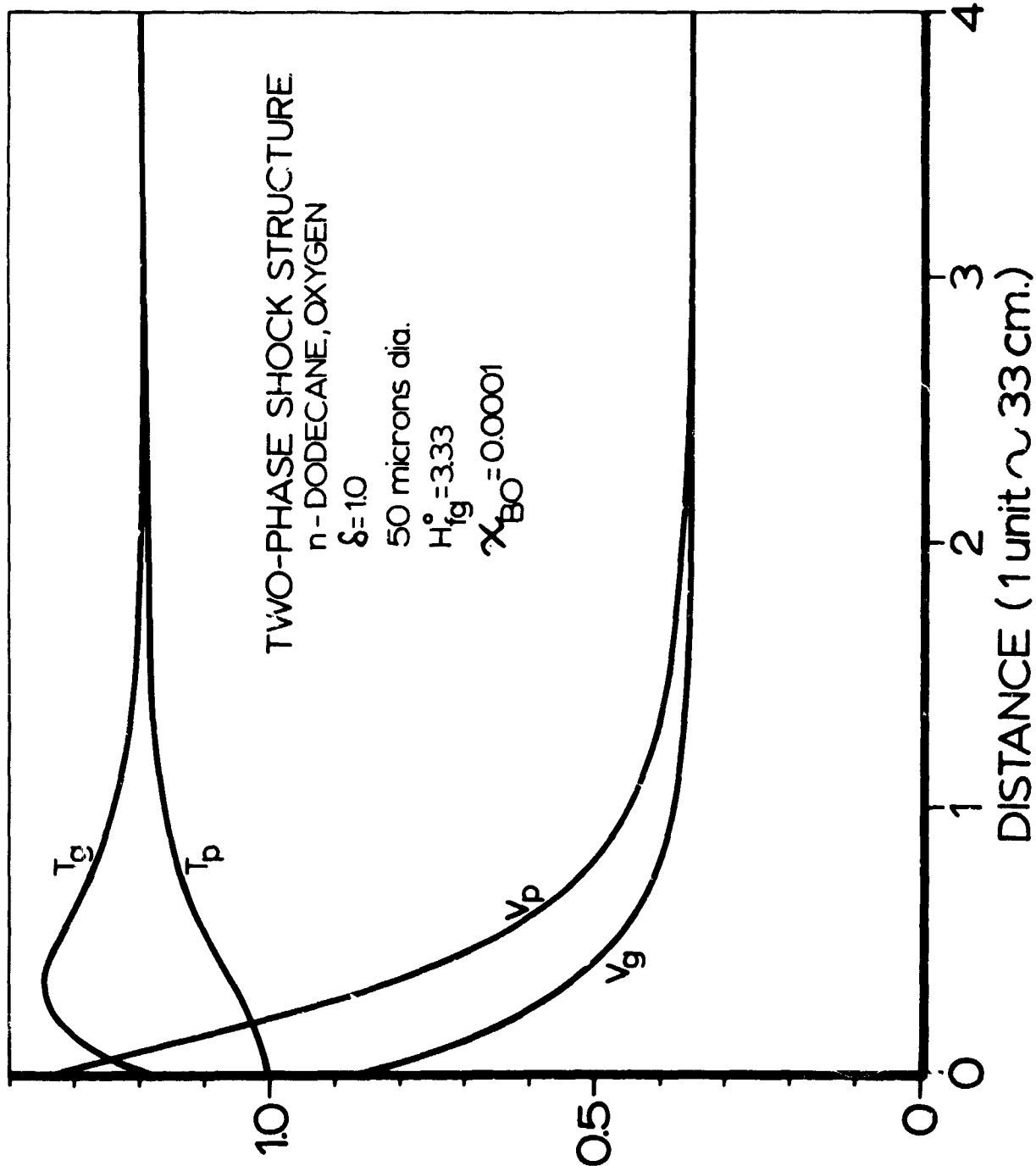








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## APPENDIX A

Proof Concerning Interphase Momentum  
Transport by Vaporization

In this appendix it will be proved that the integral over the particle surface of the mass flux times the  $x$ -component of the velocity is the same as the mass transfer function times the particle velocity:

$$\lim_{\Delta x \rightarrow 0} \frac{1}{\Delta x} \sum_i \int_{S_{pi}} \rho_g v_{gx} (\underline{v}_g - \underline{v}_s) \cdot \underline{n}_g dS = \langle v_x \rangle \Psi \quad (\text{A-1})$$

It will be assumed that the particles are all the same size; this assumption can be easily removed and is not essential to the proof.

Before the actual proof is given, it is desirable to digress in order to prove a lemma concerning the relationship of the liquid and particle velocities. The particle-phase velocity was defined by integrating the local liquid velocity across a cross-section of the particle. It will be assumed that the liquid velocity at the particle surface is constant and it will then be proved that for each particle  $i$ , the liquid surface velocity is equal to the average liquid velocity across any cross-section:

$$\langle v_{ax} \rangle_i = \frac{1}{A_{xi}} \int \underline{v}_a \cdot \underline{i} dS = \underline{v}_{ax \text{ SURFACE}} \quad (\text{A-2})$$

Figure A-1 shows the velocity vectors at a point on the particle surface. The liquid velocity  $\underline{v}_l$  and the gas velocity  $\underline{v}_g$  are different from the surface velocity  $\underline{v}_s$  because of vaporization.

The vaporization (or condensation) causes normal components

$\underline{v}_{ln}$  and  $\underline{v}_{gn}$ . Also shown in Figure A-1 is a spherical cap formed by a plane intersecting the particle. The areas are denoted by  $A_{\chi_i}$  and  $A_z$ .

