Mixing and Combustion in Two-Phase Flows with Application to the B-O-H-N System

RAYMOND B. EDELMAN,* CONSTANTINO ECONOMOS,† AND JOHN BOCCIO‡
General Applied Science Laboratories Inc., Westbury, N. Y.

This paper is a report upon some of the interrelated analytical and experimental studies designed to provide information on the combustion of boron particles in a high-speed air stream. The program upon which this work is based involved single particle ignition and combustion studies, B2O3 condensation studies, and axial and lateral injection of the effluent from a B-O-H-N gas generator into a supersonic air stream. This paper will emphasize the axial and lateral injection studies. Experimental data include profile measurements associated with both axial and lateral injection of hot and cold particle-laden primary streams injected into a variable temperature high-speed airstream. In addition, still color photographs and movies have been obtained. The analyses include treatments of coaxial mixing and combustion, and penetration for the description of the axial and lateral injection configurations, respectively. The coaxial analysis includes a special formulation for the turbulent diffusion of the particulate phase and the lateral injection analysis includes a treatment of the coupled gas-particle trajectories. Comparison of the analysis with the experiments shows very good agreement for both the coaxial and lateral injection flows provided the former is based upon the new mixing analysis and the latter employs a drag law based upon experiments with particulate clouds undergoing large accelerations.

Nomenclature

b = width of jet, Fig. 2

 $C_D = \text{drag coefficients}$

 $d_{j,p}$ = orifice diameter or particle diameter

Re =Reynolds number

s = distance along jet axis

T = temperaturev = intrinsic velocity

x,y =axial and normal coordinate

 α = angle subtended by velocity vector and streamwise co-

ordinate

 δ_p = particle bulk density

λ = primary stream-secondary stream mass flow ratio

 μ_t = turbulent viscosity

 $\rho = \text{density}$

Subscripts

a = refers to conditions external to lateral jet

g = refers to gas-phase

p = refers to particle or primary gas stream

pc = refers to potential core

n = refers to conditions normal to gas-phase jet axis

s = refers to secondary stream or distance along jet

t = total conditions

∞ = freestream conditions

Superscript

 $(\overline{})$ = nondimensionalize with respect to d_i

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Index categories: Multiphase Flows; Reactive Flows; Jets, Wakes, and Viscid-Inviscid Flow Interactions.

* Manager, Thermochemistry and Viscous Flow Section. Member AIAA.

† Supervisor, Thermochemistry and Viscous Flow Section. Member AIAA.

‡ Senior Scientist, Thermochemistry and Viscous Flow Section. Member AIAA.

I. Introduction

THERE are many practical systems which involve the flow of fluids containing particles in suspension. Such multiphase flows are relevant to problems ranging from propulsion system component design to the description of the formation and dispersion of pollutants from various industrial process equipment. Generally, the related flows involve a number of coupled processes including homogeneous gas-phase chemical reactions, heterogeneous chemical reactions, phase transition, and mixing within and between the phases.

A review of the available literature of the past ten years shows that the bulk of that work has focused upon the most basic flow configurations such as nozzle flows and shocks.^{1–4} In general, the problems that were studied were limited to cases involving inert particles suspended in an otherwise inviscid fluid. Thus, the coupling of combustion with turbulent dispersion of the particulate matter was not treated. More recently, however, attempts have been made to treat the more relevant problem including effects of mixing and combustion in turbulent flows.^{5–8}

The application in this paper is concerned with propulsion systems and includes work appropriate to the analysis of the mixing, combustion, and nozzle expansion processes. In particular, emphasis is on systems where the fuel as well as the products of combustion involve particulate matter in suspension

