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Problems of Closing Models that Describe Detonation of Gas Suspensions of Ultrafine Aluminum Particles (Review)

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Abstract: Various publications dealing with physicomathematical modeling of detonation processes in gas suspensions of fine, submicron, and nano-sized aluminum particles within the framework of mechanics of continuous and heterogeneous media are reviewed. Important issues of the description of thermal dynamics, transport properties, and ignition mechanisms are discussed. Specific features of combustion regimes of micron- and nano-sized particles are considered. Closing relations for a semi-empirical model of detonation of suspensions of aluminum nanoparticles in oxygen are presented.

Keywords: detonation, gas suspension, aluminum, microparticle, nanoparticle, mathematical modeling.

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INTRODUCTION

Various issues of ignition and combustion of fine (micron- and nano-sized) aluminum particles are intensely discussed in the literature. The interest to these problems is caused by the prospects of using these species in mixtures of composite solid propellants for improving the characteristics of ignition and combustion, increasing the combustion efficiency, etc. [1–3]. It was noted [4, 5] that addition of micron- and nano-sized aluminum particles exerts contradictory effects on the performance of various explosives, which has not been yet found reasonable explanations. There are numerous recent studies that include observations and theoretical description of combustion of nano-sized particles and the analysis of the related processes (melting, fragmentation, clusterization, etc.). However, the number of publications dealing with various aspects of detonation of gas media in the presence of nanoparticles or gas suspensions of sub-micron or nano-sized particles is not very large. Closing of physicomathematical models of heterogeneous detonation requires an adequate description of the processes of interphase interaction. Publications dealing with ignition and combustion of aluminum particles in gas media in detonation and shock waves are reviewed in the present paper. In addition, thermophysical properties and specific features of heat transfer and drag of nano-sized particles under dynamic conditions of wave flows are also considered.

The theoretical description for most problems of shock wave and detonation phenomena in gas suspensions of fine particles is based on the approaches of mechanics of continuous/heterogeneous media [6–11]. The constitutive equations describe the laws of conservation of mass, momentum, and energy for each phase and each species; they are supplemented with equations of state and are closed with relations that describe the processes of mass transfer between the species (melting, evaporation, condensation, ignition, and combustion), momentum exchange (drag forces), and heat transfer between the gas and the particles. These approaches can be used to describe gas mixtures with micron- and nano-sized particles with adequate allowance for molecular effects in interphase interaction.

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For one-dimensional unsteady flows of reacting gas suspensions with a low concentration of particles, the constitutive equations have the following form [12, 13]:

$$\frac{\partial \rho_1}{\partial t} + \frac{\partial(\rho_1 u_1)}{\partial x} = J_2, \quad \frac{\partial \rho_2}{\partial t} + \frac{\partial(\rho_2 u_2)}{\partial x} = -J_2,$$

$$\frac{\partial \rho_1 u_1}{\partial t} + \frac{\partial(p + \rho_1 u_1^2)}{\partial x} = -f_2 + J_2 u_2,$$

$$\frac{\partial \rho_2 u_2}{\partial t} + \frac{\partial(\rho_2 u_2^2)}{\partial x} = f_2 - J_2 u_2, \qquad (1)$$

$$\frac{\partial \rho_1 E_1}{\partial t} + \frac{\partial[\rho_1 u_1(E_1 + p/\rho_1)]}{\partial x} = -q_2 - f_2 u_2 + J_2 E_2,$$

$$\frac{\partial \rho_2 E_2}{\partial t} + \frac{\partial(\rho_2 u_2 E_2)}{\partial x} = q_2 + f_2 u_2 - J_2 E_2,$$

$$p = \rho_1 R T_1,$$

$$E_1 = \frac{u_1^2}{2} + c_{v,1} T_1, \quad E_2 = \frac{u_2^2}{2} + c_{v,2} T_2 + Q$$

(the subscripts 1 and 2 refer to the gas and particles, respectively). The following variables are used: p is the pressure, $\rho_i = m_i \rho_{ii}$, u_i, E_i, T_i, $c_{v,i}$, m_i, and ρ_{ii} are the mean density, velocity, total energy per unit mass, temperature, thermal conductivity, volume concentration, and true density of the ith species ($i = 1, 2$), f, J, and q are the force of interphase interaction, mass transfer, and specific heat flux of interphase heat transfer, and R is the universal gas constant; the variable Q includes the thermal effect of the reduced kinetics of the particle burning reaction and also the heat losses on melting and evaporation of the particle material.