First it is assumed that the liquid is incompressible. Then from the continuity equation:

$$\nabla \cdot \underline{v}_l = 0$$

Thus Gauss's theorem may be applied to the integral over the volume:

$$0 = \int \nabla \cdot \underline{v}_l \, dV = \int \underline{n} \cdot \underline{v}_l \, dS$$

(A-3)

$$0 = \int_{A_{\chi_i}} \underline{n} \cdot \underline{v}_l \, dS + \int_{A_z} \underline{n} \cdot \underline{v}_l \, dS$$

The velocity of the liquid is assumed constant over the surface of the particle. This implies that the particles are moving in translation motion without distorting. Next, the integral over the spherical cap is explicitly written out:

$$-\int_{A_{xi}} \underline{n} \cdot \underline{v}_e dS = v_{exs} \int_{A_2} n_x dS + v_{eyz} \int_{A_2} n_y dS + v_{ezs} \int_{A_2} n_z dS \quad (A-4)$$

Because the surface  $A_2$  has symmetry about the  $x$ -axis, the last two integrals are zero. Thus for a single particle  $i$ , we have

$$\langle v_{ex} \rangle = \frac{1}{A_{xi}} \int_{A_{xi}} \underline{i} \cdot \underline{v}_e dS = -\frac{1}{A_{xi}} \int_{A_{xi}} \underline{n} \cdot \underline{v}_e dS = (v_{exs})_i \quad (A-5)$$

Now, returning to the original problem, consider

$$\sum_i \int_{S_{pi}} \rho_g v_{gx} (\underline{v}_g - \underline{v}_s) \cdot \underline{n}_g dS \quad (A-6)$$

The mass flux due to vaporization is constant over the surface, i.e.,

$$\begin{aligned} \rho_g (\underline{v}_g - \underline{v}_s) \cdot \underline{n}_g &= \rho_e (\underline{v}_e - \underline{v}_s) \cdot \underline{n}_e = \text{constant} \\ &= \psi_i \end{aligned} \quad (A-7)$$

Also it is noted that the gas and liquid velocities at the surface obey the following (see Fig. A-1):

$$\underline{v}_g = \underline{v}_e + \underline{v}_{gn} - \underline{v}_{en} \quad (\text{A-8})$$

Substituting these relations gives

$$\begin{aligned} \sum_i \int_{S_{pi}} \rho_g v_{gx} (\underline{v}_g - \underline{v}_s) \cdot \underline{n}_g dS \\ = \sum_i \psi_i \int_{S_{pi}} [v_{ex} + (\underline{v}_{gn} - \underline{v}_{en})_x] dS \end{aligned} \quad (\text{A-9})$$

The uniform vaporization assumption implies that the magnitude of  $\underline{v}_{gn} - \underline{v}_{en}$  is constant over the particle surface. The integral of the  $x$ -component of such a normal vector over a closed surface is zero. Now the equation is

$$\begin{aligned} \sum_i \int_{S_{pi}} \rho_g v_{gx} (\underline{v}_g - \underline{v}_s) \cdot \underline{n}_g dS &= \sum_i \psi_i (v_{exs})_i \int_{S_{pi}} dS \\ &= \sum_i \psi_i (v_{exs})_i A_{Si} \end{aligned} \quad (\text{A-10})$$

On the right-hand side are the product of the vaporization flux, the liquid surface velocity, and the particle surface area summed over all the particles. Refer now to Figure A-1 which shows a section of the flow between  $x$  and  $x + \Delta x$ . Let several planes  $a, b, c, \dots$  partition this region so that all the particles are intersected. Then the sum is split up into a separate term at each partition:

$$\begin{aligned} \sum_i \Psi_i (v_{2xs})_i A_{si} &= \sum_{ia} \Psi_i (v_{2xs})_i A_{si} \\ &+ \sum_{ib} \Psi_i (v_{2xs})_i A_{si} \\ &+ \sum_{ic} \quad + \dots + \dots \end{aligned} \quad (A-11)$$

The surface area of all the particles is the same and it is assumed that the vaporization rate at each  $x$  cross-section  $a, b, c, \dots$  is the same. Then

$$\begin{aligned} \sum_i \Psi_i (v_{2xs})_i A_{si} &= (A_{si} \Psi_i)_a \sum_{ia} (v_{2xs})_i \\ &+ (A_{si} \Psi_i)_b \sum_{ib} (v_{2xs})_i \\ &+ \dots + \end{aligned} \quad (A-12)$$

Using the lemma that was proved in the first part of this appendix, replace  $(v_{ix})_i$  by  $\langle v_{ix} \rangle_i$  and note that the overall particle velocity is defined by

$$\langle v_{ix} \rangle = \frac{1}{\mathcal{N}} \sum_i \langle v_{ix} \rangle_i \quad (\text{A-13})$$

where  $\mathcal{N}$  is the number of particles cut by the plane. Hence

$$\begin{aligned} \sum_i \Psi_i (v_{ix})_i A_{Si} &= \left( A_{Si} \Psi_i v_a \langle v_{ix} \rangle \right)_{x=a} \\ &+ \left( A_{Si} \Psi_i v_b \langle v_{ix} \rangle \right)_{x=b} \\ &+ \left( \phantom{A_{Si} \Psi_i v_c \langle v_{ix} \rangle} \right)_{x=c} \\ &+ \dots + \dots \end{aligned} \quad (\text{A-14})$$

Next, the particle velocity at each cross-section  $a, b, c, \dots$  is expanded in a Taylor's series about the end of the control volume:

$$\begin{aligned} \sum_i \Psi_i (v_{ix})_i A_{Si} &= \langle v_{ix} \rangle \Big|_{x=x} \left\{ v_a A_{Si} \Psi_{i_a} + v_b A_{Si} \Psi_{i_b} \right. \\ &\quad \left. + \dots + \dots \right\} \\ &+ \frac{\partial \langle v_{ix} \rangle}{\partial x} \Big|_{x=x} \left\{ (b-x) [v_b A_{Si} \Psi_{i_b}] + (c-x) [v_c A_{Si} \Psi_{i_c}] \right. \\ &\quad \left. + \dots + \dots \right\} \end{aligned} \quad (\text{A-15})$$