The desirability of reducing combustion-chamber lengths necessitates the process of mixing, ignition and combustion, to occur at each axial station. Accordingly, a diffusion flame is appropriate and this requires consideration of axial and lateral modes of injection as shown schematically in Fig. 1. The axial mode is desirable because it provides a smooth heat release distribution, minimum losses, and can be most easily analyzed. The disadvantage of this mode is that it provides a relatively short residence time for mixing and combustion compared with the lateral mode of injection. Advantages of the lateral mode are relatively deep penetration in a short distance and the aerodynamic flame holding characteristics in the region near the injection point. In addition, for high-speed flow, near stagnation conditions are recovered in the vicinity of the injection point. This effect together with the

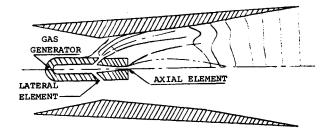


Fig. 1 Schematic of ramburner flowfield showing axial and lateral injector elements.

longer residence time can provide conditions necessary for local ignition of the fuel. In fact, this has already been demonstrated for the case of direct liquid hydrocarbon injection into a supersonic air stream.⁸ The disadvantages of this mode of injection are the attendant losses associated with the strong interaction with the secondary air stream, the high local heat-transfer rates associated with recirculation zones and shock impingement points, and finally, the difficulty of analysis.

Considering the advantages and disadvantages of both techniques, it appears that some combination of axial and lateral injection will be required to provide an optimum design concept. For the purposes of determining some of the fundamental parameters controlling the respective modes of injection, each has been considered here separately, both analytically and experimentally.

II. Analysis

A. Axial Injection

An analysis based upon a study of the conservation equations for a multicomponent gas phase containing a dispersion of particles under conditions of thermal and dynamic non-equilibrium including turbulent transport and chemical and phase transition kinetics, has led to a set of describing equations which appear to be the most suited for the present problem.^{8,9} The primary assumptions leading to the current set of working equations are listed as follows: 1) the particulate phases form a dilute, continuum suspension in the multicomponent gaseous carrier. 2) A state of near dynamic equilibrium in the mean motion prevails between the particulate and gaseous phases. 3) Each particle class and the gas phase is treated as a binary subsystem to which Fick's Law may be applied. 4) Diffusive processes are important only in the lateral direction and boundary-layer concepts apply.

The unique features of the analysis include the extension of Fick's Law for the treatment of different diffusivities for the particles and gas-phase components, and the retention of the particulate phase energy equations. Although dynamic equilibrium may be appropriate, the temperature of the particles can be significantly different from the local gas-phase temperature depending upon the processes occurring on the particle scale. Only in the case of inert, nonradiating particles is there similarity in the particle drag and heating processes for which "near" dynamic equilibrium would imply "near" thermal equilibrium. For example, for liquid hydrocarbon droplets and for metal particles like aluminum and magnesium, vapor-phase combustion is appropriate and the particle temperature can be approximated by taking it equal to the local saturation temperature. This temperature will be different from the local gas-phase temperature. For metals like boron and zirconium, surface reactions will dominate the oxidation process until temperatures of 3931 and 5200°K, respectively, are attained. Above these temperatures, vapor-phase reactions will dominate. During the important period when surface reactions are dominant the particle temperature will be different from the local gas-phase temperature.

Boron is of particular interest here and unlike most other metals its vaporization temperature is higher than the oxide boiling point temperature. This fact lends credence to the importance of surface reactions. In addition, the boron oxide layer can be a potential barrier inhibiting the oxygen from reaching the surface at temperature levels below about 1750°K. This point is of particular relevance regarding interpretation of "single" particle experiments designed to yield information on ignition delay. Generally, the particles are injected cold into the test environment. Thus, the oxide and metal must be heated and brought to a condition where the oxygen can reach the metal before any significant oxidation can be initiated. In a practical configuration, however, the particles will be treated both thermally and chemically in a primary rocket or gas generator. Furthermore, the primary flow entering the ramburner will contain combustible gases which will readily ignite with the secondary air providing further heating of the particles. Finally, the presence of water vapor in the primary stream will act chemically to remove the oxide layer via the formation of metaboric acid (HBO₂) which is significantly more volatile than B₂O₃. Thus, a reasonable assumption for the ramburner analysis is that the particles are not protected by the oxide coating. However, assuming spherical particles, the effects of convective heating, finite rate evaporation, finite rate surface reaction and radiation are included.10

This system has been solved for a number of special cases involving both free and ducted configurations. Calculations are presented in Sec IV A and C in connection with the current experimental program.