The majority of detonation models for gas mixtures and gas suspensions of solid particles are based on the combustion description within the framework of models of reduced kinetics. This allows one to obtain hydrodynamic patterns of the flow at macroscopic scales corresponding to the sizes of various engineering devices or to the volumes of space used to study explosion processes. The use of detailed multi-stage kinetic schemes for conditions of unsteady nonuniform flows of heterogeneous detonation is not always justified. The reaction constants known from available publications were determined for limited ranges of pressure and temperature, while the kinetic schemes were usually verified for conditions of laminar flame propagation. In the case of detonation, these parameters vary within wide limits, and their values may go outside the ranges in which the rate constants were determined. The deviations can be rather significant if the number of reactions is large and the activation energy is high. The experience of numerical simulations of cellular gas detonation shows that simplified models sometimes reproduce the cell size even more effectively than detailed kinetic models.

In the theoretical approaches to constructing mathematical models of reduced kinetics aimed at describing particle combustion with the minimum possible number of chemical reactions, the basic principle is a correct representation of the ignition criterion, as well as the mass transfer, heat transfer, and heat release. Thus, experimental data on combustion and detonation of gas suspensions of aluminum particles, which allow verification of models in terms of a set of various parameters, are of undoubted interest. To develop models of detonation combustion of aluminum suspensions within the framework of reduced kinetics, one has to take into account the specific features of ignition and combustion of particles of various sizes behind the shock wave.

1. DEVELOPMENT OF MATHEMATICAL MODELS OF IGNITION AND COMBUSTION OF FINE PARTICLE SUSPENSIONS

1.1. Mechanisms of Combustion of Micron-Sized Aluminum Particles

Various issues of combustion of fine aluminum particles (10–300 μm) were studied in numerous experimental and theoretical investigations, which were reviewed in [14, 15]. Pokhil et al. [14] analyzed the data on combustion of individual particles in air under static conditions (in a burner flame). The burning time was found to be a power-law function of the particle diameter with an exponent of 1.5–2 [14]. In most cases, the solid combustion products are small spherical particles consisting of aluminum oxide. It was noted that the final products contain no AlO and Al_2O sub-oxides. Vice versa, the data of thermodynamic calculations [16] and thermodynamic analysis of detonation [17] reveal the presence of sub-oxides in detonation products, which confirms that detonation combustion of aluminum particles differs essentially from combustion under static conditions.

Pokhil et al. [14] tend to present combustion of an aluminum particle in the vapor-phase regime, based on the Glassman hypothesis [18]. Some models of combustion within the framework of this concept were described, in particular, the model developed in [19], which takes into account partial diffusion of vapor-phase products of combustion toward the metal surface.

Experimental observations of combustion of aluminum particles contained in rocket propellants were performed in [20, 21] and described in [22], where the contradictory character of many aspects of the process was noted. One of the main intermediate processes is metal interaction with aluminum oxide (Al_2O_3) with formation of gaseous products (Al and AlO). Babuk [22] developed a model of combustion of a single aluminum particle in oxygen, where a key role in aluminum oxidation belongs to the presence of an oxide film, which, on the one hand, prevents interaction of aluminum and oxygen owing to reacting surface area reduction and, on the other hand, participates in aluminum oxidation with formation of the intermediate product AlO. Accumulation and breakthrough of the gaseous sub-oxide AlO can lead to violation of the oxide film integrity and formation of an asymmetric combustion region. (The possibility of symmetry violation in the case of aluminum particle combustion was discussed in [14].)