Now it is noted that the mass transfer function originally defined by equation (1-8) is described equivalently by the notation

$$\Psi = - \lim_{\Delta x \rightarrow 0} \frac{1}{\Delta x} \left\{ \nu_a A_{si} \Psi_{ia} + \nu_b A_{si} \Psi_{ib} + \dots \right\} \quad (\text{A-16})$$

By substituting this result, dividing by  $\Delta x$ , and limiting, we get

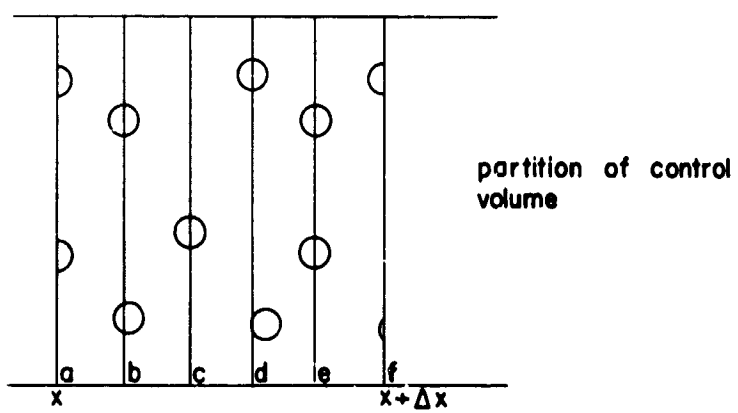
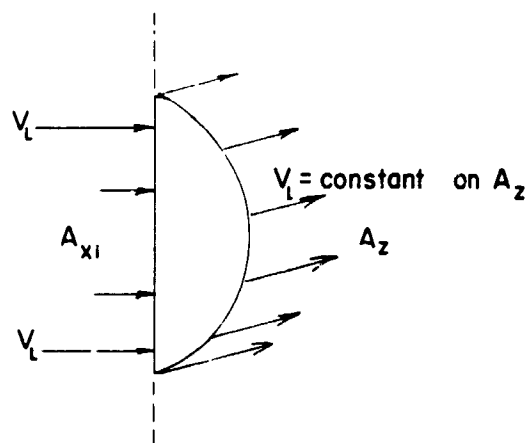
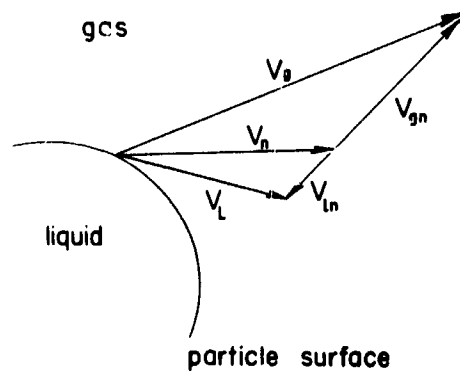
$$\begin{aligned} & \lim_{\Delta x \rightarrow 0} \frac{1}{\Delta x} \sum_i \int_{S_{pi}} \rho_g v_{gx} (\underline{v}_g - \underline{v}_s) \cdot \underline{n}_g \, dS \\ &= \lim_{\Delta x \rightarrow 0} \left\{ \left\{ \langle v_{gx} \rangle \Big|_x \cdot \frac{1}{\Delta x} \left\{ \nu_a A_{si} \Psi_{ia} + \nu_b A_{si} \Psi_{ib} \right. \right. \right. \\ & \quad \left. \left. \left. + \dots \right\} + \frac{\partial \langle v_{gx} \rangle}{\partial x} \Big|_x \cdot \left\{ \frac{(b-x)}{\Delta x} \nu_b A_{si} \Psi_{ib} \right. \right. \\ & \quad \left. \left. + \frac{(c-x)}{\Delta x} \nu_c A_{si} \Psi_{ic} + \dots \right\} + \dots \right\} \\ &= \langle v_{gx} \rangle \Psi \end{aligned} \quad (\text{A-17})$$

This proves the desired result. In the last step the second term may be estimated as follows:

$$\begin{aligned}
 & \left. \frac{\partial \langle v_{cx} \rangle}{\partial x} \right|_x \cdot \left\{ \frac{(b-x)}{\Delta x} \tau_b A_{si} \psi_{ib} + \frac{(c-x)}{\Delta x} \tau_c A_{si} \psi_{ic} + \dots \right\} \\
 & \leq \left. \frac{\partial \langle v_{cx} \rangle}{\partial x} \right|_x \frac{\Delta x}{\Delta x} \left\{ \tau_b A_{si} \psi_{ib} + \tau_c A_{si} \psi_{ic} + \dots \right\} \quad (\text{A-18}) \\
 & \leq \left. \frac{\partial \langle v_{cx} \rangle}{\partial x} \right|_x \cdot \psi \cdot \Delta x
 \end{aligned}$$

And so all the higher terms approach 0 as  $\Delta x \rightarrow 0$ .

