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ON THE APPLICATION OF FLOWS AFTER STRONG DISCONTINUITIES FOR TREATING DISPERSED-PHASE MATERIAL. I. SHOCK-WAVE (AND RAREFACTION-WAVE) ACTION ON PARTICLES

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On the basis of mathematical modeling and numerical experiments, the action of the gas flow after strong discontinuities on particles has been investigated.

Introduction. The destructive action of strong shock and detonation waves in gases is a matter of common knowledge and has been fairly well studied. For instance, methods of detonation deposition are being developed fruitfully and aspects of the practical use of detonation combustion of gases or gasified liquid fuels in rocket and aircraft engines are being discussed [1, 2]. At the same time, investigations (excluding the works with our co-authorship, e.g., [3–6]) connected with the use of shock and detonation waves in gases for technological action on materials with the aim of changing their composition, the aggregate state, and the dispersion degree are not known to the authors.

Note that the use of the detonation of condensed explosives for synthesis and structural transformations of materials has been studied fairly intensively [7–10], whereas the use of *gas* detonation has many advantages in terms of applications, among which is the possibility of organizing a cyclic process with a frequency of up to 100 Hz [2] and relatively "soft" regimes (for instance, pressures in the Chapman–Jouguet plane differ by more than three orders of magnitude) that guarantee a longer service life of equipment.

To assess the possibility of using the shock-detonation phenomena in gases in particular technological processes and choosing their parameters, one has to study the interaction of the flows after strong discontinuities with the particles of the material being treated. Note that in the literature investigations of the interaction of gas flows after shock and detonation waves and rarefaction waves with a cloud of suspended particles are widely presented. For instance, in [11–37] the interaction of waves with a gas suspension of solid particles is investigated (including, in [15, 26, 29, 34], upon expansion of a compressed volume of a gas suspension and, in [38–41], the interaction of waves with an evaporating gas suspension of liquid particles). However, in investigating the action of strong waves with the aim of transforming the source material into a final product, this approach may turn out to be ineffective. For instance, in [42, 43], in investigating the motion of particles deposited on a surface, to determine their trajectory the authors had to introduce labeled particles, i.e., carry out additional procedures that complicate the investigation. Therefore, ignoring the influence of the cloud of suspended particles on the gaseous medium and the shock- or detonation-wave intensity but focusing only on the behavior of particles, it will be more logical and easier to investigate the wave action (acceleration, heating, evaporation, crushing, chemical and phase transformation) on a single particle. In so doing, the results obtained will also be applicable to the case of the particle cloud, for which the approximation of "single" particles is still admissible. According to the results of [19], it holds where the interparticle spacing l_{part} exceeds their size by two orders of magnitude, i.e., $l_{\text{part}}/2r \geq 10^2$, and the ratio of the total mass of particles m_{part} to the gas mass m_{g} in the volume $m_{\text{part}}/m_{\text{g}} \leq 10^{-2}$.

Mathematical Model and Numerical Computing Methods. Let us represent a system of equations describing the action of a gas flow with discontinuities on a single particle. If we ignore the action of the particle on the gas flow and assume that its heat conductivity is infinitely large, then the system of equations can be given in the following form:

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$$\frac{\partial \rho_g}{\partial t} + \frac{\partial (\rho_g v_g)}{\partial x} = 0 , \tag{1}$$

$$\frac{\partial (\rho_g v_g)}{\partial t} + \frac{\partial}{\partial x} (\rho_g v_g^2 + P) = 0 , \tag{2}$$

$$\frac{\partial}{\partial t}\left[\rho_g \left(e + \frac{1}{2} v_g^2\right)\right] + \frac{\partial}{\partial x}\left\{v_g \left[\rho_g \left(e + \frac{1}{2} v_g^2\right) + P\right]\right\} = 0 , \tag{3}$$

$$e = c_{Vg} T_g = \frac{P}{(\gamma - 1)\, \rho_g} , \tag{4}$$

$$\frac{dv_{part}}{dt} = \frac{3}{8} \frac{\rho_g}{\rho_{part}} \frac{C_d}{r} (v_g - v_{part}) \left| v_g - v_{part} \right| , \tag{5}$$