A modification of the vapor-phase model of aluminum particle combustion on the basis of the concepts described in [18, 19] was presented in [15]. In that work, oxide condensation was assumed to occur on the particle surface with formation of an asymmetric structure ("cap").

The physicomathematical model developed in [23, 24] takes into account accumulation of the oxide on the aluminum particle surface. The results calculated by the model [24] with allowance for evaporation kinetics and surface chemical reactions agree well with the experimental data [14, 25] on the dependence of the burning time on the pressure and oxidizer concentration; the results on the burning time dependence on the particle size predicted by that model are within reasonable scatter of data.

Specific features of combustion of individual coarse (80–250 μm) aluminum particles in oxygen and oxygen-containing media were noted in [26–28]. It was demonstrated [26, 27] that aluminum combustion includes several stages. The first stage proceeds at temperatures of the order of 3000 K, most probably, in the vapor-phase regime. At the second stage, the temperature decreases to 2800 K, the combustion process is asymmetric, and the particle rotates, which is associated with the formation of an oxide "cap" on the surface. At the third stage, radiation becomes less intense, the temperature decreases to 2300 K, and the oxide is accumulated on the surface (which is confirmed by additional experiments under microgravity conditions and by the analysis of the particle composition at different stages of combustion in [27]). For combustion of aluminum particles in pure oxygen or oxygen mixtures with nitrogen, argon, and helium, Dreizin [28] derived a quadratic dependence of the burning time on the particle diameter. The particle burning time in pure oxygen was found to be several times shorter than in air. It was also demonstrated that the change in the oxide film thickness is comparable to the particle size.

For combustion of aluminum as a component of composite propellants, the burning time was found to be a power-law function of the particle diameter with a smaller exponent: up to 1.5 [14]. In their experiments, Servaites et al. [29] established a dependence with an exponent of 1.65 ± 0.55; they found that the burning rate weakly changes with oxygen concentration, but depends linearly on pressure in the measurement range used. The fact of the weak dependence of the burning rate on the oxygen concentration allowed the authors to conclude that oxygen is probably not the primary oxidizer in combustion of aluminum as a component of composite rocket propellants. Their calculations predicted higher rates of aluminum interaction with other reagents: CO_2 and H_2O.

An extensive review of results on the burning time of aluminum particles in air and oxygen media was performed in [30]. It can be concluded from the analysis that the exponent of 1.5 is more typical for air mixtures, whereas the exponent for oxygen media is closer to 2. Nevertheless, extension of this dependence to the particle size interval from 1 to 10 μm is questionable. Beckstead et al. [31] presented a model of combustion of a single aluminum particle in various oxidizer media, which is based on the kinetic mechanisms of heterogeneous (surface) and gas-phase reactions with formation of sub-oxides with due allowance for condensation and dissociation. Numerical calculations and comparisons with experimental data were performed for comparatively coarse particles (60–230 μm) under the conditions of a turbulent wake flow.

The data on combustion of aluminum particles up to 10 μm in size under various conditions presented in [32, 33] confirm the transitional character of combustion. It was found [32] that the change in the combustion regime may occur at even coarser particle sizes than 10 μm, depending on the test conditions. The experimental data reported in [33] show that the transition from the diffusion-limited gas-phase combustion of aluminum particles to the kinetic regime begins at the particle size of 10 μm and pressure of 8.5 atm. The measurements of the burning time of dust with the particle sizes of 10 and 2.8 μm show that the exponent in the dependence of the burning time on the particle diameter is of the order of unity in media with carbon dioxide and decreases to 0.7 in oxygen–nitrogen mixtures.