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## APPENDIX B

Summary of Two-phase Equations  
for One-dimensional Flow

Gas Phase Equations

Continuity:

$$\frac{\partial}{\partial t} \langle \tilde{\rho}_g \rangle = - \frac{\partial}{\partial x} (\langle \tilde{\rho}_g \rangle \langle \tilde{v}_{gx} \rangle) - \frac{\dot{\Psi}}{A_x}$$

Momentum: (inviscid)

$$\begin{aligned} \frac{\partial}{\partial t} (\langle \tilde{\rho}_g \rangle \langle \tilde{v}_{gx}^2 \rangle) &= - \frac{\partial}{\partial x} (\langle \tilde{\rho}_g \rangle \langle \tilde{v}_{gx}^2 \rangle) \\ &\quad - \frac{\partial}{\partial x} (\langle \tilde{\rho}_g \rangle \langle \tilde{v}_{gx}'' \tilde{v}_{gx}'' \rangle) - \frac{\partial}{\partial x} \langle \tilde{\rho}_g \rangle \\ &\quad - \frac{\dot{\Psi}}{A_x} \langle \tilde{v}_{gx} \rangle - \frac{\dot{\Gamma}}{A_x} \end{aligned}$$

Particle Phase Equations

Continuity:

$$\frac{\partial}{\partial t} \langle \tilde{\rho}_p \rangle = - \frac{\partial}{\partial x} (\langle \tilde{\rho}_p \rangle \langle \tilde{v}_{px} \rangle) + \frac{\dot{\Psi}}{A_x}$$

Momentum:

$$\begin{aligned} \frac{\partial}{\partial t} (\langle \tilde{\rho}_p \rangle \langle \tilde{v}_{px} \rangle) &= - \frac{\partial}{\partial x} (\langle \tilde{\rho}_p \rangle \langle \tilde{v}_{px}^2 \rangle) - \frac{\partial}{\partial x} (\langle \tilde{\rho}_p \rangle \langle \tilde{v}_{px}'' \tilde{v}_{px}'' \rangle) \\ &\quad - \frac{\partial}{\partial x} \langle \tilde{\rho}_p \rangle + \frac{\dot{\Psi}}{A_x} \langle \tilde{v}_{px} \rangle + \frac{\dot{\Gamma}}{A_x} \end{aligned}$$

Thermal Energy:

$$\begin{aligned} \frac{\partial}{\partial t} (\langle \tilde{\sigma}_r \rangle \langle \tilde{h}_2 \rangle) &= - \frac{\partial}{\partial x} (\langle \tilde{\sigma}_r \rangle \langle \tilde{v}_{2x} \rangle \langle \tilde{h}_2 \rangle_i) \\ &\quad + \frac{\bar{Q}}{A_x} + \frac{\bar{\Psi}}{A_x} h_{03} - \frac{\partial}{\partial x} (\langle \tilde{\sigma}_r \rangle \langle \tilde{v}_{2x}'' h_2 \rangle_r) \end{aligned}$$

### Overall Equations

Continuity:

$$\frac{\partial}{\partial t} (\langle \tilde{\sigma}_r \rangle + \langle \tilde{\sigma}_y \rangle) = - \frac{\partial}{\partial x} (\langle \tilde{\sigma}_r \rangle \langle \tilde{v}_{2x} \rangle_r + \langle \tilde{\sigma}_y \rangle \langle \tilde{v}_{2y} \rangle_r)$$

Momentum:

$$\begin{aligned} &\frac{\partial}{\partial t} (\langle \tilde{\sigma}_r \rangle \langle \tilde{v}_{2x} \rangle + \langle \tilde{\sigma}_y \rangle \langle \tilde{v}_{2y} \rangle_r) \\ &= - \frac{\partial}{\partial x} [(\langle \tilde{\sigma}_r \rangle \langle \tilde{v}_{2x}^2 \rangle + \langle \tilde{\sigma}_y \rangle \langle \tilde{v}_{2y}^2 \rangle_r) + \langle \tilde{\pi}_r \rangle + \langle \tilde{\pi}_y \rangle] \\ &\quad - \frac{\partial}{\partial x} [\langle \tilde{\sigma}_r \rangle \langle \tilde{v}_{2x}'' \tilde{v}_{2x}'' \rangle + \langle \tilde{\sigma}_y \rangle \langle \tilde{v}_{2y}'' \tilde{v}_{2y}'' \rangle] \end{aligned}$$

Energy (neglecting velocity fluctuations)

$$\begin{aligned} &\frac{\partial}{\partial t} [\langle \tilde{\sigma}_r \rangle \langle \tilde{e}_2 \rangle + \frac{1}{2} \langle \tilde{v}_{2x}^2 \rangle + \langle \tilde{\sigma}_y \rangle (\langle \tilde{e}_y \rangle_r + \frac{1}{2} \langle \tilde{v}_{2y}^2 \rangle_r)] \\ &= - \frac{\partial}{\partial x} [\langle \tilde{\sigma}_r \rangle (\langle \tilde{v}_{2x} \rangle \langle \tilde{h}_2 \rangle_i + \langle \tilde{v}_{2x}'' h_2'' \rangle_r)] \\ &\quad - \frac{\partial}{\partial x} [\langle \tilde{\sigma}_y \rangle (\langle \tilde{v}_{2y} \rangle \langle \tilde{h}_y \rangle_i + \langle \tilde{v}_{2y}'' h_y'' \rangle_r)] \\ &\quad - \frac{\partial}{\partial x} [\frac{1}{2} \langle \tilde{\sigma}_y \rangle \langle \tilde{v}_{2y} \tilde{v}_{2y}^2 \rangle_r + \frac{1}{2} \langle \tilde{\sigma}_r \rangle \langle \tilde{v}_{2x} \tilde{v}_{2x}^2 \rangle_r] \end{aligned}$$

Thermodynamic Equations

Gas

$$\langle \tilde{\pi}_g \rangle = \langle \tilde{\sigma}_g \rangle R \langle \tilde{T}_g \rangle$$

$$\langle \tilde{h}_g \rangle = C_{p2} \langle \tilde{T}_g \rangle + h_{REF}$$

Particles

$\langle \tilde{\pi}_p \rangle =$  assumed relation to external pressure and flow field

$$\langle \tilde{\sigma}_p \rangle = \frac{\rho_x}{A_x} \bar{A}_{px} = m_i \langle \tilde{n} \rangle$$