B. Lateral Injection

This mode of injection has not been analyzed in depth because of its complex three-dimensional character. However, injection of single-phase jets into supersonic streams has been analyzed with relatively simple models yielding a reasonable degree of success.^{11–14} Generally, these models rely upon the similarity that exists between the jet discharging into a quiescent medium to that issuing into a moving stream.

Apparently very little has been done in the way of analysis of the lateral injection process for two-phase flows. The purpose of the present discussion is to extend an existing gasphase model¹⁴ to include some of the effects of the presence of particles in the injected stream.

The model is intended to provide information on gross properties including penetration and spreading for both the gas and particulate phases.

Two limits are considered in terms of the behavior of the particles in the gas-phase stream. In the first, or frozen, limit the coupling between the gas and the particles is unilateral wherein the gas-phase trajectory is assumed unaffected by the particles. In the second limit, a trajectory is computed based upon dynamic equilibrium between the gas and

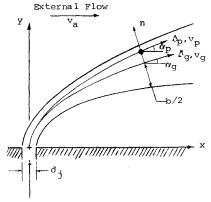


Fig. 2 Schematic of lateral jet.

particles. Finally, for both cases, the ability of the particles to follow the respective trajectories is determined. Thus, in addition to predicting penetrations, the residence time of the particles within the primary stream is given.

The basic concept behind the models that have been employed involves the assumption that the injected stream retains its identity at least until it becomes parallel to the main-stream flow (Fig. 2). However, the deformation of the jet due to pressure and viscous shear forces can be accounted for empirically.14

The trajectories of the particles within the jet can be readily determined as a function of the dynamics of the carrier gas. The equations of motion for the particles are given by:

$$dv_p/d\bar{s}_g = (\frac{3}{4})(C_{Dp})_s(\rho_j/\delta_p)(d_j/d_p) \times [v_g \cos(\alpha_p - \alpha_g) - v_p]^2[v_p \cos(\alpha_p - \alpha_g)]^{-1}$$
(1)
$$d\alpha_p/d\bar{s}_g = -(\frac{3}{4})(C_{Dp})_n(\rho_j/\delta_p)(d_j/d_p) \times$$

$$[v_g \sin(\alpha_p - \alpha_g)]^2 [v_p^2 \cos(\alpha_p - \alpha_g)]^{-1}$$
 (2)

Equations (1) and (2) have been coupled to the gas-phase equation of motion developed in Ref. 14. The resulting system of equations provides the necessary relations to determine, α_p , α_g , v_p and v_g , ¹⁰ and has been solved using two different particle drag laws.

Although Stokes Law is a poor approximation when the particle Reynolds numbers, Re_p , is greater than unity, it is one of the two laws that were used. In addition to the Reynolds number limitation, this law in no way accounts for large accelerations and cooperative effects which are of potential importance in particle clouds. However, it was incorporated into the analysis to see its effect on the comparison between theory and experiment. Large accelerations and cooperative effects were implicitly accounted for by taking as the second candidate for the drag coefficient the Rudinger drag law which was derived from experiments involving clouds undergoing large acceleration, Ref. 15, viz:

$$C_{Dp} = 6000 Re_p^{-1.7} (3)$$

To apply the above analysis to underexpanded jets, the concept of an effective back pressure is employed. This con-

