JTTEE5 5:185-195

Gas-Particle Interaction in Detonation Spraying Systems

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A model is developed to describe dynamic interaction of particles with the carrier gas during detonation spraying. Equations of mass, energy, and momentum conservation are integrated numerically for the two-phase particle-gas flow with the Hugoniot boundary conditions at the detonation wave front. Velocity and temperature of the sprayed powder and the gas parameters are calculated self-consistently, taking into account effects of friction and cooling of the gas in the vicinity of the gun barrel and effects of particle-gas interaction on the parameters of the gas phase. Calculations are performed for tungsten carbide particles of 30 μm diam and a 1.8 m long detonation gun using a stoichiometric mixture of oxygen and propane. Distributions of gas and particle parameters along the barrel are calculated for various moments of time. Tungsten carbide particles of 30 μm reach an exit velocity of 1278 m/s and a temperature of 1950 K. Exit particle velocity is a nonmonotonic function of the loading distance, *L*, with a distinct maximum at *L* = 75 cm. The proposed model can be applied to a broad range of problems related to detonation coating technology and allows evaluation of the effectiveness of various designs and optimization of operational parameters of detonation spraying systems.

1. Introduction

FUTURE PROGRESS of thermal spray technology and design of more advanced thermal spray equipment depends on understanding the fundamental principles of thermal spray processes and, in particular, knowledge about gas dynamics and thermodynamics of the two-phase gas-particle flow inside the spraying device. For example, use of a Laval nozzle (Ref 1), combination of subsonic and supersonic accelerating channels, and use of additional heating channels (Ref 2) allow improvements in the quality of the high-velocity oxygen fuel (HVOF) process and allow better control of the sprayed powder parameters. Knowledge about predetonation distances, critical cross sections for detonation wave propagation, and limits of detonability in various gas mixtures is essential for good design of gas detonation coating systems.

While many investigations have focused on studying the gas dynamics and modeling the HVOF thermal spray process (Ref 3-5), little research was directed to the study of the gas detonation coating process (Ref 6-8). Consequently, there is little understanding of the fundamental principles of detonation gun operation and the mechanisms of detonation coating formation. This paper presents a model that analyzes gas dynamics of the conventional detonation gun during the spraying process. The model allows the calculation of the thermodynamic parameters of the gas mixture and sprayed particles. Results are presented for a 1.8 m long detonation coating gun operating on oxygen propane mixture and spraying tungsten carbide particles with the diameter of 30 μm.

This paper is organized as follows. Section 2 describes several designs of detonation coating systems and some parameters of their operation. Section 3 reviews known analytical solutions for the parameters of detonation products behind the detonation wave front. These solutions can be used for rough evaluation of detonation parameters and a fast estimate of the velocity and

Nomenclature

c	Speed of sound, m/s
C_d	Drag coefficient
c_p	Specific heat at constant pressure, J/kg · K
c_v	Specific heat at constant volume, J/kg · K
D	Velocity of detonation wave front, m/s
F_d	Gas particle drag force
h	Specific enthalpy, J/kg
k	Coefficient of heat conduction, W/m · K
n	Concentration, m^{-3}
Nu	Nusselt number
p	Pressure, Pa
Q	Specific energy of detonation, J/kg
r	Powder particle radius, m
Re	Reynolds number
S	Entropy
T	Temperature, K
t	Time, s
u	Velocity, m/s
x	Coordinate along the gun barrel, m

Greek symbols

γ	$\gamma = c_p/c_v$ coefficient
ε	Specific internal energy, J/kg
μ	Viscosity, kg/m · s
ν	Specific volume, m^3/kg
ρ	Density, kg/m^3
τ	Friction force
λ	Heat exchange with particles

Subscripts

g	Gas parameters
p	Particle parameters
1	Gas parameters before the detonation front

Keywords Chapman-Jouguet point, detonation gun, gas detonation, shock wave

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temperature of the sprayed particles. Section 4 formulates basic equations describing the dynamics of two phase flow inside the detonation gun. The described approach accounts for the effects of friction and cooling of the gas in the vicinity of a gun barrel and effects of particles on the parameters of detonation products. Section 5 describes the boundary conditions and the numerical procedure that was used to solve gas dynamics equations. Section 6 presents calculation results. Better understanding of fundamental principles of the complex gas detonation coating process will allow optimization of gas detonation coating technology and expand its application.

2. Background

2.1 *Principles and Operational Parameters of Detonation Spraying Systems*

Whereas most of the thermal spray techniques use continuous sources of energy to accelerate sprayed powder, the gas detonation coating process is intermittent by nature. The typical detonation coating gun (Fig. 1) consists of (1) the accelerating channel of rectangular or round cross section, which is closed at one end, combined with the systems of (3) powder and (2) gas supply, and (4) the ignition system, which periodically generates the ignition spark inside the channel. Particular designs of gas and powder supply systems as well as the gun barrel geometry vary and are discussed here. The operating cycle of the detonation gun includes the following stages (Ref 9). The channel is filled with a fuel mixture at atmospheric pressure and room temperature, and the powder is injected into the accelerating channel. The mixture is then ignited by a spark plug. This produces a wave of deflagration (combustion) that propagates along the channel. If the detonation conditions are satisfied (limits of detonation in gas composition, pressure, temperature), the deflagration wave transforms into a detonation wave after passing a distance called the predetonation distance, *L*. The detonation wave is characterized by the very stable thermodynamic parameters and represents a shock wave, which initiates a chemical reaction in the gas mixture by the action of great pressure and temperature in the wave front. The detonation wave and hot detonation products accelerate and heat the powder particles, which form (6) a hard coating upon collision with (5) the substrate. Then, the barrel is purged with inert gas (this stage can be eliminated in some designs) and filled with a fuel gas, and the process repeats with the frequency of 1 to 15 Hz. The extreme parameters of the detonation wave (supersonic speed, strong gas compression) typically produce excellent quality coatings (Ref 7, 10) of metals, carbides, oxides, or compounds.

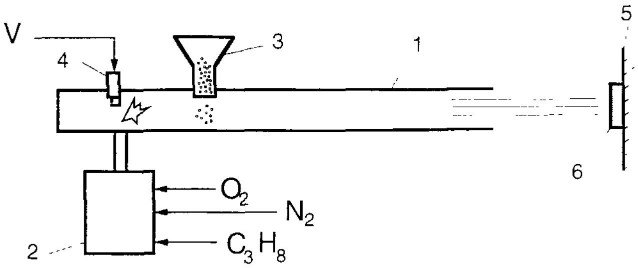

Fig. 1 Schematic diagram of gas detonation coating process 1, accelerating channel; 2, gas supply system, 3, powder feeder, 4, spark plug; 5, substrate; 6, coating

Two unique features separate the gas detonation coating process from other coating technologies. Firstof them is an extremely low amount of heat transfer to the gun barrel and to the sprayed substrate. The detonation process occurs on a very short time scale and is "almost adiabatic." The velocity of the detonation wave depends on the type of fuel gas used and on the volume fraction of the fuel gas in the combustible mixture. It ranges from 1090 m/s in the reaction of carbon monoxide and oxygen, $2CO + O_2$, to 3525 m/s in the detonation of hydrogen, $H_2 + 0.5O_2 + 2.5H_2$. For such velocities, it takes the detonation products and the powder particles an average of 0.5 to 4.0 ms to exit the barrel. This point is illustrated in Fig. 2, which shows exit of detonation products from the detonation gun barrel. The time interval between the photographs is 50 μs. During this short time, the amount of heat transferred to the sample and the gun barrel is very low. Typically the substrate temperature stays below 150 °C, and with additional cooling, it can be brought down to room temperature. This fact makes the detonation process very suitable for spraying low-melting point materials and precision parts without the risk of causing chemical transformations and deformations in them. It makes it possible to spray powders that may evaporate at high temperatures, for example boron carbide. The intermittent nature of the process also allows simplification of the gun cooling system or even complete elimination of it.