Overall

$$\langle \tilde{\pi}_m \rangle = \langle \tilde{\pi}_p \rangle + \langle \tilde{\pi}_g \rangle$$

$$\langle \tilde{\sigma}_m \rangle = \langle \tilde{\sigma}_p \rangle + \langle \tilde{\sigma}_m \rangle$$

$$\langle \tilde{\sigma}_m \rangle \langle \tilde{T}_m \rangle = \langle \tilde{\sigma}_p \rangle \langle \tilde{h}_e \rangle + \langle \tilde{\sigma}_g \rangle \langle \tilde{h}_g \rangle$$

Ancillary Relations for  $\langle \tilde{n} \rangle$  and  $m_i$ 

$$\frac{\partial}{\partial t} \langle \tilde{n} \rangle + \frac{\partial}{\partial x} (\langle \tilde{n} \rangle \langle \tilde{v}_{ex} \rangle) = 0$$

$$\frac{\partial m_i}{\partial t} + \langle \tilde{v}_{ex} \rangle \frac{\partial m_i}{\partial x} = \frac{\psi}{A_x \langle \tilde{n} \rangle}$$

## APPENDIX C

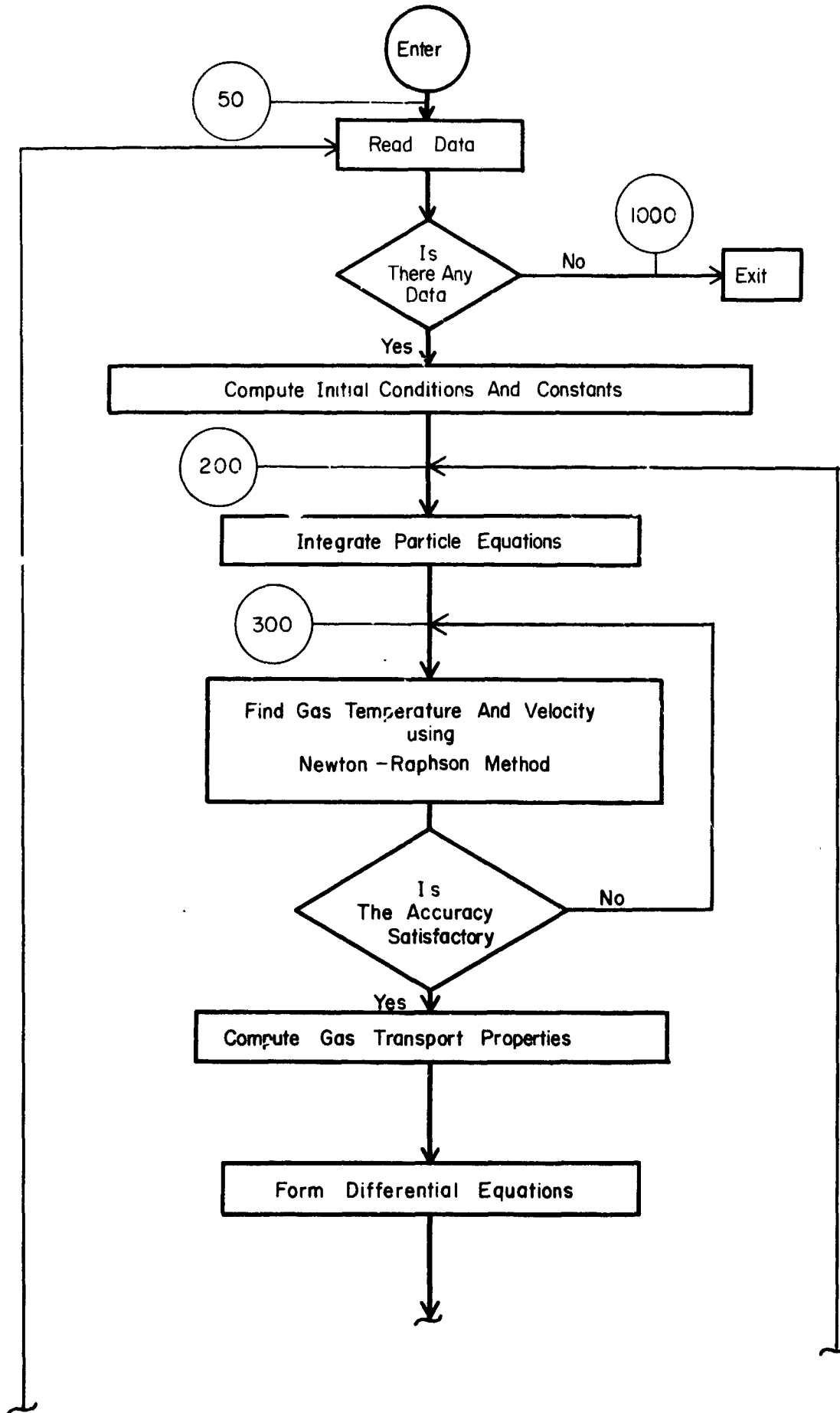
## Dictionary of FORTRAN Symbols

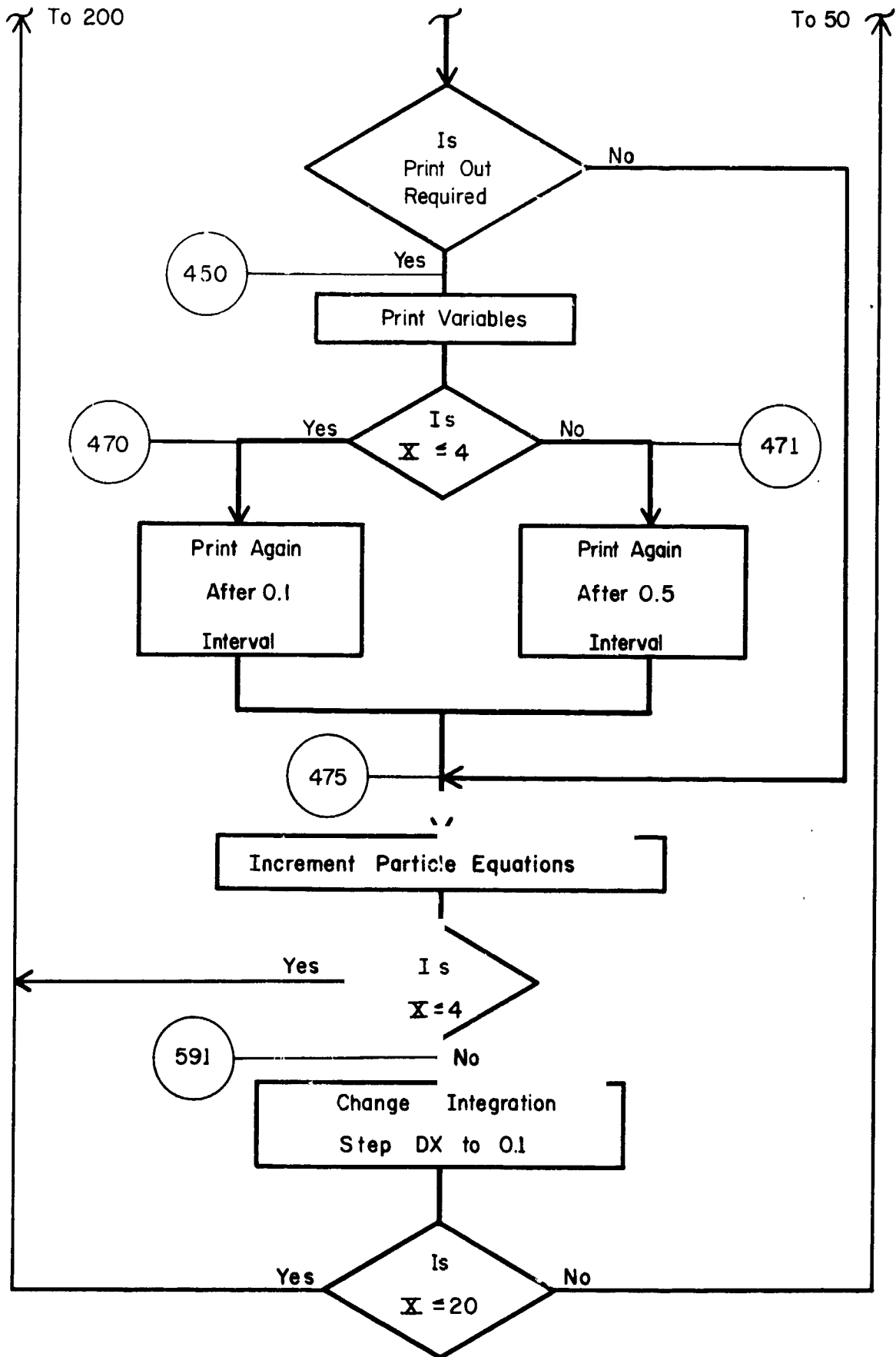
AI = I	DHL(I) = $dH_{pi} / dX'$