$$\frac{dT_{part}}{dt} = \frac{3\alpha}{r \rho_{part} c_{ppart}} (T_g - T_{part}) , \tag{6}$$

$$C_d = 0.48 + 28.0 \mathrm{Re}^{-0.85} , \tag{7}$$

$$\mathrm{Nu} = 2 + 0.6 \mathrm{Re}^{0.5} \mathrm{Pr}^{0.33} , \tag{8}$$

$$\alpha = \frac{\lambda_g \mathrm{Nu}}{2r} , \tag{9}$$

$$\mathrm{Re} = \frac{\rho_g \left| v_g - v_{part} \right| 2r}{\mu_g} , \quad \mathrm{Pr} = \frac{\mu_g c_{pg}}{\lambda_g} . \tag{10}$$

Note that the choice of expression (7) from the numerous relations for the aerodynamic drag coefficient is due to the fact that it is applicable in a wide range of Reynolds numbers and was used in investigating the relaxation zones after shock waves with Mach numbers M from 1.05 [40]–2.0 [17, 30, 39, 40] to 4.5–5 [23, 27] and even 8 [28], and — in the last three works — in simulating the evaporation and combustion after the shock-wave front. In considering the heat exchange between phases, the Ranz–Marshall formula (8) is one of the most widely used formulas [17, 23, 39, 40].

We assumed the following initial conditions. The particle and the gas in the initial state have the same temperature T_1 = 293.17 K and velocity v_1 = 0. As a gas, we use air (M = 28.96 kg/kmole) with a density ρ_1 = 1.20 kg/m^3 at a pressure $P_1 = 1.01 \cdot 10^5$ Pa. A shock wave with intensity P_2/P_1 propagates through the gas and at time t = 0 begins to act on a particle of radius r. We considered tungsten, beryllium, glass, and silicon particles with a density of 19,026, 1840, 2500, and 2333 kg/m^3 and a specific heat capacity of 154, 1675, 670, and 712 J/(kg·K), respectively [44–46]. Because of the model character of the problem, the phenomena of dissociation and ionization in the air after the shock waves were not considered.

The system of Euler equations (1)–(4) was solved by the numerical flow correction technique (FCT) described in [47, 48] and chosen after its consideration and comparison (also in terms of the program operation) with other tech-

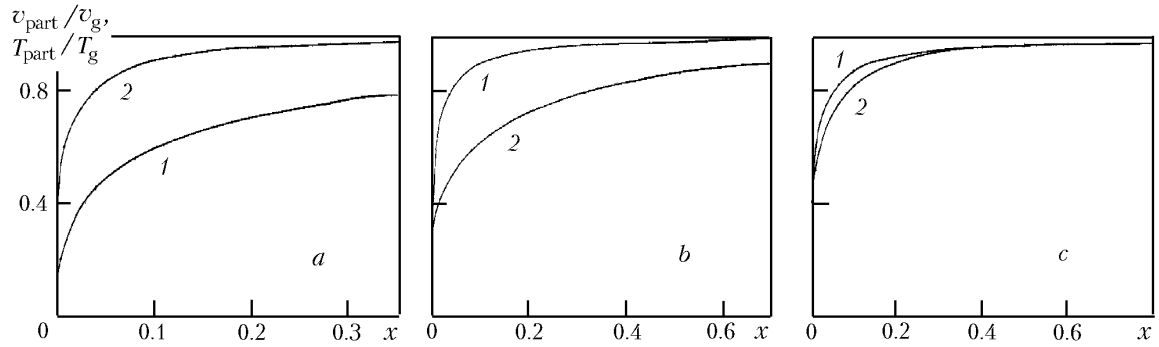

Fig. 1. Change in the velocity (1) and temperature (2) of particles moving along the tube: a) tungsten; b) beryllium; c) glass. x, m.

niques, including the Godunov method [49], MUSCL [50], and the TVD method, whose principles were presented by Harten in [51]. Among the advantages of the FCT is the fact that it is not tedious, is easy to program and is graphical, and its programs can be used as blocks in other programs. Calculations based on it require less computer time as compared to the other methods listed above. In performing large volumes of computing experiments, this is a serious argument in favor of the FCT.