A second feature of the process is the simplicity of operation and reliability. High-pressure gas and cooling water supply systems are not needed. Typical gas pressures are 1 atm, and the cooling water flow rate is 0.1 to 0.2 gal/min, which is much lower than for a typical HVOF spraying system. Consumption of electrical power is minimized to 100 W (Ref 11). These features make the process very economical in industrial conditions. Good designs of gas detonation systems should provide the conditions necessary for stable existence of the detonation wave and for maximum utilization of energetic potential of the particular gaseous mixture used. Geometry of the gun barrel and design of the powder supply system, which influences reliability and efficiency of the detonation system, can greatly affect the overall quality of the system.

Selection of geometrical parameters of the system is closely related to the properties of the combustible mixture. Numerous gases have the detonation effect in reaction with oxygen at normal conditions. Among them are hydrogen H_2, carbon monoxide CO, methane CH_4, acetylene C_2H_2, propane C_3H_8, penthane C_5H_{12}, benzene C_6H_6, carbon disulfide CS_2, dicyan C_2N_2, and others. In principle, they all can be used for detonation spraying, and they produce reactions at different temperatures and detonation speeds. For example, reaction temperature in the reaction $H_2 + 0.5O_2$ in the presence of nitrogen is 2596 K whereas in the reaction of dicyan $C_2N_2 + O_2$, the temperature is 5960 K (Ref 12). Among the commonly used detonation spraying fuel gases is acetylene, which produces high velocity (3091 m/s) detonation wave, high temperature of the reaction (5570 K), and large compression ratio (55.4) (Ref 12). Acetylene has a very short predetonation distance of a few centimeters and can be detonated easily. Other commonly used fuel gases are propane, butane, methane, propylene, and their mixtures. These natural gases are safer in use and cheaper. However, they have longer predetonation distances of 40 to 80 cm, which must be taken into account in the design of the detonation barrel.

Experiments indicate that predetonation distance in a given fuel mixture depends on many parameters (Ref 13). Pressure increase reduces predetonation distance, whereas temperature increase makes predetonation distance longer. Increase of pressure at room temperature from 1 to 6.5 atm reduces predetonation distance in the $2H_2 + O_2$ mixture from 70 to 27 cm, and temperature increase at 1 atm from 15 to 180 °C results in an increase of L from 60 to 78 cm. A great influence is exerted on predetonation distance by the length and diameter of the detonation barrel (Ref 14). When the barrel becomes too short, the detonation disappears, and there is a transition to vibration type propagation (Ref 15). An increase in the barrel length and diameter results in an increase of predetonation length. The detonation velocity is affected very little by the pressure and temperature of the mixture before ignition and is mainly determined by the mixture composition; i.e., the type of fuel gas and the fuel/oxygen mass ratio in the final mixture. The detonation velocity increases slightly with increasing pressure; however, this effect is most noticeable at low pressures and gradually fades with increasing pressure. For the $2H_2 + O_2$ mixture at 2 atm pressure, this effect disappears. An increase in temperature decreases the velocity slightly.

Internal roughness of the barrel walls has a large effect on both the velocity of the wave, which decreases with the increase of roughness, and the predetonation length. In polished tubes, the value of L is usually 20 to 40 tube diameters. Increase in the internal barrel wall roughness reduces the predetonation length greatly. In rough tubes, the detonation may originate at a distance of 2 to 4 diameters from the ignition source (Ref 16). Typically powder is injected into the barrel with the help of additional carrier gas, for example nitrogen (Ref 18, 29). Also, neutral noncombustible gases could be used to purge the barrel after the detonation cycle is complete. Some of this gas blends with the new portion of fuel mixture and affects parameters of detonation. Experiments and calculations (Ref 12) show that the addition of light gases, such as hydrogen, increases the detonation speed, although the reaction temperature is reduced. Addition of heavy gases, such as nitrogen, reduces both the temperature and the velocity of detonation. These ideas are reflected in designs of detonation coating systems, which are briefly reviewed here.