AJ = J	DTG = $\Delta \hat{T}_g$
ALPHA = $\alpha$	DV = $\Delta \hat{V}_g$
AU = $\mu^*$	DVD(I) = $dV_{pi} / dX'$
AUX = $\sqrt{\mu^*}$	DWD(I) = $dW_{pi} / dX'$
AUMDT = internal quantity	DX = $\Delta X'$
AUMDV = internal quantity	ETA = $\eta$
CAPPA = internal quantity	FDRG = $f$
CON1 = constant for testing	F1 = $F_1$
CONA = $k_A$ ; CONB = $k_B$	F2 = $F_2$
COND = k	GAMMA = $\gamma_0$
CPA = $C_{pA}^*$	H = $H_1$
CPB = $C_{pB}^*$	HA = $H_A$
CPF = $C_{pf}^*$	HAO = $H_{A0}$
CPG = $C_{pg}^*$	HB = $H_0$
CPL = $C_{pl}^*$	HBO = $H_{B0}$
D1, D2, D3 = dummy spaces	HFGO = $H_{fg}^0$
DELTA = $\delta$	HFG(I) = $H_{fg}(T_{pi})$
DEN = $\rho_2 / \rho_{g0}$	HL(I) = $H_{pi}$
DET = internal quantity	HO = $H_{g0}$
DF1DT = $\partial F_1 / \partial \hat{T}_g$	HU(I) = $N_{u_i}$
DF1DV = $\partial F_1 / \partial \hat{V}_g$	HUD(I) = $N_{u_j}$
DF2DT = $\partial F_2 / \partial \hat{T}_g$	NUM = number of particle sizes
DF2DV = $\partial F_2 / \partial \hat{V}_g$	P = p