The system of equations (5)–(10) was solved by the Runge–Kutta method of fourth order of accuracy. The general scheme of solving the system of equations (1)–(10) consisted in that at each time step first the distribution of the quantities ρ_g, v_g, P, and T_g was defined by formulas (1)–(4) and then the new values of the particle velocity, location, and temperature were computed by (5)–(10) on the basis of the data obtained.

Results of the Computing Experiments. Before presenting the results, we stipulate that, because of the absence of a more exact and comprehensive definition, the processes of equalization of the particle velocity and temperature with the gas parameters will be termed the mechanical and thermal relaxation of the particle. As a criterion of the corresponding relaxation of the particle, the attainment of a 1% difference from the flow parameters δv and δT will be considered. The transition to a rougher level, e.g., to a difference of δv and δT of 10% leads, to a reduction of the characteristic times and domains with preservation of the main mechanisms of the process.

Figure 1 presents the results of the experiments on the action on particles of shock waves with intensity $P_2/P_1 = 20$ ($P_2 = 20.2 \cdot 10^5$ Pa, $v_2 = 1120$ m/sec, $r_2 = 5.37$ kg/m^3, $T_2 = 1262.97$ K) and shows the typical behavior of tungsten, beryllium, and glass particles of radius 10 μm after the shock-wave front. The temperature and velocity of particles are related to the gas parameters after the shock wave, which permits graphical representation of the approximation of the particle parameters to the gas parameters. Heating and acceleration of particles begin immediately after the wave front; then the acceleration and the heating intensity steadily decrease and the particle parameters approach the gas parameters more and more slowly. Such a behavior is easy to predict and follows from the form of the mechanisms of hydrodynamic and thermal gas-particle interaction that are used.

Note that, depending on the properties of particles, the rates of the thermal and mechanical relaxation processes may differently correlate with each other. For the tungsten particle, heating proceeds faster than acceleration; for the beryllium particle, vice versa, it proceeds more slowly; and for the glass particle, the rates of these two processes have the same order.

The subsequent numerical excitements were aimed at elucidating the features of the mechanical and thermal processes depending on the properties and sizes of the particles.

We have considered the dependence of the relaxation characteristics of the processes for various types of particles on their size. Some of the experimental results are given in Table 1. It has been established that with increasing radius of the particle the times and lengths of the relaxation zones increase, i.e., the retardation of the relaxation processes due to the increase in the particle mass and heat capacity is more substantial than the acceleration of these processes as a result of the increase in the force action and the heat-exchange intensity. In so doing, as follows from the analysis of the results presented, for the mechanisms of hydrodynamic and thermal interaction used in the model, the increase in the heat capacity of particles with increasing radius is compensated due to the intensification of the heat

TABLE 1. Length of Mechanical and Thermal Relaxation Zones for Different Particles

Material	r, μm	l_v, m	l_T, m	l_v/l_T
Tungsten	1	0.160	0.0042	38
	50	59	7.8	7.6
Beryllium	1	0.016	0.032	0.5
	50	5.5	61	0.09
Glass	1	0.021	0.0089	2.4
	50	7.9	15	0.5

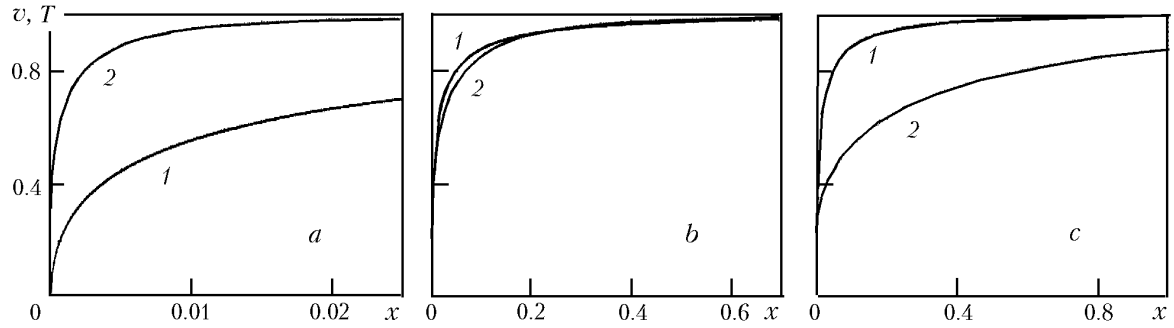

Fig. 2. Change in the velocity (1) and temperature (2) of the quasi-glass particle under the action of the shock wave at various specific heat capacities: a) c_p = 100; b) 600; c) 2000 J/(kg·K). x, m.