The burning rate of micron-sized particles also depends on pressure. Lynch et al. [34] performed an experimental study of combustion of 3- and 11-μm particles. Based on these experimental results, they found correlations for the dependence of the burning time on the pressure P, fraction of oxygen $X_{\rm ox}$, and particle diameter d: $t_b = a_0 X_{\rm ox}^{a_1} (P/P_0)^{a_2} d^n$, where the values for oxygen are $a_1 = 0.5$, $a_2 = -0.5$, and $a_0 = 200\ \mu$s; the particle diameter d is measured in micrometers. A universal formula was derived for the exponent: $n = 2\exp(-4.3X_{\rm ox})(P/P_0)^{-0.3}$.

1.2. Mathematical Models of Combustion of Suspensions of Microscopic Particles under Dynamic Conditions

Theoretical approaches to the description of suspensions of aluminum particles behind shock and detonation waves have been developed since the mid-1980s. Medvedev et al. [11] proposed a model of interpenetrating continua with an Arrhenius-type equation of reduced kinetics. The model took into account incomplete combustion of particles caused both by the oxidizer deficit and by oxide accumulation on the particle surface. The relationship between the pre-exponent and the particle size was not considered.

Simultaneously the model of ignition and combustion of an aluminum particle behind a shock wave was presented in [35] and later in [36]. Several factors were taken into account, such as particle melting and evaporation, Al_2O formation, and Al_2O_3 condensation. Particle burning was controlled by diffusion within the film. The model was applied in problems of particle ignition and combustion behind a shock wave, but the detonation structure was not analyzed, and comparisons with experimental data on detonation were not performed.

In modeling detonation in gas suspensions of aluminum particles in hydrogen–oxygen and hydrogen–air mixtures with addition of aluminum [37, 38] and also in air and oxygen [39], the combustion process was described on the basis of the concepts of [14]. The reaction rate was assumed to be described by the formula derived in [14] with the constant found in [25]: $\tau_{\rm comb} = K\dfrac{d^{1.5}}{(a_k)^{0.9}}$. It should be noted that this formula was derived in [25] on the basis of processing experimental data on combustion of aluminum contained in combustion products of condensed systems, where the main oxygen-containing reagents were H_2O and CO_2. In [38, 39], the presence and role of the oxide film on the particle surface were ignored, whereas the condensed reaction products (consisting of small particles of aluminum dioxide identical to the oxide film) were considered as part of the gas phase. If the aluminum dioxide boiling point was reached, the possibility of its decomposition into sub-oxides was taken into account.

The detonation model [38] was used by Benkiewicz and Hayashi [40] for numerical simulations of two-dimensional processes in heterogeneous detonation of the gas suspension of aluminum particles. They indicated that oxygen was considered as a carrier phase and the particle concentration used in the study (0.3 kg/m^3) was several times smaller than the stoichiometric value. The detonation velocity predicted numerically (1.74 km/s) was consistent with the thermodynamic calculations [39, 41].

A simple two-stage model of reduced kinetics for the description of detonation combustion of aluminum particles in oxygen with allowance for aluminum oxide decomposition was analyzed in [42]. Parametric investigations were performed to study the influence of various parameters on the results of modeling the Chapman–Jouguet and cellular detonation structures. It was found that the reaction rate constant exerts a minor effect on the detonation structure, whereas the role of temperature responsible for aluminum oxide decomposition into sub-oxides is fairly important.

A model of detonation combustion of a suspension of aluminum particles in oxygen with one Arrhenius-type equation of reduced kinetics was used in [43–50]. The expression for the mass transfer J in Eqs. (1) has the form

$$J = \begin{cases} \dfrac{\rho}{\tau_\xi}(\xi - \xi_k)\exp\left(-\dfrac{E_a}{RT_2}\right), \\ \qquad\qquad T_2 \geqslant T_{\rm ign},\ \xi \geqslant \xi_k, \\ 0,\ T_2 < T_{\rm ign} \text{ or } \xi < \xi_k. \end{cases} \tag{2}$$