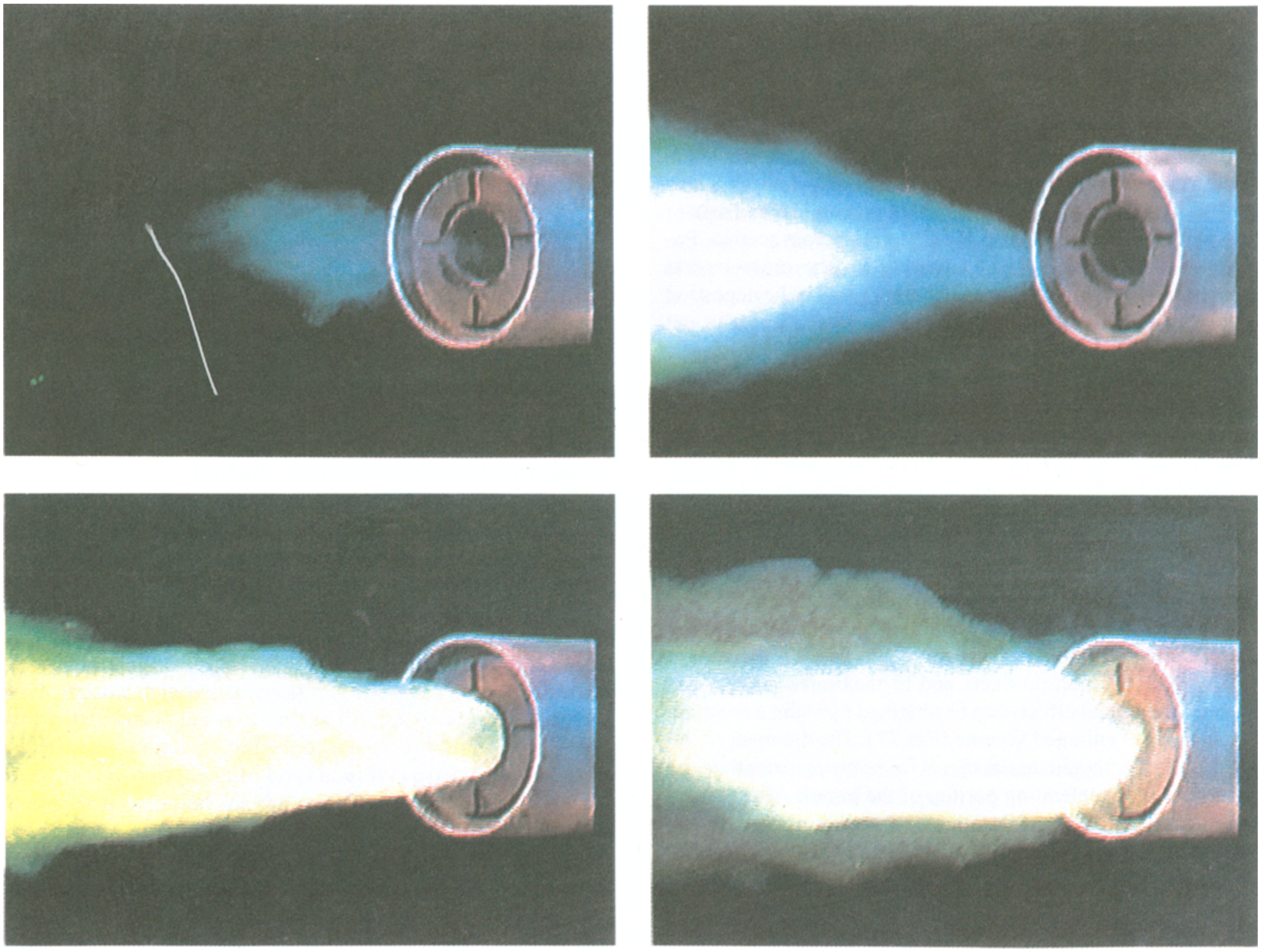

Fig. 2 Products of gas detonation at the exit from the coating gun Photographs are taken with the time interval of 50 μs.

2.2 *Designs to Produce Gas Detonations*

Gas detonation coating systems and some of their applications are described in Ref 17 to 31. Part of this work covers particular detonation coatings for applications (Ref 19-21) or devices for powder or gas injection (Ref 25, 27, 31) to be used with detonation systems. Principal designs of detonation coating systems are described in Ref 18, 22, 27, 28, and 29. All of these designs provide the conditions necessary for the existence of stable detonation in the barrel and for the prevention of backfiring, namely propagation of the detonation into the gas supply means.

Backfiring creates an operational hazard, may destroy gas supply means, and represents an important problem to be considered in each design. The original design by Pelton and Cowden (Ref 18) is an automatic gas detonation system with internal fuel mixture formation and radial powder injection. Nitrogen is used to purge the apparatus, and backfiring is prevented by the system of mechanically controlled valves. Oxygen and acetylene are supplied at equal pressure to the barrel. Imprecise operation of the pressure reducers in the gas lines for such a design may result in propagation of oxygen into the fuel line and vice versa. This may create the detonation in the gas lines and damage the equipment. Injection of fuel mixture components into the combustion chamber, which is used successfully in HVOF-type devices, turned out to be inefficient and did not guarantee safe operation of detonation systems. The buffer tube can be used to prevent backfiring. The tube is installed between the gas mixing chamber and the main barrel and is filled with nitrogen gas periodically. Application of special flame quenchers made of porous materials and narrow ducts as damping devices is also possible (Ref 28). A detonation barrel of rectangular and square cross section can be used instead of the round cross section. Parameters of detonation depend weakly on the cross-section shape; however, a square-shaped chamber enables the deposited material to be utilized more completely and efficiently and makes it possible to obtain a coating more uniform in thickness than that obtained with a round-shaped combustion chamber.

The following features can be used to classify detonation systems: (a) way to form a fuel gas mixture; that is, systems with direct mixture formation (Ref 18, 19) and with preliminary gas mixing (Ref 23); (b) way to supply mixture into the barrel; that is, systems with continuous (Ref 28), or intermittent fuel supply (Ref 18); (c) way to inject powder into the barrel; that is, systems with radial or axial powder injection; (d) way to ignite the mixture, that is direct or forecamera "preliminary" ignition.

Reference 23 describes the system with forecamera ignition and injection type of mixture formation. It is possible to increase velocity of detonation products and to maximize powder parameters. Beneficial effects can be obtained by using a combustion chamber of enlarged volume (Ref 27). The diameter of the combustion chamber in this design is four times greater than the diameter of the accelerating portion of the barrel. After the 1:1 oxygen-acetylene mixture is ignited, detonation starts in the combustion chamber. Velocity of the detonation products behind the wave is 1230 m/s. Pressure is 4.3 MPa, and temperature is 4500 K. After the narrow part of the chamber is entered, velocity, pressure, and temperature can be increased greatly. For example, a four-fold decrease in a channel cross section will increase the pressure to 6.8 MPa, and the temperature to 5150 K. Typically, the cooling system is necessary to keep the barrel temperature low and to prevent self-ignition and continuous combustion of the gas.

Practical experience and experiments indicate that the promising direction of industrial detonation system designs is through creating systems with internal mixture formation, continuous gas supply, and propane-butane-oxygen fuel mixture operation (Ref 9). All modern gas detonation coating systems utilize the same principle; i.e., acceleration of powder by the detonation wave in the gaseous mixture and, by following it, hot products of detonation. Thus, detailed analysis of interactions in such a system represents great practical importance and is considered in detail in Section 3.

3. Propagation of the Detonation Wave inside the Coating Gun: Analytical Solutions

Propagation of the detonation wave in a coating gun barrel can be described in one-dimensional approximation because the length of the detonation barrel is typically greater than its diameter by a factor of 40 to 80. In this case, the curvature of the detonation wave front can be neglected, and gas properties can be calculated as a function of two major parameters: coordinate along the barrel, x, and time, t. Such a one-dimensional problem has an analytical solution, provided that effects of friction and viscosity are neglected and the gas is considered to be ideal.

Various aspects of this problem are treated in detail in Ref 32 to 36. Reference 32 provides calculations of detonation wave parameters in a shock tube and compares the results with experimental data. Computer code is developed in Ref 38, which calculates properties of the detonation wave inside the barrel. This section reviews only basic gasdynamic equations, which are further modified in section 4 to account for the effects of friction and viscosity, and the solutions for gas parameters in the case of strong detonations. These solutions have practical importance in evaluating a detonation system operation and can be used to estimate particle parameters quickly (Ref 37).

Propagation of the detonation wave in a gun barrel is a strongly nonequilibrium process on a millisecond time scale. During such a process, all major gas parameters, such as speed u, pressure p, density ρ, and local speed of sound c are functions of both the coordinate x and the time t. These quantities obey fundamental equations of mass, momentum, and energy conservation, which in the one-dimensional case are:

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u)}{\partial x} = 0 \qquad \text{(Eq 1)}$$

$$\frac{\partial(u\rho)}{\partial t} + \frac{\partial}{\partial x}(p + \rho u^2) = 0 \qquad \text{(Eq 2)}$$

$$\frac{\partial}{\partial t}\left(\rho\varepsilon + \frac{\rho u^2}{2}\right) + \frac{\partial}{\partial x}\left(\rho u\left(\varepsilon + \frac{u^2}{2}\right) + pu\right) = \rho Q \qquad \text{(Eq 3)}$$

where ε is the specific internal energy of the gas and Q is specific energy released in the combustion reaction.