exchange between the phases less effectively than the increase in the mass — by the growth of the force action on the increased surface of the particle.

The results of the calculation at a fixed specific heat capacity and a varied particle density have shown that the lengths of the relaxation zones increase with their density. This is easy to understand if we take into account the increase with increasing particle density in its mass and heat capacity. However, unlike the case described below, where the specific heat capacity changes with increasing density, the ratio between the thermal and mechanical relaxation rates remains unaltered.

It has been shown that in the case of a fixed density of particles and a variation of their specific heat capacity the scales of the thermal relaxation zones increase with increasing heat capacity.

The results illustrating the dependence of the type of the dominant relaxation process on the specific heat capacity of the particles (with the example of quasi-glass) are shown in Fig. 2 (the quasi-particle is a particle in which all properties correspond to the properties of a certain material, except one which varies over some reasonable range). As above, the velocity and temperature of particles are related to the gas parameters after the shock wave. The velocity curves at different c_p differ only in the scale of the x-axis.

At low heat capacities (e.g., at c_p = 100 J/(kg·K)), the thermal equalization proceeds faster than the equalization of velocities. Then, at some values of c_p close to 600 J/(kg·K), the relaxation rates of the thermal and mechanical processes have one order. Finally, at high heat capacities (the case of c_p = 2000 J/(kg·K) is given), the particle accelerates faster than it is heated. In so doing, the increase in the thermal relaxation time is due not only to the increase in the quantity of energy to be supplied to the particle in order to increase its temperature to the given value but also to the decrease in the rate of heat exchange of the particle with the gas. At low heat capacities, the particle is heated mainly in the zone of large relative velocities of the gas and the particle, where the intensity of the heat exchange between the phases is high. But if the particle has a high heat capacity, then the heating region is extended to the space where its velocity relative to the gas is low; therefore, the heat exchange is small, which considerably decreases the heating rate and increases the relaxation time. Analogous results, i.e., a faster thermal relaxation at c_p = 100 J/(kg·K), almost equal rates of mechanical and thermal processes at c_p = 600 J/(kg·K), and a lag of the heating processes at c_p = 2000 J/(kg·K), have been obtained in numerous experiments for quasi-tungsten and quasi-beryllium particles. Only the scales of the relaxation zones differ. While for the quasi-beryllium they are about 20% smaller than in the quasi-

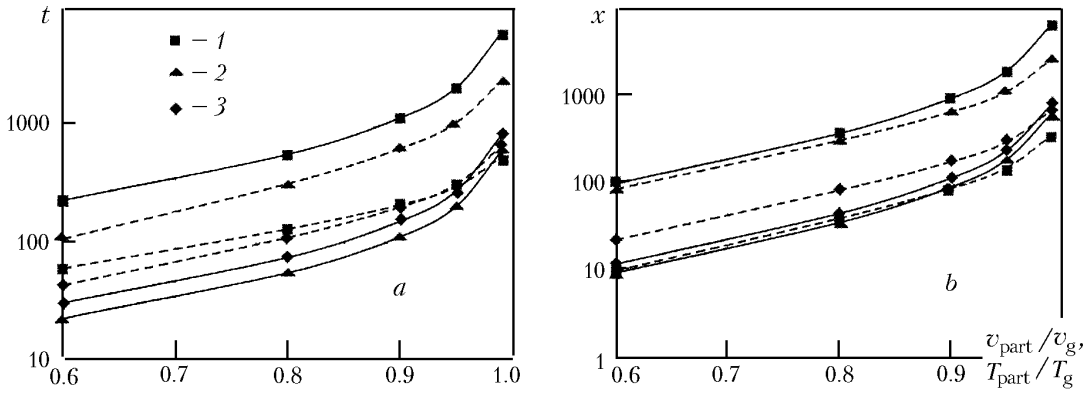

Fig. 3. Particle acceleration and heating time (a) and particle path under acceleration and heating (b) needed for tungsten (1), beryllium (2) and silicon (3) particles to attain a given velocity (solid curves) temperature (dashed lines) relative to the gas parameters. t, μsec; x, mm.