Here ρ is the density of the mixture as a whole and ξ_k is the residual relative mass concentration of unburned particles. The process of aluminum oxide formation on the particle surface (shaped as a "cap" or a film), which prevents complete burning of the particle, was modeled by introducing the term ξ_k into the equation for the particle concentration. The model constants ensure the consistency of the results of thermodynamic calculations of the detonation velocity [41], initiation energy, and detonation cell size estimate with the experimental data [51]. A quadratic dependence of the burning time of the aluminum particle on its size was taken in accordance with the data on combustion in pure oxygen [25, 27]; this dependence was also extended to particles 1–10 μm in diameter. The characteristic constant of the burning rate was chosen in such a way that agreement with the experimental data [25] was ensured. The formation of aluminum sub-oxides was taken into account in an integral manner (the heat release with allowance for oxide decomposition was determined from empirical data on the detonation velocity). The following results were obtained by the model: Chapman–Jouguet detonation structure, detonation initiation scenarios, two-dimensional flows with interaction of the shock wave with bounded clouds of particles, and cellular detonation in channels with constant and variable geometry in monodispersed and polydispersed suspensions of aluminum particles in oxygen. The results were consistent with available experimental and numerical data of other researchers on the characteristic scales of the cellular structure, initiation energy, and other characteristics of detonation.

Detonation of suspensions of aluminum particles in air was also studied by Zhang et al. [52, 53]. The experimental data on propagation of spin detonation in gas suspensions of aluminum particles 100 nm and 2 μm at different pressures were reported in [52]. The dependence of the critical diameter of the tube or detonation cell size on the particle diameter was discussed; it was noted that the exponent in the dependence on the particle diameter for particles 1–2 μm in size was significantly smaller than 2 (it was estimated as 1.3 in the range of particle sizes from 100 nm to 2 μm). In [53], these and other experimental data of the same authors were used to construct a semi-empirical model of detonation with hybrid reduced kinetics, which was also used in [54]. A specific feature of the hybrid kinetic model is the allowance for two reaction types (diffusion-controlled and Arrhenius-type reactions). The rate of the diffusion-controlled reaction is assumed to be a power-law function of the particle radius (with an exponent of -2), whereas the rate of the kinetic reaction is independent of this factor. The characteristic particle burning time is determined by the sum (i.e., the rate of the hybrid reaction is equal to the mean geometric value of the two reaction rates). Thus, the model takes into account the transition from the diffusion type of combustion (typical for coarse particles at high temperatures) to the kinetic type (typical for combustion of fine or coarse particles at low temperatures). The estimates show that the transition from one burning mode to the other in the case of detonation combustion (at temperatures of the order of 2000 K) occurs in the particle size interval from 100 nm to 10 μm. Though this model is fairly attractive, it still has some drawbacks. It is assumed that the heat release of the reaction at the stage of low-temperature oxidation (ignition) also occurs in the gas phase, i.e., the particle heating is determined only by convective heat transfer. Moreover, the thermal effect of the reaction is determined with the possibility of formation of aluminum sub-oxides (oxide decomposition) being ignored, which leads to overestimation of the equilibrium temperature of detonation products (5000 K). One of the uncertainty parameters is the value of the activation energy of the kinetic reaction. Parametric calculations of cellular detonation revealed that the detonation cell size and type depend significantly on this parameter. A comparison of the calculated and experimental data on the period of oscillations yielded the activation energy value of 95 kJ/mol.

In [55, 56], the principles of the particle burning description within the framework of the hybrid model [53] were used to simulate the cellular and spin detonation on the basis of two-dimensional [55] and three-dimensional [56] calculations. The particle size was varied within 1.5–20 μm. A comparison of the results predicted by the two-stage model [38, 41] and the hybrid model showed that there are practically no differences in determining the burning time and the detonation cell size as functions of the particle size [55]. The lengths of the induction zone are different, but the length in the two-stage model depends on the choice of the ignition temperature.

The theoretical investigations mentioned in this Section deal with suspensions of micron-sized aluminum particles, including suspensions of flake-shaped particles (25–40 μm in diameter and approximately 1 μm thick), whose analysis was based on considering spherical analogs with an “equivalent” diameter [53, 55, 56].