Assuming that the detonation wave front has negligible thickness and integrating Eq 1 to 3 over small volume containing the wave front, one can obtain the conditions relating the gas parameters before and behind the propagating wave front:

$$\rho_2 u_2 = \rho_1 u_1 \qquad \text{(Eq 4)}$$

$$p_2 + \rho_2 u_2^2 = p_1 + \rho_1 u_1^2 \qquad \text{(Eq 5)}$$

$$h_2 + \frac{u_2^2}{2} = h_1 + \frac{u_1^2}{2} + Q \qquad \text{(Eq 6)}$$

Here subscript 1 denotes parameters of the undisturbed gas before the detonation wave front, subscript 2 denotes parameters of the gas in the immediate vicinity behind the front, u is velocity of gas with respect to the detonation wave front, and $h = \varepsilon + pv$ is the specific enthalpy.

Eliminating the velocities u_1 and u_2 from Eq 4 to 6, the Hugoniot conditions can be obtained:

$$h_1 - h_2 + Q = \frac{p_1 - p_2}{2}(v_1 + v_2) \qquad \text{(Eq 7)}$$

$$\varepsilon_1 - \varepsilon_2 + Q = \frac{p_2 + p_1}{2}(v_2 - v_1) \qquad \text{(Eq 8)}$$

where v is the specific volume. These conditions describe the Hugoniot adiabat and relate the pressure and specific volume of the detonation products to the parameters of initial mixture p_1 and v_1 and the reaction energy Q.

At the Chapman-Jouguet point (Ref 39) on the Hugoniot curve, an additional condition is introduced:

$$\left(\frac{\partial p_2}{\partial v_2}\right)_S = \frac{p_2 - p_1}{v_1 - v_2} \qquad \text{(Eq 9)}$$

where S is the entropy. When this condition is used in Eq 1 to 6, all major parameters of the detonation products are calculated and expressed as a function of Q, p_1, v_1, and $\gamma = c_p/c_v$, where c_p and c_v are the gas specific heats at constant pressure and volume. All expressions are greatly simplified for the case of strong detonations; i.e., the detonation reactions in which the amount of energy Q released in the reaction is much greater than the internal gas energy. The condition of strong detonation is expressed as $Q/\varepsilon >> 1$, which is equivalent to the condition $Q/c_1^2 >> 1$, where $c_1 = \sqrt{(\gamma_1 p_1/\rho)}$ is the speed of sound in the initial mixture. It is easy to see that this condition is satisfied for the reactions of acetylene-oxygen and propane-oxygen used in a modern detonation system. In the reaction $C_3H_8 + 5O_2 \leftrightarrow 3CO_2 + 4H_2O$, the amount of energy released is 2.05 MJ/mol. Estimating the speed of sound in the initial mixture at normal conditions to be 275 m/s, we obtain $Q/c_1^2 \approx 40$; thus the limit of strong detonations (Ref 33) can be used in further calculations. Solution of Eq 1 to 6 with the condition in Eq 7 and the equation of state for ideal gas results in the following expressions. The velocity of detonation wave front in the laboratory coordinate system is $D = u_1$:

$$D = \sqrt{2Q(\gamma_2^2 - 1)} \qquad \text{(Eq 10)}$$

Pressure of the detonation products is:

$$p_2 = 2\gamma_1(\gamma_2 - 1)\frac{Q}{c_1^2}p_1 \qquad \text{(Eq 11)}$$

Velocity of the detonation products in the laboratory coordinate system is:

$$u_2^* = c_1\sqrt{2\frac{\gamma_2 - 1}{\gamma_2 + 1}\frac{Q}{c_1^2}} \qquad \text{(Eq 12)}$$

Specific volume of detonation products is:

$$v_2 = \frac{\gamma_2}{\gamma_2 + 1}v_1 \qquad \text{(Eq 13)}$$

Density of detonation products is found from $\rho_2/\rho_1 = v_1/v_2$. Temperature of the reaction is:

$$T_2 = \frac{2\gamma_2}{\gamma_2 + 1}\frac{Q}{c_{v^2}} \qquad \text{(Eq 14)}$$

On the basis of these simple relations, parameters of the detonations in different gases can easily be evaluated, and selection of the optimized mixture composition can be made for a particular detonation coating application. Accelerating action of the gas can be characterized by the number $\rho_2 u_2^2$ (gas dynamic pressure), which is proportional to the gas kinetic energy density. Calculation of this number for acetylene, propane, and dicyan results in 3.090, 2.72, and 4.25 ($\times 10^6$ kg/ms^2), respectively. This shows good potential of the C_2N_2 mixture for spraying hard melting materials such as carbides. Assuming that the γ coefficient does not change during the reaction and using general solution of gasdynamics equations (Ref 34) in the form $x = (u + c)t + F(u)$ and $u = [2/(\gamma - 1)]c + \text{const}$ with the boundary conditions at $t = 0$, $x = 0$, $u = D/(\gamma + 1)$, and $c = \gamma D/(\gamma + 1)$, one obtains $F(u) = 0$ and $\text{const} = (D/\gamma) - 1$. Substituting this into general solution, we get:

$$u(x,t) = \frac{2}{\gamma + 1}\left(\frac{x}{t} - \frac{D}{2}\right) \qquad \text{(Eq 15)}$$

which describes velocity distribution behind the wave front. Distribution of the sound speed is:

$$c(x,t) = \frac{\gamma - 1}{\gamma + 1}\frac{x}{t} + \frac{D}{\gamma + 1} \qquad \text{(Eq 16)}$$

Distributions of density and pressure of detonation products are related to $u(x,t)$ and $c(x,t)$ by:

$$u = \frac{D}{2}\left(1 + \ln\frac{\rho}{\rho_2}\right) \qquad \text{(Eq 17)}$$

and $c^2 = \gamma p/\rho$.

Figure 3 shows calculated distributions of velocity and speed of sound. The velocity profile in the detonation pulse and the speed of sound are linear functions of coordinate x. The coordinate of the detonation wave front is given by Dt. Behind the wave front, velocity of detonation products linearly decreases and reaches zero at point $x = Dt/2$. From $x = 0$ to $x = Dt/2$, velocity of gas is equal to zero, and speed of sound is constant. Since the dependence on time and coordinate enters all expressions in a form x/t, the motion of the gas in a detonation gun barrel represents an example of self-similar motion (Ref 34). The width of detonation pulse increases as it propagates.