PBP(I) = $P_{BSj}$	V = $V_g$
PCOR(I) = internal variable	VD(I) = $V_{Pj}$
PIE = $P / P_0$	VDO = $V_{p0}$
PHI(I) = $\psi_j$	VO = $V_0$
PHIAB = $\phi_{AB}$	VISA = $\mu^*_{A}$
PHIBA = $\phi_{BA}$	VISB = $\mu^*_{B}$
PO1 = $P_1$	WA = $\omega_A$
POO = $P_0$	WAO = $\omega_{A0}$
PR = $P_r$	WB = $\omega_B$
Q(I) = $Q_j$	WBO = $\omega_{B0}$
R = $R$	WDD = $\dot{M}_P$
RAD(I) = $R_{adj}$	WDDO = $\dot{M}_{p0}$
REALX = $X$	WD(I) = $\dot{M}_{Pj}$
REF = $r_0$ (dimensional)	WDM = $\dot{M}_g$
REY(I) = $Rey_j$	WDMO = $\dot{M}_{g0}$
RODAB = $(\rho_{g0} D_{A0})^*$	WGG = $\dot{M}_g / \dot{M}_{g0}$
RREF(I) = $Ref_j$	W(I) = breakup parameter
SC = $S_c$	X = $X' = X \sqrt{\mu^*_{A}}$
SUMA(I) = internal quantity	XA = $\chi_A$
SUMB(I) = internal quantity	XAO = $\chi_{A0}$
SUM1 = internal quantity	XB = $\chi_B$
SUM2 = internal quantity	XBO = $\chi_{B0}$
TEN = dimensionless surface tension	XOUT = punch out interval
TG = $\Theta_g$	YOLE = $m_g / m_B$
TGO = $\Theta_{g0}$	YOLEO = $m_{g0} / m_B$
TL(I) = $\Theta_{2j}$	ZETA = $\zeta = m_B / m_A$
TLO = $\Theta_{s0}$	

# COMPUTER PROGRAM FLOW CHART





APPENDIX E  
FORTRAN PROGRAM

```

C      TWO PHASE SHOCK STRUCTURE
C      VARIABLE TRANSPORT PROPERTIES
C      N PARTICLE SIZES
      DIMENSION WD(2),ALPHA(2),VD(2),TL(2),HL(2),RAD(2),SUMA(2),SUMB(2)
1      ,PCOR(2),XBP(2),RFY(2),CDRG(2),HU(2),HUD(2),PHI(2),FDRG(2),Q(2), D
1      WD(2),DVD(2),DHL(2),RREF(2),PBP(2),W(2),HFG(2)
      PRINT 10
      PRINT 11
      PRINT 12
      PRINT 13
      PRINT 14
      PRINT 15
      PRINT 16
      PRINT 18
      PRINT 12
50     READ 100 ,D1,D2,D3,CPA,CPB,CPL,HFGO,ZFTA,GAMMA,TEN,TGO,TLO,VO,VDO,
1     DELTA,XBO,CON1,DX,REF,DEN,VISA,VISB,RODAB
      PRINT 100,D1,D2,D3,CPA,CPB,CPL,HFGO,ZETA,GAMMA,TEN,TGO,TLO,VO,VDO,
1     DELTA,XBO,CON1,DX,REF,DEN,VISA,VISB,RODAB
      IF(VO)1000,1000,51
51     CONTINUE
      READ 101,NUM
      PRINT 101,NUM
      DO 55 I=1,NUM
      READ 102,ALPHA(I),RREF(I)
55     PRINT 102,ALPHA(I),RRFF(I)
      PRINT 12
      PRINT 17
      PRINT 19
      PRINT 12
10     FORMAT (80H      TWO PHASE SHOCK STRUCTURE      VARIABLE PROPERTIES
1      )
11     FORMAT (80H      N PARTICLE SIZES
1      )
12     FORMAT (1H )
13     FORMAT(80H      D1          D2          D3          CPA          CPB          CPL
1      HFGO
14     FORMAT(80H      ZFTA          GAMMA          TEN          TGO          TLO          VO
1      VDO
15     FORMAT (80H      DELTA          XBP          CON1          DX          REF          DEN
1      VISA
5      FORMAT (3X,4HVISA,5X,5HRODAB)
16     FORMAT (8X,3HNUM)
18     FORMAT (2X,8HALPHA(I),3X,7HRREF(I))
17     FORMAT(130H      REALX          X          PIF          V          TG          WGG
1      XB          AU          PR          SC
1      )
19     FORMAT(4X,1HI,13X,5HVD(I),10X,5HTL(I),10X,6HRAD(I),9X,6HREY(I),9X,
1     4HW(I),11X,5HWD(I),10X,6HXBP(I))
100    FORMAT (7F10.5)
101    FORMAT (I10)
102    FORMAT (2F10.6)
500    FORMAT (2F10.4,8F10.6)
501    FORMAT (I5,5X,7F15.6)

```

```

C      COMPUTE INITIAL CONDITIONS AND CONSTANTS
      LOGICAL BFGIN
      RFAL INOV
      X=0
      XOUT=-.000005
      WDDO=DELTA*VDO
      WDMO=VDO
      POO=WDMO/(GAMMA*VDO)
      XAO=1.-XBO
      WAO=XAO/(ZFTA-XAO*(ZFTA-1.))
      YOLFO=XAO*(1.-ZFTA)/ZFTA+1.
      FTA=GAMMA/YOLFO*HFGO
      WDD=WDDO
      V=VO
      TG=TGO
      WA=WAO
      PO1=WDMO*TGO/(GAMMA*VO)
      WR0=1.-WAO
      HAO=CPA*(TGO-1.)
      HR0=CPR*(TGO-1.)+HFGO
      HO=WAO*HAO+WR0*HR0
      AJ=WDMO*(HO+.5*VO**2)+WDDO*.5*VDO**2.
      AI=WDMO*VO+WDDO*VDO+PO1
      DO 170 I=1,NUM
      WD(I)=WDDO*ALPHA(I)
      VD(I)=VDO
      TL(I)=TLO
170    HL(I)=CPL*(TL(I)-1.)
C      BEGIN INTEGRATION LOOP
200    WDD=0.
      DO 210 I=1,NUM
210    WDD=WD(I)+WDD
      WDM=VDO*(1.+DELTA)-WDD
      WA=WAO*WDMO/WDM
      WB=1.-WA
      XA=ZFTA*WA/(1.+WA*(ZFTA-1.))
      XB=1.-XA
      YOLF=XAO*(1.-ZETA)/ZETA+1.
      R=YOLEO/YOLF
      DO 220 I=1,NUM
220    RAD(I)=(WD(I)/WDDO/ALPHA(I))**.5*(1./3.)*RRFF(I)
C      FIND GAS PROPERTIES BY N-R METHOD
300    HA=CPA*(TG-1.)
      HB=CPR*(TG-1.)+HFGO
      H=WA*HA+WB*HB
      SUM1=0.
      DO 330 I=1,NUM
330    SUMA(I)=WD(I)*(HL(I)+.5*VD(I)**2)
      SUM1=SUM1+SUMA(I)
      F1=H+.5*V**2-AJ/WDM+SUM1/WDM
      DF1DT=WA*(CPA-CPR)+CPR
      DF1DV=V
      SUM2=0.
      DO 360 I=1,NUM
360    SUMB(I)=WD(I)*VD(I)
      SUM2=SUM2+SUMB(I)
      F2=V**2+R*TG/GAMMA+V*(SUM2-AI)/WDM
      DF2DT=R/GAMMA
      DF2DV=.5*V+(SUM2-AI)/WDM