glass, for the quasi-tungsten particles the sizes of the thermal zones are 7–8 times larger (for each of the above values of c_p) than for the quasi-glass. Thus, the main parameter of the particle influencing the relation between the mechanical and thermal relaxation rates is its specific heat capacity.

The following numerical experiments were conducted to elucidate the dependence of the character of the thermal and mechanical behavior of particles on the shock-wave parameters.

We investigated the behavior of tungsten, beryllium, and silicon particles at various parameters of shock perturbations. The calculations have shown that in more intensive waves the particles are heated and accelerated faster. Moreover, it follows from them that in the entire investigated range of intensities P_2/P_1 the attainment of higher velocity and temperature is impossible without an increase in the length and time of action.

To form ideas about the temporal and spatial scales of the final stage of the relaxation process, Fig. 3 shows the times and spacings needed for particles of diameter 10 μm to attain a given level of velocities and temperatures with respect to the parameters after a shock wave with intensity $P_2/P_1 = 20$. From the graphs it is seen that from 65 to 85% of the time and spacing are expended in heating and accelerating the particles for attaining from 90 to 99% of the gas parameters. It is clear that, proceeding from the necessary conditions for the technological process being developed, one can choose a reasonable combination of shock-wave parameters and the length of the channel in which it will be realized. Thus, in the case of an insignificant excess (by a few percent) of the wave intensity needed according to the calculation, one can attain equal effects of the action on a particle by reducing the treatment times and spacings by 50%.

It was shown above that the behavior of the particle after the shock wave is influenced by the particle–gas interaction intensity, which is determined by the gas viscosity and heat conductivity. Let us consider the influence of the above gas properties on the particle in more detail.

With increasing viscosity, the scales of mechanical relaxation decrease and those of thermal relaxation increase, and at a certain value of viscosity the thermal and mechanical relaxation rates are equal. At a small viscosity of the gas, the force of its action on the particle is also small, due to which the particle accelerates slowly. As a consequence of this, the relative velocities of the particle and the gas remain high for a fairly long time, which, in turn, leads to an intensive heat exchange between the gas and the particle and to a small time and spacing of its heating. With increasing viscosity there is an increase in the drag force and the particle accelerates faster; therefore, the convective heat exchange decreases. All of this is responsible for the decrease in the characteristic parameters of the mechanical relaxation and the increase in the thermal relaxation parameters.

At a low heat conductivity of the gas, the heat-exchange intensity is also low. Therefore, the time and the length of the thermal relaxation zone are large, markedly exceeding the scales of the mechanical relaxation. With increasing heat conductivity, the relation between them changes, and at a certain value of the heat conductivity the orders of these processes become equal, as the calculations show. Its further increase leads to the fact that the scales of the mechanical processes exceed those of the thermal ones.