Figure 4 shows the calculated distribution of pressure for three different moments of time in the stoichiometric propane-oxygen mixture. The above solutions are valid only until the front of the detonation wave reaches the exit cross section of the gun. After this happens, the rarefaction low-pressure wave starts to propagate inside the barrel. Equations 4 to 6 are no longer valid because the flow cross section changes and solutions have to be found by numerical integration of Eq 1 to 3. A peculiar form of velocity and pressure distributions result in the non-monotonic nature of powder acceleration in a detonation spraying device (Ref 37). Since the gas temperature during the detonation reaction reaches 3000 to 5000 K while the initial temperature of the injected particles is low and the temperature of the internal barrel wall is below 400 K, the large thermal gradients are created inside the gun. The estimate shows that close to the barrel wall, value of thermal gradient may reach 10^5 degrees/m. Such high values of thermal gradients affect the gas phase temperature and have to be taken into account in the detonation process model. Calculations also demonstrate that gas parameters are affected strongly by the presence of particles and friction at the barrel walls (Ref 40, 41). These effects change parameters of the detonation wave and can be described by including special terms in the conservation laws, which are described in section 4.

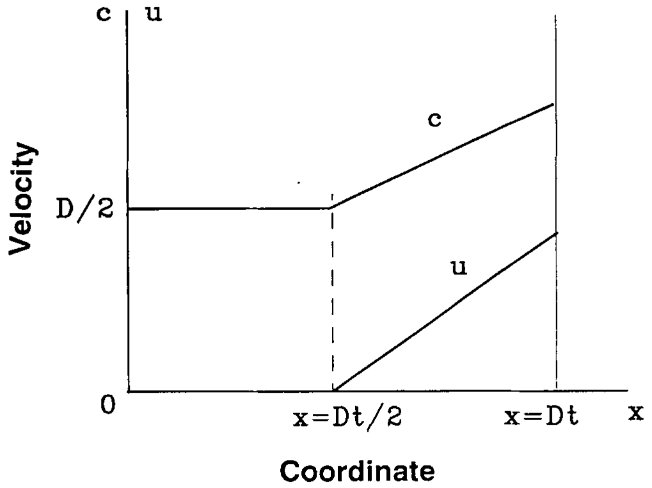

Fig. 3 Qualitative distributions of speed of sound and gas in one-dimensional detonation pulse c is speed of sound, u is speed of gas, D is speed of detonation wave front, and x is coordinate along the direction of wave propagation.

4. Basic Equations and Computational Technique

4.1 *Conservation Laws for Two-Phase Flow inside the Detonation Coating Gun*

The problem of detonation spraying can be formulated as follows. Initially the gun barrel is filled with a gas mixture and powder particles, which are located at some point x_0 inside the barrel or distributed uniformly with the density n. Conditions and composition of the mixture are known. At $t = 0$, the detonation wave is initiated at a closed end of the barrel and starts to propagate toward the open end of the barrel. The goal is to calculate parameters p, u, T, and ρ for the gas and u and T for particles at time $t > 0$. Since the parameters of the gas are affected by the particles while particle acceleration is caused by the action of hot gas detonation products, the natural way to approach this problem is to solve equations describing gas and particle phases simultaneously (Ref 42, 43). We use a two-phase continuum model that assumes that the continuous gas phase having the concentration n_g is mixed with continuous second phase (particles), having the concentration n. There is friction between the gas phase and the barrel walls, and the gas phase and the particles. Therefore two additional "friction" terms have to be introduced into momentum conservation Eq 2. Gas-particle drag force F_d is described by (Ref 37):

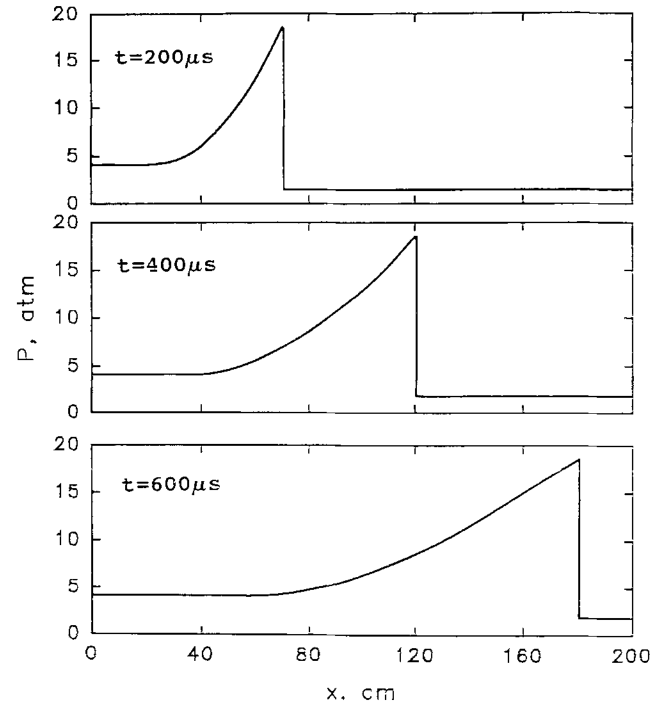

Fig. 4 Distribution of pressure P (atm) in the propane-oxygen detonation pulse at three different moments of time: t = 200 μs, t = 400 μs, t = 600 μs x (cm) is the coordinate along the direction of wave propagation

$$F_d = \frac{\pi r^2 n C_d |u_g - u_p|(u_g - u_p)}{2n_g} \qquad \text{(Eq 18)}$$

where subscript p refers to particles, subscript g refers to gas, r is the particle radius, C_d is the drag coefficient (Ref 44), and n is powder concentration. The friction force τ in the vicinity of the barrel walls was covered in Ref 45 and is given by:

$$\tau = -0.5 f n_g \rho_g |u_g| u_g \qquad \text{(Eq 19)}$$

where f is the coefficient equal to $0.046 \times \mathrm{Re}^{-0.2}$. Two corresponding energy terms have to be added to Eq 3. This equation also has to be completed with terms describing heat exchange processes of the gas with particles and the gun barrel. Heat exchange with particles (Ref 46) is described by:

$$\lambda = \frac{2\pi r n k \ \mathrm{Nu}\ (T_p - T_g)}{n_g \rho_g} \qquad \text{(Eq 20)}$$

where k is the coefficient of heat conduction and Nu is Nusselt number. Heat exchange with the gun barrel (Ref 46) is described by:

$$\lambda_1 = \frac{\tau c_p (T_b - T_g)}{u_g} \qquad \text{(Eq 21)}$$

where T_b is the barrel temperature, which is assumed to be constant. We also assume that $n_g \approx 1 >> n_p$, and that the amount of energy Q supplied to the system is zero behind the detonation wave front. There is some uncertainty in the values of coefficients τ, λ, and λ_1 employed. It comes from the unsteadiness of the viscous flow near the wall, which can be out of phase with the mean flow away from the wall. The friction coefficient f was determined in Ref 45. Experimental research of this effect and gas heating effects was carried out in Ref 49. Finally, the system of equation describing the gas phase is written as:

$$\frac{\partial \rho_g}{\partial t} + \frac{\partial(\rho_g u_g)}{\partial x} = 0 \qquad \text{(Eq 22)}$$

$$\frac{\partial(\rho_g u_g)}{\partial t} + \frac{\partial}{\partial x}(p + \rho_g u_g^2) = \rho_g F_d + \frac{2\tau}{R} \qquad \text{(Eq 23)}$$

$$\frac{\partial}{\partial t}\left[\rho_g\left(\varepsilon_g + \frac{u_g^2}{2}\right)\right] + \frac{\partial}{\partial x}\left[\rho_g u_g\left(\varepsilon_g + \frac{u_g^2}{2} + \frac{p}{\rho_g}\right)\right]$$

$$= \rho_g u_g F_d + \frac{2u_g\tau}{R} + \rho_g\lambda + \frac{2\lambda_1}{R} \qquad \text{(Eq 24)}$$