1.3. Mechanisms of Aluminum Particle Ignition under Dynamic Conditions

Mathematical modeling of detonation processes requires an adequate description of ignition, which occurs under velocity and thermal nonequilibrium conditions. Aluminum ignition was mainly studied under static conditions of slow heating. It was noted [14] that ignition may occur at the instant of oxide film oxidation. In the course of slow heating, thermal expansion of the metal is accompanied by surface oxidation reactions recovering the oxide film integrity. Faster heating leads to the emergence of surface disturbances at a temperature of about 950 K and subsequent cracking. This allows one to conclude that ignition may occur at temperatures below the metal boiling point. It was also noted that the aluminum surface may become partly naked in regimes with high-velocity heating, which facilitates evaporation or direct contact of the metal with the oxidizer medium. The data on the ignition temperature were reported in [14] for static conditions of slow heating. Nevertheless, the analysis of these data made it possible to conclude that ignition may occur at temperatures of the order of 1300 K, which is significantly lower than the melting point of aluminum oxide.

In the case of fast heating, ignition may occur at even lower temperatures. The oxide film under standard conditions (at temperatures around 300 K) consists of the amorphous oxide Al_2O_3. After heating (when the particle reaches the temperature of $\approx$500–600°C), amorphous oxide transforms to crystalline oxide, and the protective properties of the oxide film appreciably decrease [57, 58]. Moreover, violation of the film integrity (cracking) becomes possible in the case of fast heating owing to a three-fold difference in the linear expansion coefficients of aluminum and aluminum oxide [59]; this may occur already at 500°C. Thus, a region not covered by aluminum oxide may appear on the particle surface, which favors initiation of the aluminum oxidation reaction. At the stage of ignition, the oxidation reaction proceeds with solid oxide formation directly on the particle surface. The heat from the low-temperature oxidation reaction passes to the particle, i.e., it is completely spent on particle heating and melting. The possibility of low-temperature ignition of micron-sized aluminum particles in shock waves was also noted in [60]. Moreover, the presence of AlO directly behind the shock wave was also noted in [60], which testifies to the possibility of aluminum sub-oxide formation at temperatures below the aluminum oxide boiling point.

1.4. Modeling of Particle Ignition in Detonation Processes

Medvedev et al. [11] developed a physicomathematical model of ignition and combustion of gas suspensions of metal particles under various conditions, including detonation waves. Three mechanisms of ignition of aluminum particles under dynamic conditions behind shock and detonation waves were discussed: thermal explosion, reaching the critical temperature, and particle fragmentation. Ranges of initial parameters determining this or that ignition mechanism were identified. The model of aluminum ignition presented in [61] is based on the concept of oxidizer diffusion through the oxide film, which describes two experimental parameters: limiting temperature of ignition and ignition delay time as a function of the particle radius.

Mathematical modeling of particle ignition in shock waves and gas detonation waves with allowance for pre-flame oxidation and melting was performed in [35, 36]. Afanas'eva and Levin considered only single particles in [35] and analyzed the influence of the particle concentration on ignition of the gas suspension in [36]. The calculations within the framework of this model did not reveal violation of thermal equilibrium under the ignition conditions considered in the study, and the transition to the diffusion-controlled regime of particle combustion was associated with reaching the oxide film melting temperature of 2300 K by the particle, which does not agree with the ignition criteria of the hybrid and heterogeneous models of detonation of aluminum particle suspensions [37–39]. No comparisons with experimental data were performed in [36], and comparisons of the data [36] with the experimental results [62] for the ignition delay time of the gas suspension of aluminum particles with the mean particle diameter of the order of 10 μm show that the calculated values [36] (100–200 μs) was significantly higher than the experimental values [62] (20–40 μs).

The model [38] for aluminum particles is also based on the temperature criterion of ignition. The critical ignition temperature was set equal to 1350 K, which is appreciably lower than the melting point of the oxide film. However, this ensured better agreement with the experimental data on the detonation velocity and particle ignition than the value corresponding to the limiting temperature of particle ignition under static conditions [63].