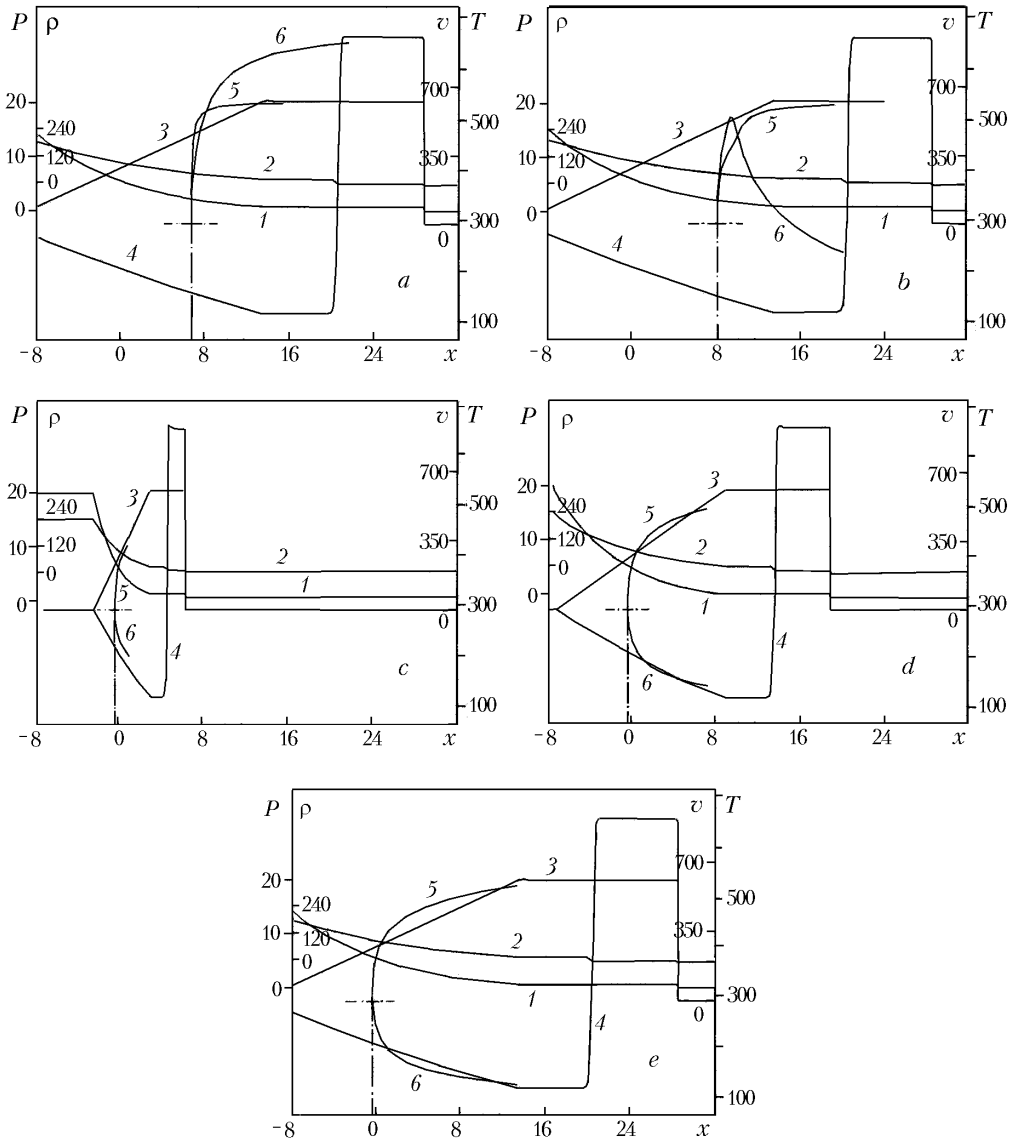

Fig. 4. Typical behavior of particles under the action of a shock wave (a, b) (particles of a different mass) and a rarefaction wave (c, d, e) (process dynamics for the tungsten particle of radius 40 μm) formed upon continuity break: a) silicon particle of radius 60 μm in the region of constant parameters after the shock wave; b) tungsten particle of radius 90 μm in the region of constant parameters after the rarefaction wave; c, d) particle in the region of the rarefaction wave fan; e) the particle catches up with the region of constant parameters after the rarefaction wave [1) gas pressure P; 2) gas density ρ_g; 3) gas velocity v_g; 4) gas temperature T; 5) particle velocity v_{part}; 6) particle temperature T_{part}]. x, m; P, MPa; ρ_g, kg/m^3; T_g, K; v_g, v_{part}, m/sec.

Thus, the relation between the thermal and mechanical relaxation times depends on the properties of both the particle and the gas. If it is possible to change the particle's properties, one can select the conditions under which the thermal processes will proceed faster than the mechanical ones, and vice versa. If the properties of the material are fixed, then the ratio between the rates of the relaxation processes can be changed by selecting the gas.