Here R is the radius of the detonation gun barrel. Energy of the gas phase is related to its pressure and density by the equation of state. For the particle phase, the corresponding equations are:

$$\frac{\partial n}{\partial t} + \frac{\partial(n u_p)}{\partial x} = 0 \qquad \text{(Eq 25)}$$

$$\frac{\partial(u_p)}{\partial t} + \frac{\partial(u_p^2)}{\partial x} = nF_{dp} \qquad \text{(Eq 26)}$$

$$\frac{\partial}{\partial t}\left[n\left(\varepsilon_p + \frac{u_p^2}{2}\right)\right] + \frac{\partial}{\partial x}\left[u_p\left(\varepsilon + \frac{u_p^2}{2}\right)\right] = u\lambda + u_p F_{dp} \qquad \text{(Eq 27)}$$

The drag F_{dp} exerted on the particles by the gas phase is related to drag F_d by the relation $F_{dp} = -(\rho_g F_d / n_p \rho_p)$. The particle internal energy is given by $\varepsilon_p = c_p T$, where c_p is particle specific heat. Equations 22 to 27 describe the behavior of gas and particles inside the detonation gun during the detonation pulse propagation and are connected through their right-hand side and must be solved simultaneously.

5. Numerical Procedure and Boundary Conditions

After transformations and renormalization of parameters are put into dimensionless form, the system of equations 22 to 24 is reduced to:

$$\frac{\partial u_g}{\partial t} + \frac{1}{\rho c}\frac{\partial p}{\partial t} +$$

$$(u_g + c)\left(\frac{\partial u_g}{\partial x} + \frac{1}{\rho c}\frac{\partial p}{\partial x}\right) = \alpha_0\alpha + \beta_0\beta + \gamma_0\gamma + \omega_0\omega \qquad \text{(Eq 28)}$$

$$\frac{\partial u_g}{\partial t} - \frac{1}{\rho c}\frac{\partial p}{\partial t} +$$

$$(u_g - c)\left(\frac{\partial u_g}{\partial x} - \frac{1}{\rho c}\frac{\partial p}{\partial x}\right) = -\alpha_0\alpha + \beta_0\beta + \gamma_0\gamma - \omega_0\omega \qquad \text{(Eq 29)}$$

$$\frac{\partial S}{\partial t} = u_g \frac{\partial S}{\partial x} = \xi_0\xi \qquad \text{(Eq 30)}$$

where S is the entropy, and α_0, β_0, γ_0, ω_0, and ξ_0, renormalization coefficients and parameters on the right-hand side, are given by:

$$\alpha = \frac{n\mathrm{Nu}(T_p - T_g)}{\rho_g c} \qquad \text{(Eq 31)}$$

$$\beta = nC_d |u_p - u_g| (u_g - u_p) \qquad \text{(Eq 32)}$$

$$\gamma = -f|u_g|u_g \qquad \text{(Eq 33)}$$

$$\omega = \frac{f|u_g|(T_b - T_g)}{c} \qquad \text{(Eq 34)}$$

$$\xi = \frac{n\mathrm{Nu}(T_p - T_g)}{\rho T_g} \qquad \text{(Eq 35)}$$

The system of equations describing the particle phase after transformations and renormalization is reduced to:

$$\frac{du_p}{dt} = \eta_0 \eta \qquad \text{(Eq 36)}$$

$$\frac{dn}{dt} = -n\frac{\partial u_p}{\partial x} \qquad \text{(Eq 37)}$$

$$\frac{dT_p}{dt} = \delta_0 \delta \qquad \text{(Eq 38)}$$

Here d/dt is equal to $\partial/\partial t + u_p(\partial/\partial x)$, coefficients η_0 and δ_0 are renormalization constants, and:

$$\eta = \rho C_d |u_p - u_g|(u_g - u_p) \qquad \text{(Eq 39)}$$

$$\delta = \mathrm{Nu}(T_g - T_p) \qquad \text{(Eq 40)}$$

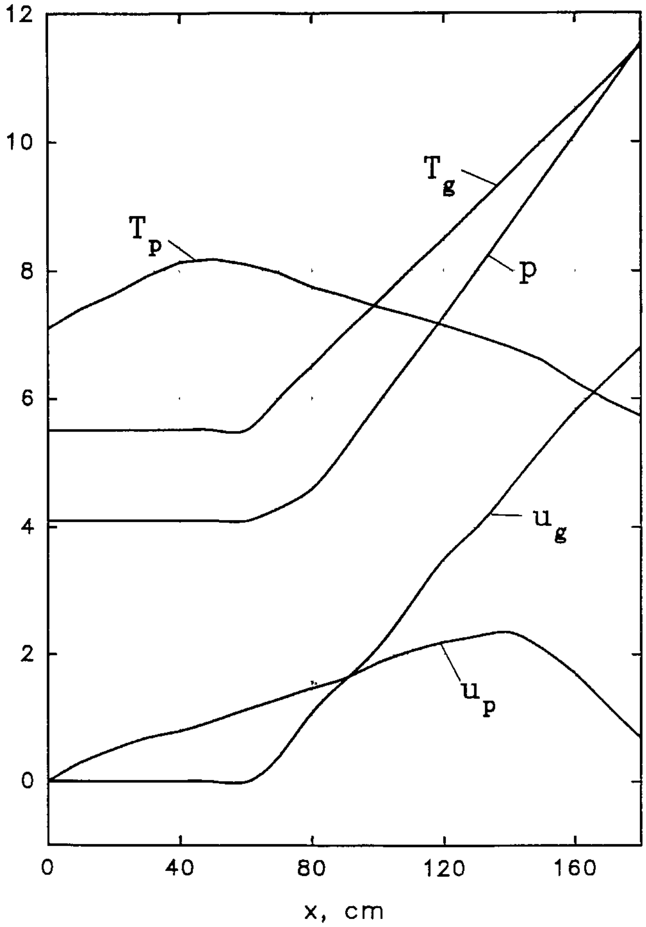

Fig. 5 Gas parameters (p is pressure, T_g is temperature, u_g is velocity) and particle parameters (T_p is temperature, u_p is velocity) at $t = 0$. Vertical axis is in dimensionless units. To obtain real parameter values, the dimensionless values have to be multiplied by corresponding factors p by 1.58 atm, T_p and T_g by 195 K, u_g by 283 m/s, and u_p by 180 m/s

Equations 28 to 30 and 36 to 38 were solved numerically by the method described in Ref 40, 47, and 48. The "predictor-corrector" algorithm (Ref 46, 47) on a three-layer moving difference grid was used to integrate Eq 28 to 30, and the method of characteristics developed in Ref 48 was used to integrate Eq 36 to 38. Finite difference equations of the characteristics method allow calculation of properties of particles at the moment of time $t + \delta t$ using parameters of the two-phase flow at the moment t. Then the values of particle parameters are used on the right-hand sides of Eq 28 to 30, and the gas parameters are calculated at time $t + \delta t$. Calculation is run until the detonation wave and the particles exit the gun barrel.