Veyssiere and Khasainov [38] discussed some known physical mechanisms responsible for low-temperature ignition of particles under dynamic conditions (shock waves), in particular, violation of the oxide film integrity due to the difference in the linear expansion coefficients of aluminum and its oxide. The model [38] was used to analyze heterogeneous detonation of suspensions of aluminum particles in air and oxygen in [39], where steady propagation of the detonation wave with a velocity of about 1600 m/s (corresponding to the experiments [51]) was obtained in calculations only for the ignition temperature of 950 K.

Benkiewicz and Hayashi [64] performed a numerical study of ignition of a suspension of aluminum particles behind reflected shock waves based on the model [38] with the ignition criterion $T_{\text{ign}} = 1350$ K. The same value of the ignition temperature was used in [40] for numerical simulation of cellular detonation in lean suspensions of aluminum particles in oxygen (the velocity of stationary detonation was 1735 m/s).

In the model used in [43–49], ignition is described by a simplified scheme: particle melting and heat release in low-temperature reactions of particle oxidation are neglected. The temperature criterion of ignition is taken to be $T_{\text{ign}} = 900$ K, which is lower than the melting point, but is close to the ignition temperature of 950 K used in [39]. Ignition of the gas suspension of aluminum particles in the heterogeneous detonation wave was analyzed in [50] within the framework of the model [43–49] and model [35] with allowance for particle melting and pre-flame oxidation. Based on comparisons of these data and of data on some experiments on ignition in transient and reflected waves and in detonation processes, the temperature criterion of ignition and the adequacy of the choice of the critical temperature $T_{\text{ign}} = 900$ K for the description of detonation of aluminum suspensions in oxygen were justified.

2. MATHEMATICAL MODELING OF THE DYNAMICS OF SUSPENSION OF ALUMINUM NANOPARTICLES

2.1. Specific Features of Ignition and Combustion of Sub-Micron and Nano-Sized Aluminum Particles

The transition to nano-sized particle suspensions requires the analysis of specific features of ignition and combustion of nano-sized aluminum particles. The data on ignition and combustion of sub-micron and nano-sized aluminum particles both under static conditions and behind shock waves are reviewed in the present Section. Of greatest interest are data that can be used to construct simplified models of reduced kinetics of detonation combustion.

The data of various researchers that show that the ignition temperature decreases with a decrease in the aluminum particle size were reported in [65, 66]. Ignition at temperatures around 900 K may occur already for particles smaller than 500 nm, which may be associated with the size effect.

Sundaram et al. [66] also provided an extensive review of data on combustion of nano-sized aluminum particles. It is seen from the experimental data analyzed in [66] that the transition from the diffusion-limited to kinetic combustion occurs smoothly, i.e., there exists a transitional region. In the particle size range from 1 to 10 μm, either the diffusion-limited regime of combustion may be retained or the transitional regime may be observed, depending on test conditions. The power-law dependence of the burning time of particles smaller than 1 μm on the particle diameter is characterized by a significantly smaller exponent.

Park et al. [67] presented experimental data on combustion of nano-sized aluminum particles of various diameters (19–150 nm) in air under the conditions of an aerosol flow in a reactor. The burning time was measured by mass spectrometry of individual particles. It was found that the burning time decreases with a decrease in the particle size, and the calculated approximating values of the activation energy of the Arrhenius reaction also decrease (from 120–175 kJ/mol for 100–150 nm to 25–32 kJ/mol for 19 nm). It was noted that particles 19 nm in diameter burn down almost completely already at a temperature of about 900 K, though particles greater than 50 nm burn only partly even at 1100 K. Nevertheless, Park et al. [67] argued that combustion is a diffusion-controlled process.