Table 1 Environmental conditions for mixing experiments

CONFIGURATION NUMBER	MIXING GEOMETRY (L) LATERAL; (A) AXIAL	(N) NONREACTING (R) REACTING	SECONDARY STREAM TOTAL TEMPERATURE (K)	PRIMARY STREAM PARAMETERS								
				total temperature (^o k)	TOTAL PRESSURE (ATM)	PARTICLE FLOW RATE (pps)	PARTICLE PHASE (B) BORON (G) GRAPHITE	CARRIER GAS	LOADING RATIO	FUEL/OXIDIZER RATIO	B/H RATIO OR C/H RATIO	H ₂ /O ₂ RATIO
1	A	N	610	310	2	0	_	Aiı	0	_	_	
2		"	*1				-	H_2	o	-	-	-
3	"	"	11		- 0	н	-	co2		-	-	-
4		"		11		.034	G	Air	0.3	-	-	-
5 6		R	1220					co2	"	-	-	-
	16	к.		1100		.013		N_2	0.45		9	0.1
7		.,	295	1900	"		В	"	0	"	18	0.2
8		"	610			"		"		"	**	н
9			1220		"	"	0	"	н	"		n
10		"	610	11		"		н	ti	и	9	0.1
11	"		1220	"		н	n	**	"		23	"
12	L	N	610	295	"	0	-	Air	0	-	• -	-
13				10	ti	0	-	H_2	0	-	-	-
14	"	"			"		-	co_2	"	-	-	-
15	"			0	12	"	~	Air	a	-	-	-
16	11	"		"	11	н	~	H_2	"	-	-	-
17			**	11	16		~	co_2	11	-	-	-
18			13		3	.056	G	Air	.7	_	~	
19	0.5	н			18	.013	10		.3	_	-	_
20	**	R	H	1900	2		В	N_2	.45	2	9	0.1

Particle flow rates are average values. All flow ratios given by mass.

Nominal secondary stream stagnation pressure is 8.2 atmospheres

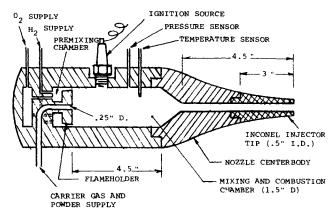


Fig. 3 Schematic of gas generator.

cept has been found to be a valid empirical method of correlating experimentally determined Mach disc locations as determined from measurements obtained in quiescent environments. 11, 12, 16 The location of the Mach disc and the state downstream of the normal shock constitute the initial conditions used in the above analysis. The results using both of these laws will be discussed in the subsequent section.

III. Description of Experiments

A. Wind-Tunnel Facility

The desired enthalpy levels of the secondary stream were provided by means of vitiated heating using a hydrogen combustion heater. The vitiated stream was then allowed to expand to atmosphere at approximately Mach 2 by means of either a two-dimensional contourned nozzle having a 3 in. X 3 in. exit cross section or a plug-nozzle arrangement with an exit diameter of approximately 3.5 in. Lateral jet-mixing studies used the former nozzle arrangement whereas the latter configuration was employed for the axial mixing experiments. In this case the center body, or plug, was designed internally so that both the reacting and nonreacting multiphase primary streams could issue concentric to the secondary gas stream; for the lateral jet-mixing studies, a similar primary gas generator was affixed externally to the lower nozzle block.

B. Primary Gas Generator

The basic features of the gas generator which supplied the primary stream are shown in Fig. 3. The essential components of this device include a small chamber for premixing the combustibles (H2-O2), a circular disc flame holder, a mixing and combustion chamber $3\frac{1}{2}$ -in. long by $1\frac{1}{2}$ -in. diam and an aircraft-type spark plug for initiating combustion. Note that the particulate phase enters the combustion chamber through a 0.25 in. orifice located in the center of the flameholder. The powders utilized in these studies (1-5 μ graphite, 1 μ Trona§ boron) were transported to the gas generator by entrainment in various carrier gases. This entrainment was accomplished by means of a combined gravity-pneumatic feed system augmented by a mechanical vibrator. The average flow rate of the particulate phase was determined by weighing of the powder contained in the reservoir before and after each test. The flow rates of the gaseous components were obtained by means of standard venturi meters.