The grid is bounded by the closed end of the detonation chamber from the left and by the propagating front of the detonation wave from the right. Until the detonation wave front reaches the open end of the barrel, analytical expressions (Eq 10-12) are valid and describe the right boundary conditions. After the wave front reaches the open end of the barrel at the time $t = L_0/D$, these conditions are not valid any more because the flow cross section changes. In this case, the right boundary condition is found with the help of an additional grid point located at a distance h from the barrel exit. It was assumed that after exiting the barrel, gas is expanding isentropically inside the cone with apex angle ϕ. If the additional point of the grid is numbered $N + 1$, then the gas parameters at this point will be given by the conditions of isentropic expansion:

$$S^*_{N+1} = S_N \qquad \text{(Eq 41)}$$

$$p^*_{N+1} = p_N\left(\frac{d}{d_n}\right)^{2\gamma} \qquad \text{(Eq 42)}$$

$$u^*_{N+1} = u_N + \frac{p_N - p^*_N}{\rho_N c_N} \qquad \text{(Eq 43)}$$

where d_n is the diameter of the gas stream at $x = d + h$, h is the coordinate step of the difference grid, and * denotes parameter value at time $t + \delta t/2$. Time step of the grid is not constant and is equal to $\delta t = h/u_N$. Value of the angle ϕ, which defines the right boundary condition after the detonation wave front reaches the barrel exit, depends on the parameters of the surrounding media and the parameters of the gas flow. Since there is no reliable experimental data on values of ϕ, the effect of ϕ variation on the parameters of gas flow at the vicinity of the barrel open end was investigated. Calculations showed that variation of ϕ by ±10° around 20° had little effect upon the gas parameters, which is in good agreement with the results of Ref 50. In further calculations, angle ϕ was assumed to be equal to 20°. Effects of possible particle melting and evaporation were neglected. Calculations indicate that during spraying of WC particles by propane-oxygen mixture, particles with the diameter larger than 10 μm did not reach the melting point; therefore, the above assumption is valid. During the detonation of propane, the reaction, $C_3H_8 + 5O_2 \leftrightarrow 3CO_2 + 4H_2O + Q$, occurs where $Q = 93.5$ MJ/m^3. The lower concentration limit of detonation for combustion of propane is 3.2 vol% of fuel in the mixture; the upper limit of detonation is 37 vol% of fuel. The velocity of detonation wave at the upper limit is 2210 m/s. Parameters of the gas were: $\gamma = 1.35$, $\rho_g = 1.23$ kg/m^3, kinematic viscosity $\mu = 18.6 \times 10^{-6}$ kg/m · s, and $\rho_2/\rho_1 = 5.4$. Length of the detonation gun barrel was 1.8 m. Initial uniform particle concentration was $n_0 = 10^{-4}$ m^{-3}. Density of WC particles was $\rho_p = 15.1 \times 10^3$ kg/m^3.

A computer code was developed to apply the method described above. To check the stability and precision of numerical algorithm, initial calculations of gas parameters were performed neglecting effects of friction and viscosity. Corresponding terms on the right-hand side of Eq 28 to 30 were taken to be zero. Numerical solutions obtained were compared with analytical solutions (Eq 15, 17). Deviation of numerical solutions for density and pressure distributions from corresponding analytical solutions at different moments of time did not exceed 3%. Initially the particles were assumed to be distributed uniformly inside the barrel, and parameters of gas and particles were calculated for different moments of time. $t = 0$ denotes the time when the detonation wave front reaches the open end of the gun barrel. Also the effect of the loading distance variation on the final particle velocity was investigated. During this calculation, effects of particles on the gas parameters were neglected, and all particles were initially placed within a thin layer δx located at a distance L from the closed end of the barrel. Calculation results are presented in section 6.

6. Results and Discussion

Figure 5 shows the distribution of parameters for gas and particles at the time $t = 0$ when the detonation wave front reaches the open end of the barrel. All parameters are plotted in dimensionless units. In order to obtain real values of parameters, the dimensionless numbers have to be multiplied by: temperature $T_{p0} = T_{g0} = 195$ K, velocity $u_{g0} = 283$ m/s, $u_{p0} = 180$ m/s, and pressure $p = 1.58$ atm. At $t = 0$, gas velocity, pressure, and temperature are monotonically increasing functions of x. Between $x = 0$ and $x = 64$ cm, there is an undisturbed portion of gas with $u_g = 0$. In this region, gas pressure and temperature are constant. At the open end of the barrel, $p = 18.2$ atm, $T_g = 2242.5$ K, and $u_g = 1924$ m/s. Velocity of the particles increases with x and has a maximum at $x = 138$ cm.

Figure 6 shows distributions of gas pressure and particle parameters at time $t = 0.2$ ms when the detonation products started to exit the gun barrel and the rarefaction wave starts to penetrate inside. Gas pressure and temperature quickly drop to 8.53 atm and 1462 K at the exit cross section. Velocity of particles at the exit cross section reaches 612 m/s. Velocity of particles now is a monotonically increasing function of the coordinate. This can be attributed to the accelerating action of the rarefaction wave as it propagates inside the barrel. The temperature of particles further increases and reaches 1618 K for the particles located at $x = 80$ cm.

Figure 7 shows the parameter distribution at $t = 0.9$ ms when the rarefaction wave already reached the closed end of the barrel. At this point, gas temperature and pressure are monotonically decreasing functions of the coordinate. All gas inside the barrel is in motion. Particle speed at the exit reaches 1278 m/s, and temperature is 1950 K.

Figure 8 shows exit velocity of tungsten carbide particles as a function of the loading distance L, which is defined as a distance between the point of detonation wave initiation and the point of particle injection. $V(L)$ has a distinct maximum at $L = 75$ cm. This maximum is caused by the peculiar profile of gas velocity and pressure in the detonation pulse and by the nonmonotonic nature of particle acceleration (Ref 37). Too short loading distance causes the particles to be accelerated by a "narrow" detonation pulse, which reduces final velocity. Large loading corresponds to a shorter accelerating path, which again results in the reduced final particle velocity. Our results are in good agreement with the experiments of Ref 51 and 52 and with numerical results in Ref 37. Experimental investigations of exit particle velocity clearly exhibit nonmonotonic dependence on loading distance. The exact position of the peak in velocity depends mostly on the composition of the gaseous mixture.