```

```

DET=DF1DT*DF2DV-DF2DT*DF1DV
AUMDT=-F1*DF2DV+F2*DF1DV
AUMDV=-F2*DF1DT+F1*DF2DT
DTG=AUMDT/DET
DV=AUMDV/DET
TG=TG+DTG
V=V+DV
IF(ABS(DTG)-CON1)400,400,300
400 IF(ABS(DV)-CON1)410,410,300
C COMPUTE TRANSPORT PROPERTIES OF THE GAS MIXTURE
410 CPG=WA*CPA+WB*CPB
SIGMA=VISA/VISB
PHIRA=(1.+1./ZETA**(.25)/SQRT(SIGMA))**2/SQRT(8.+8.*ZETA)
PHIAR=(1.+SQRT(SIGMA)*ZETA**(.25))**2/SQRT(8.+8./ZETA)
AU=XA*VISA/(XA+XB*PHIAB)+XB*VISB/(XB+XA*PHIBA)
CONA=VISA*(CPA+5./4.*YOLEO*ZETA/GAMMA)
CONB=VISB*(CPB+5./4.*YOLEO/GAMMA)
COND=XA*CONA/(XA+XB*PHIAB)+XB*CONB/(XB+XA*PHIBA)
PR=AU*CPG/COND
SC=AU/RODAB
C FORM DIFFERENTIAL EQUATIONS FOR DROPLET PROPERTIES
P=WDM*R*TG/(GAMMA*V)
CPF=CPG
PIE=P/POO
YOLFF=YOLF
CAPPA=GAMMA/YOLFO*(CPB-CPL)
DO 430 I=1,NUM
TL(I)=HL(I)/CPL+1.
HFG(I)=HFGO+(CPB-CPL)*(TL(I)-1.)
PCOR(I)=TL(I)**CAPPA*FXP(CAPPA*(1./TL(I)-1.))
PBP(I)=(1.-XAO)*POO*FXP(ETA*(1.-1./TL(I)))*PCOR(I)
XBP(I)=PBP(I)/P
REY(I)=2.*RAD(I)*WDM*ABS(V-VD(I))/AU/V
CDRG(I)=.48+28./REY(I)**(.85)
HU(I)=2.+6*PR**(1./3.)*SQRT(REY(I))
HUD(I)=2.+6*SC**(1./3.)*SQRT(REY(I))
PHI(I)=3./2.*WD(I)/RAD(I)**2*HUD(I)/SC*AU/VD(I)*(XBP(I)-XB)/(1.-X
1 BP(I))
FDRG(I)=3.*WD(I)*WDM*CDRG(I)*(V-VD(I))*ABS(V-VD(I))/(8.*RAD(I)*V*
1 VD(I))
Q(I)=1.5*WD(I)/RAD(I)**2*HU(I)/PR*AU/VD(I)*CPF*(TL(I)-TG)
430 W(I)=AU/TEN*ABS(V-VD(I))
AUX=SQRT(VISA)
WGG=WDM/VDO
REALX=X*REF*DEN/AUX
IF(XOUT-X)450,450,475
450 PRINT 12
PRINT 500,REALX,X,PIF,V,TG,WGG,XB,AU,PR,SC
DO 460 I=1,NUM
460 PRINT 501,I,VD(I),TL(I),RAD(I),REY(I),W(I),WD(I),XBP(I)
PRINT 12
IF(X-4.)470,470,471
470 XOUT=XOUT+.1
GO TO 475
471 XOUT=XOUT+.5
475 CONTINUE
X=X+DX
DO 490 I=1,NUM
DWD(I)=-PHI(I)/AUX
DVD(I)=FDRG(I)/WD(I)/AUX

```

```

DHL(I)=- (PHI(I)*HFG(I)/WD(I)+Q(I)/WD(I))/AUX
WD(I)=WD(I)+DWD(I)*DX
VD(I)=VD(I)+DVD(I)*DX
490 HL(I)=HL(I)+DHL(I)*DX
IF(4.-X)591,591,200
591 DX=.1
IF(20.-Y)600,600,200
600 GO TO 50
1000 CALL EXIT
STOP
END

```

\$DATA

5.3	3	1.4	.001	2.5	4.49	5.69	3.33
.2		.0001	.0001	1.1909	1.	.8575	1.3
.0	0 045	.00047		.001	.0025	570.	.00192
	1						
1.		1.					
5.3	3	1.4	.001	2.5	4.40	5.69	3.33
1.		.0001	.0001	1.1909	1.	.8575	1.3
.0	0 045	.00047		.001	.0025	570.	.00192
	1						
1.		1.					