C. Environmental Conditions

The parameters which were varied in the mixing experiments included secondary and primary stream total temperatures and primary stream stagnation pressure and composi-The latter was varied not only by utilizing a variety of

[§] Trade name American Potash and Chemical Corporation.

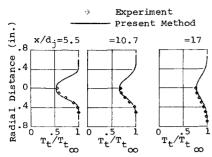


Fig. 4 Comparison, theory/experiment, nonreacting axial mixing, Configuration 1.

carrier gases and (gaseous) fuel/oxidizer ratios but also by the use of two different solid fuels, i.e., graphite powder and boron powder. In particular, all nonreacting studies were conducted with graphite as the solid constituent, while in the reacting test series both graphite and boron were utilized. The stagnation pressure of the primary stream was maintained at values greater than or equal to approximately two atmospheres. Thus, the primary jet always operated at a choked condition (i.e., $M_p \approx 1.0$) but with varying degrees of underexpansion. The environmental conditions for the entire test series have been summarized in detail in Table 1.

D. Instrumentation and Measurements

For both single and two-phase nonreacting tests, surveys of impact pressure, stagnation temperature and static pressure were made across the jet in the vertical plane of symmetry at several axial locations downstream of the primary jet exit. For this purpose a three-pronged rake, on which a 0.0625-in. diam impact probe, a bare junction, 30 gage chrome-alumel thermocouple and a 0.0625-in,-diam cone-cylinder static pressure probe were mounted, was traversed slowly (~ 0.15 ips) through the flow. Surveys of local gas composition were also obtained for the single phase lateral nonreacting configurations (i.e., Configurations 13, 14, 16 and 17 of Table 1). this case a rake with six 0.0625-in. diam Pitot-type probes spaced 0.25 in. apart was utilized to collect the gas samples. Analysis of the samples was by means of a Beckman GC-2 Gas Chromatograph. For all nonreacting two-phase configurations (Configurations 4, 5, 18, 19), black and white polaroid photographs were obtained.

Surveys of the mixing zones with a temperature probe were also attempted for the reacting tests. However, such attempts proved unsuccessful due to the high heating loads that the probe and probe support had to withstand. Moreover, the heavy coating of boron and its oxides on the sensing surface precluded an accurate assessment of the temperature profiles within the jet.

Qualitative information with regard to the reacting tests was obtained by optical means. Specifically, the flame patterns which were observed were photographed in color utilizing both still and cine-photography. For the still photographs, Type 48 Polaroid color film was utilized while the

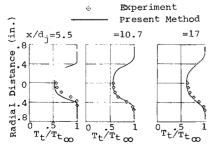


Fig. 5 Comparison, theory/experiment, nonreacting axial mixing, Configuration 2.

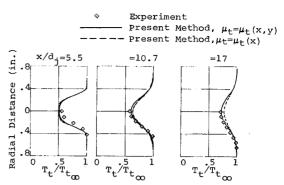


Fig. 6 Comparison, theory/experiment, nonreacting axial mixing, Configuration 4.

motion pictures were obtained using a Bell and Howell Super 8, Model 431, with Kodachrome II color film at 36 frames per sec. All color pictures were of the self-luminosity type.

IV. Experimental Results and Comparison with Theory

A. Nonreacting Coaxial Mixing

Representative results obtained during this test series are shown in Figs. 4–6, which show the total temperature profiles at three axial stations. These experimental data have been compared with theoretical predictions generated by the analysis described in Ref. 10.