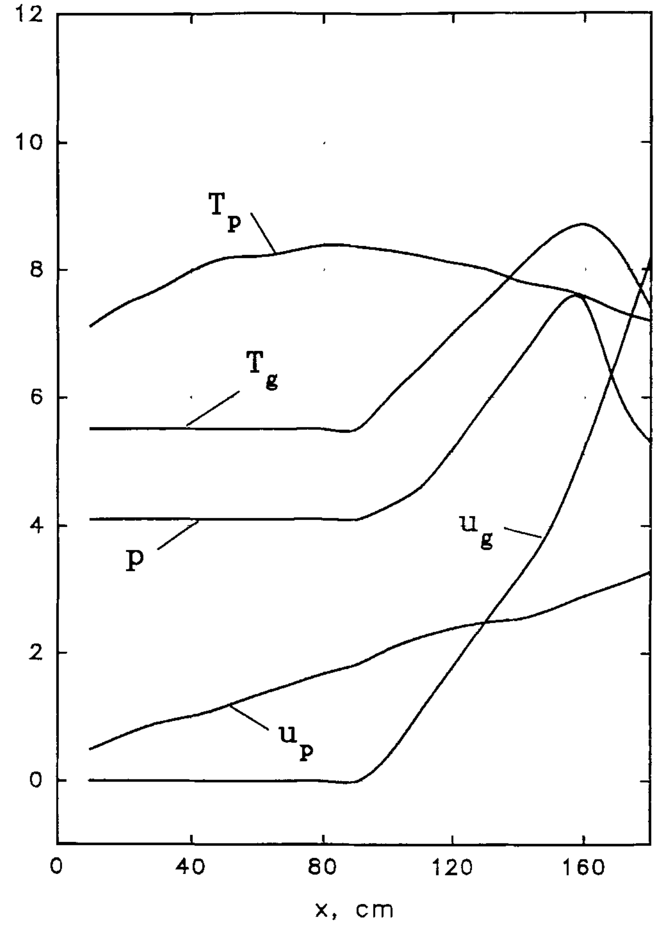

Fig. 6 Gas parameters (p is pressure, T_g is temperature, u_g is velocity) and particle parameters (T_p is temperature, u_p is velocity) at $t = 0.2$ ms. Vertical axis is in dimensionless units. To obtain real parameter values, the dimensionless values have to be multiplied by corresponding factors: p by 1.58 atm, T_p and T_g by 195 K, u_g by 283 m/s, and u_p by 180 m/s

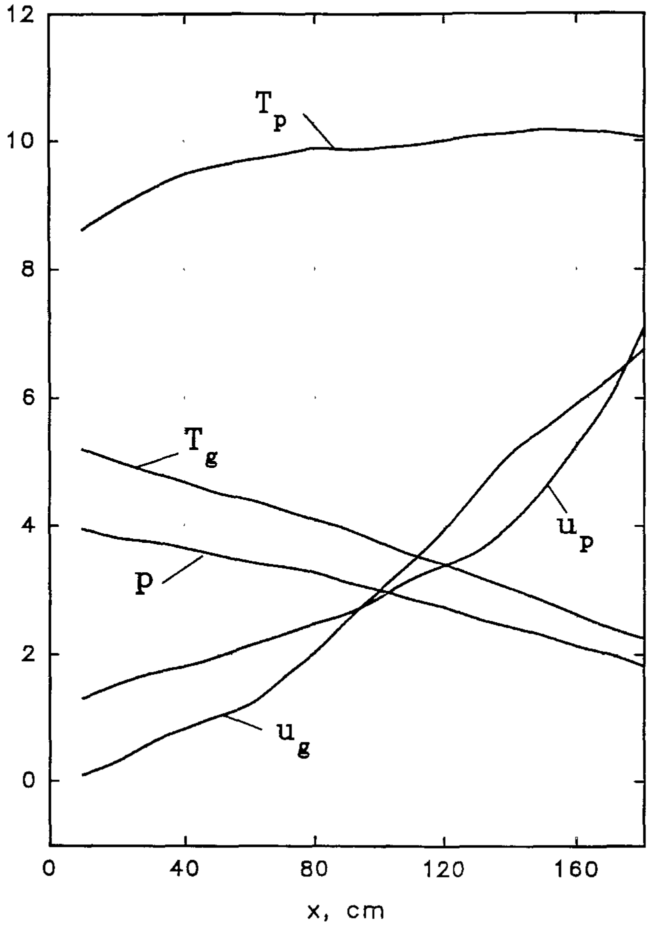

Fig. 7 Gas parameters (p is pressure, T_g is temperature, u_g is velocity) and particle parameters (T_p is temperature, u_p is velocity) at $t = 0.9$ ms. Vertical axis is in dimensionless units. To obtain real parameter values, the dimensionless values have to be multiplied by corresponding factors: p by 1.58 atm, T_p and T_g by 195 K, u_g by 283 m/s, and u_p by 180 m/s

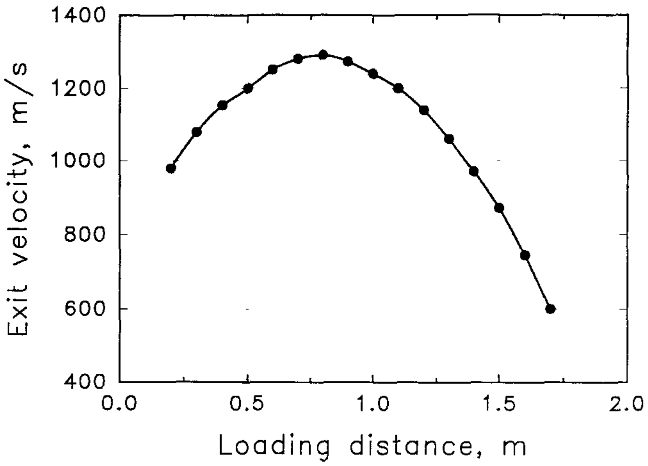

Fig. 8 Exit velocity of 30 μm tungsten carbide particles as a function of the loading distance L

The above calculations show that although during the detonation spraying with the propane-oxygen mixture, 30 μm tungsten carbide particles reach high supersonic speeds of approximately 1200 m/s; their final temperature still remains below the melting point. Thus, to improve the quality of tungsten carbide coating further at this condition, it is beneficial either to reduce particle diameter or to utilize a more energetic gas mixture, such as acetylene, for detonations.

7. Conclusions

A one-dimensional model describing gas dynamics of the detonation coating process was developed and applied to calculate parameters of gas and particles during the detonation spraying of tungsten carbide particles with an oxygen-propane mixture. The model takes into account the effects of powder particles on the gas parameters and gas friction and cooling in the vicinity of barrel walls. The 30 μm tungsten carbide particles reach supersonic velocities of 1278 m/s and the temperature of 1950 K at the exit cross section of the barrel. Exit particle velocity is a nonmonotonic function of loading distance with a maximum of velocity at $L = 75$ cm. The quality of coatings under these stated conditions would be improved by either reducing particle size or utilizing a more energetic detonation mixture. The present analysis shows that the composition of the fuel mixture and the particle loading distance are the most important factors affecting particle parameters and detonation coating quality. The model can be applied to a broad range of problems related to detonation powder spraying and can be used to optimize gas detonation coating technology further.

Acknowledgments

The author is grateful to Dr. V.I. Remeslo and Dr. V.K. Kadyrov, Ukrainian Academy of Sciences, and Dr. T. Gavrilenko, Russian Academy of Sciences for numerous useful discussions.

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