Consider the features of the behavior of the investigated particles in the gas flows that are formed by the discontinuity decay when the partition (diaphragm) between the regions of motionless gas with different pressures is re-

moved. As the computing experiments have shown, the behavior of particles in such flows is much more diverse than the above-described behavior in flows after the shock wave. Additional factors appear: the particle position relative to the diaphragm (in a high-pressure chamber (HPC) or in the low-pressure chamber (LPC); distance from the diaphragm; parameters of the gas flow formed upon the diaphragm break.

If, at the initial instant of time, the particle is in the LPC, then, under the action on it of a shock wave, three variants of its motion are possible. In the first case, the particle will be accelerated by the shock wave to the gas velocity in the zone of constant parameters (to a contact discontinuity) and will stay in this region of the flow for the shock-wave lifetime (Fig. 4a). In the second variant, where the particle will have no time to accelerate in the flow after the shock wave, a contact discontinuity will catch up with it and it will "jump out" into the zone of constant parameters after the last characteristic of the rarefaction wave (Fig. 4b). It is seen that, upon passing through the contact discontinuity, the particle begins to cool down and undergoes additional acceleration. This is illustrated by the maximum on the temperature curve and the kink on the velocity curve. Finally, the case is possible where the last characteristic of the rarefaction fan will also catch up with the particle and will get into the rarefaction zone wave. Note that, in so doing, the situation where the particle accelerated by the flow in the rarefaction wave can again return to the region of constant parameters of the pushing gas is possible.

Unlike the particle motion after a solitary shock wave, where it is steadily heated, in the gas flow upon the diaphragm break the particle can be both heated and cooled, depending on in which zone of the flow it is situated. If the particle is situated between the shock-wave front and the contact surface, it is heated. In all other instances it is cooled.

As the computing experiments show, the character of the particle motion is also dependent on its position relative to the diaphragm. For instance, if the particle located in the LPC is close to the diaphragm, then it may have no time to accelerate under the action of the shock wave and "jump out" beyond the contact discontinuity. Moving it away from the diaphragm, one can obtain a variant of motion in which the particle will remain in the region of constant parameters before the contact discontinuity. This is easy to understand, taking into account that as the shock wave propagates, the zone of its constant parameters expands.

If, at the initial instant of time, the particle is in the HPC, then the character of its behavior will depend on the initial pressure ratio on the diaphragm, which will specify the rate and direction of motion of the last characteristic of the rarefaction wave. When the wave tail is moving in the direction of motion of the head, then any particle approaches the last characteristic of the rarefaction fan moving from the opposite direction and goes from the rarefaction wave into the flow region with constant parameters of the pushing gas. But if the tail is moving towards the wave front, then the particle, being accelerated by the flow in the rarefaction wave, will strive to catch up with the zone of constant parameters of the pushing gas that is moving away from it. However, practical realization of this at reasonable distances will only be possible for the lightest of particles, whose sizes (and densities) are the smaller, the higher the initial pressure ratio on the diaphragm. Such a type of behavior is given in dynamics in Fig. 4c, d, e. It is seen that in the given case the particle catches up with the last characteristic of the rarefaction fan. As the particle stays further in the region of constant parameters after the rarefaction wave, its velocity and temperature approach the pushing-gas parameters. It will be recalled that when, at the initial instant of time, the particle is in the HPC, it is cooled during the whole process.

Let us mention the following feature of the action on the particle of flows formed when the diaphragm between the gas regions with different pressures is removed. As shown above (see Fig. 4b), in the zone of constant parameters between the shock wave and the rarefaction wave, the force action of the flow between the rarefaction wave and the contact surface on the particle is more effective than the action of the flow between this surface and the wave front, which is due to the higher density of the pushing gas. Interestingly, a comparable and, in individual cases, a stronger force action on the particle can be produced by the flow directly in the zone of the rarefaction wave fan, beginning with flow velocities slightly exceeding the local velocity of sound (from Fig. 4c, d it is seen that the particle follows, with a small delay, the rapidly changing gas velocity). This is due to the fact that the dynamic pressure component of the flow has a sufficiently sloping maximum in the vicinity of the Mach number $M \cong 2.1$ (at the $1.4 \leq M \leq 2.9$ interval boundaries, the deviation of the value of $\rho_g v_g^2/2$ from the maximum value does not exceed 10%). Thus, upon discontinuity break, the flow in the supersonic region of the rarefaction wave fan and in the region of constant parameters after this wave provides a faster acceleration of the particle than after the shock wave.