Noteworthy is the excellent agreement between theory and experiment for the radial variation of total temperature (Fig. 5) for the tests involving air and H₂ as the primary exhaust effluent. This is particularly relevant since the constants which are required for 1) fixing the potential core length through the empirical relation $x_{pc}/y = k_2(\lambda)^{1/2}$, 2) for determining the axial variation of eddy viscosity through this region using a Prandtl mixing-length relation which results in a relation stating that $\mu_{pe} = k_1 \rho_s x |u_{y=0} - u_s| + 10^{-4}$ lbf- $\sec/\mathrm{ft^2}$, and finally, 3) the constant, k_3 , which describes the linear variation of eddy viscosity from the value it achieves at the end of the potential core to the value it then proceeds to take on in the fully developed region have all been obtained experimentally by only examining the air into air mixing experiment (Fig. 4). Accordingly, the excellent agreement that these figures portray for the H2 into air mixing experiment lends credence for the wide range of applicability of the mixing models chosen and for the determination of these empirical constants, which in the context of these experiments have been determined to be $k_1 = 6(10)^{-4}$ and $k_2 = 12$ with k_3 ranging from 0.018 to 0.013.

Of even more significance from the point of view of the current program are the results obtained with two-phase flow. Consider for example, the results shown in Fig. 6 which correspond to the two-phase Configuration Number 4. Here the experimentally determined radial temperature variation has been compared with two different predictions. One of these predictions (shown by the solid line) utilizes the model described in Sec II.A, corresponding to equilibrium between the phases. It is important to note here that even with equilibrium the proposed model indicates that the eddy viscosity for the mixture is explicitly affected by the presence of the solid phase. In particular, a radial variation of the viscosity level is introduced by virtue of non-zero particle concentra-Thus, the proposed multiphase mixing model must be distinguished from one in which, for example, standard gas eddy-viscosity models are applied directly to the two-phase mixture. To demonstrate this distinction an additional calculation was carried out with $\mu_{\rm mix}=\mu_{\rm gas}$ and has also been indicated in Fig. 6 by the dashed line. It is apparent that the proposed model provides improved agreement with experiment.

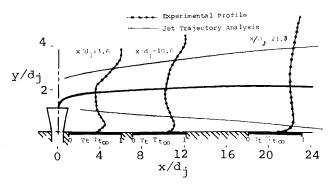


Fig. 7 Comparison, theory/experiment, nonreacting lateral mixing, Configuration 16.

Additional comparison for other configurations and for other properties of the flow such as impact pressure distribution may be found in Refs. 10 and 18. The agreement is adequate in all cases.

In summary, the following may be concluded for the range of environmental conditions examined: 1) the two phase cloud behaves as an "effective" gas, i.e., dynamic and thermal equilibrium between the phases is appropriate; 2) turbulent transport coefficients are explicitly affected by the presence of the particulate phase; and 3) the phenomenological model proposed to account for this effect appears realistic.

B. Nonreacting Lateral Mixing

Representative results obtained during this phase of the investigation are given in Figs. 7–10.

Figure 7 shows the total-temperature profiles measured at three axial stations for the single phase underexpanded configuration (Configuration 16). Superimposed on this figure are theoretical predictions for the jet plume showing both the axis of the jet as well as the lateral spread. As may be noted, reasonable agreement between experiment and theory is achieved insofar as the jet axis is concerned. That is, the points of minimum temperature indicated by the measure-

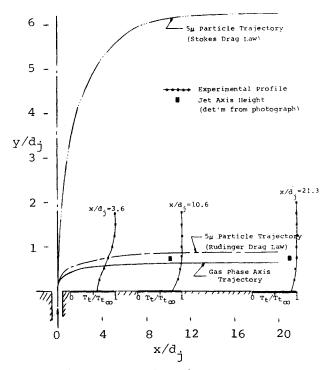


Fig. 8 Comparison, theory/experiment, nonreacting lateral mixing, Configuration 18.

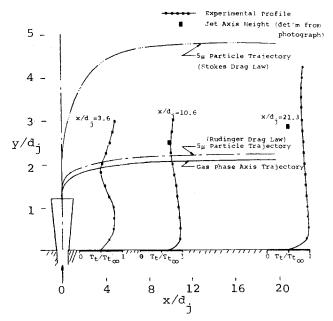


Fig. 9 Comparison, theory/experiment, nonreacting lateral mixing, Configuration 19.

ments essentially coincide with the theoretically predicted plume axis. The boundaries of the plume, of course, are underestimated by the analysis but this is consistent with the essentially inviscid character of the theoretical model. Nevertheless, it is clear that the means for making reasonable estimates for the extent of the jet spreading is provided by this analysis.

Corresponding results for two-phase flows for a matched and an underexpanded case are shown in Figs. 8 and 9, respectively. In this case the experimental data include not only the total-temperature variation but the location of the axis of the particle cloud as determined from the photographs. (Hardware configurations precluded photographic determination of the cloud axis at the first profile station.) Furthermore, two different theoretical predictions are shown corresponding to two choices of the particle drag law. Several important conclusions can be drawn from an examination of these results. First, it would appear that the solid and gas phases remain "locked" together. That is, the axis of the particle cloud determined experimentally is more or less coincident with the center of the disturbed region as reflected by the total temperature distribution. This result, of course, gives rise to a second important conclusion: viz., a Stokes

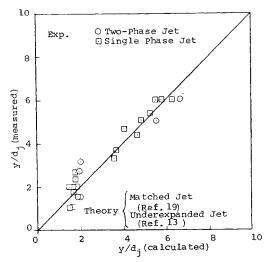


Fig. 10 Comparison, theory/experiment, jet penetration.

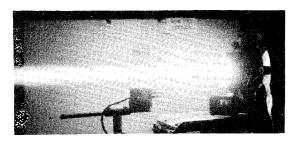


Fig. 11 Representative flame pattern obtained with boron combustion, Configuration 11.

drag law is clearly inappropriate for the configuration which is involved here. That is, since the particles are subjected to rapid acceleration, it would appear that the drag law due to Rudinger which was developed empirically from studies in which such acceleration prevailed, is the more appropriate choice.

Finally, it should be noted that for the underexpanded case (Fig. 8) the prediction underestimates somewhat the jet axis penetration. The cause of this discrepancy is not clear at this time. Nevertheless, it is suggested that the proposed model can be utilized to provide a first estimate for this behavior particularly if it is supplemented by simultaneous utilization of certain penetration correlations which are currently available. Two of these correlations (Refs. 13 and 19) have been utilized to generate predictions which have been compared with experimental data in Fig. 10. It should be noted here that a) for single-phase tests, penetration is defined as the point where the total temperature is 0.995 of the external value, b) for two-phase tests penetration corresponds to the edge of the particle cloud as determined from the photographs, and c) two different correlation laws have been applied depending upon whether the jet was underexpanded or matched, i.e., for underexpanded cases it was found that the data were best correlated by the method of Ref. 13, while for the matched cases better agreement is provided by the formulation of Ref. 19. It is also important to note here that the aforementioned correlations were developed for single-phase configurations. Thus, the agreement which is evidenced with two-phase results implies that an assumption of dynamic equilibrium between the phases would be valid.

In summary it may be concluded that for the range of environmental conditions examined: the particles remain "locked" with the gas phase stream; reasonable estimates of jet penetration can be obtained using existing empirical relations; and the particle trajectory analysis which utilizes a Rudinger drag law yields predictions which are in good agreement with experimental results.

C. Combined Mixing and Combustion

As indicated in Sec. III.D, the data retrieved in this phase of study were of the qualitative type, i.e., photographs, visual observations, etc. From the photographic evidence, of which Fig. 11 is a typical example, from visual observations, and from the high rates of attrition of the hardware components, the feasibility of burning boron in a supersonic stream has been clearly demonstrated. However, combustion efficiencies are not as yet well defined.

In summary, it is concluded that supersonic combustion of solid boron is feasible, and that, at least in a qualitative sense, the possibility of attaining substantial heat release within distances of practical interest may be anticipated. It is apparent, however, that additional work must be conducted in order to verify this latter conclusion in a quantitative sense.

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