Possible Applications of Flows after Strong Discontinuities for the Synthesis and Treatment of Materials. The analysis of the numerical experiments has revealed several variants of the behavior of particles under the action of flows in a shock tube. Varying the intensity of perturbations, the parameters of gases in the high- and low-pressure chambers, and, to a reasonable extent, the sizes of the particles being treated, as well as the region of gas suspension dislocation before the process, one can provide a wide spectrum of regimes of pulsed static and dynamic loading and high-amplitude thermal action on particles (including those with alternating heat loads), which cannot be obtained for the types of technological equipment known to us.

The use of a shock tube will apparently be especially expedient when the source material and intermediate and end products have to be kept in an inert atmosphere. The shock tube may turn out to be a difficult-to-replace element of equipment also for technological processes, in which it is required to first rapidly heat and then sharply cool the treated gas suspension (in times of the order of 10^{-3}–10^{-2} sec). One can predict its use also for the cases where it is required to atomize and freeze in the form of finely dispersed powder a just-synthesized, thermally unstable compound introduced into the high-pressure chamber just before diaphragm breaking.

Having chosen, with the help of the results presented, the necessary amplitude parameters of the process and determined the flow diaphragm of treatment (e.g., the duration and intensity of action of the heating and cooling phases), one can formulate requirements for structural materials and specify the length of the high- and low-pressure chambers for the equipment being developed.

It should be noted that when air is used as a pushing gas, its considerable heating is needed to obtain shock waves with an intensity of $P_2/P_1 \cong 10$. To obtain waves with an intensity of $P_2/P_1 \cong 20$, it is necessary to use hydrogen or heated helium in the HPC, and a further increase in the wave intensity can only be provided by heated hydrogen. However, the consideration given in the present paper to the action of flows after strong shock waves ($P_2/P_1 \geq 20$) is not incidental. Pressures close to the above value (at P_1 = 0.1 MPa) are observed after detonation waves in hydrocarbon–air mixtures; in strongly detonating mixtures, the pressure in combustion products can reach 4 MPa [54]. Having selected flow parameters after a stationary shock wave close to the Chapman–Jouget parameters for a particular combustible mixture, one can estimate the action of the flow after the detonation wave on the particle. Suggestions on the technological use of flows after strong discontinuities (based on the method of detonation synthesis of refractory oxides [3]) for obtaining finely dispersed electronic and heat-insulation ceramics are given in [55].

CONCLUSIONS

1. The possibility of using shock and detonation waves in gases for technologies of synthesis and treatment of materials has been considered.

2. On the basis of the investigation made, it has been shown that selecting parameters of gases and particle sizes, it is possible, as a rule, to attain the required force and thermal action on the particle with the aim of making phase and chemical transformations in it, as well as momentum transfer to it for mechanical treatment.

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NOTATION

C_d, aerodynamic drag coefficient; M, Mach number; Nu, Nusselt number; P, pressure, Pa; Pr, Prandtl number; Re, Reynolds number; T, temperature, K; v, velocity, m/sec; c_p and c_V, specific heat capacities at constant pressure and volume, J/(kg·K); e, internal energy, J/kg; l, length of the relaxation zone, interparticle spacing, m; m, mass, kg; M, molar mass, kg/mole; r, particle radius, m; t, time, sec; x, coordinate, m; α, heat-transfer coefficient, W/(m^2·K); δ, relative quantity; γ, ratio between specific heat capacitors; λ, heat-conductivity coefficient, W/(m·K); μ, viscosity, kg/(m·sec); ρ, density, kg/m^3; τ, relaxation time. Subscripts: 1 and 2, parameters before the shock wave and after the shock wave; g, gas; part, particle; d, drag; p, pressure; V, volume.

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