Bazyn et al. [68] reported the measured parameters of combustion of aluminum particles approximately 80 nm in size behind a reflected shock wave (in the pressure range of 4–32 atm and temperature range of 1200–2100 K) in oxidizing media containing oxygen, carbon dioxide, and nitrogen. The duration of combustion determined on the basis of luminescence was 50–500 μs depending on test conditions. For the 50:50 oxygen/nitrogen mixture, the experimental dependences of the burning time on temperature are adequately described by Arrhenius-type reactions. The burning time also depends on pressure (it decreases by a factor of 1.6–4 as the pressure increases from 8 to 32 atm). The activation energies of the combustion reactions were found to be different at pressures of 8 and 32 atm. The dependence of the burning time on the fraction of oxygen in the mixture with nitrogen in the interval from 10 to 50% was also established. Replacement of oxygen by carbon dioxide as an oxidizer revealed qualitatively different trends of the burning time as a function of temperature.

Some experimental data on aluminum particle combustion in a wide range of parameters, including the nanometer range of particle sizes, were discussed in [69]. Ignition of particles smaller than 1 μm occurs at temperatures around 900 K, and the dependence of the burning time on the particle diameter with an exponent of 0.3 correlates well with experimental data. Huang et al. [69] believe that the decrease in the exponent below unity may be associated with agglomeration of nano-sized particles, which determine the burning times observed in experiments. It was also noted that the burning time significantly depends on temperature, in contrast to combustion of micron-sized particles.

A review and discussion of combustion of various nanoparticles, including aluminum, can be found in [70]. A classification of combustion regimes on the basis of thermodynamic relations is presented; conditions of diffusion-controlled and kinetic regimes and various issues of powder formation and applications are discussed.

Sundaram et al. [71] considered various mechanisms of particle heating, ignition, and combustion under static conditions of heating, where the governing mechanism of ignition and combustion is oxidizer diffusion through the oxide film. A comparison of theoretical and experimental data shows that combustion of nano-sized particles is not controlled by diffusion; however, it does not obey the laws of free-molecular combustion either. It was noted that the kinetic constants needed to construct the combustion model had not been adequately studied. Moreover, there are several important phenomena, such as sintering and agglomeration of particles and cracking of the oxide film, which should be taken into account in comparisons with experimental data.

Kwon et al. [72] performed an experimental study of combustion of aluminum particles approximately

100 nm in size in air under static atmospheric conditions. They investigated the influence of test conditions on the final products of particle combustion. Self-sustained propagation of the combustion wave was observed for concentrations about 0.1 g/cm^3 and low temperatures. It was noted that it is necessary to take into account reactions with formation of both Al_2O_3 oxide and Al_2O sub-oxide, which then interacts with nitrogen to form AlN. At low temperatures, heat is released during the formation of Al_2O_3, Al_2O, and AlN. At high temperatures, the only exothermic reaction is that with Al_2O_3 formation. The effect of aluminum reactions with nitrogen can be traced by comparing the data reported in the review [30], where the combustion of coarse particles in air and pure oxygen differs by the slope of the straight lines (i.e., by the exponent in the dependence of the burning time on the particle diameter).

2.2. Theoretical Models of Ignition and Combustion of Aluminum Nanoparticles

At the moment, there is still no single opinion and clear understanding of the mechanisms of nanoparticle combustion [66]; the models developed by various researchers describe both diffusion-limited and kinetic mechanisms.

Huang et al. [73] performed a theoretical study of combustion of micron- and nano-sized particles in air. The velocity of flame propagation and temperature distributions in the flame front were calculated by means of the numerical solution of the energy conservation equation. The particle burning rate was modeled as a function of the particle diameter and ambient temperature. Sub-nanometer particles were asymptotically considered as large molecules. Good agreement with experimental data was obtained. It was noted that the flame velocity increases as the particle diameter decreases, and combustion transforms from the diffusion-limited to kinetic regime. It was also mentioned that ultrafine particles (several nanometers) because of their low melting point are in the liquid state, rapidly evaporate, and react with the oxidizer in the gas phase, i.e., replacement of solid-phase aluminum by its liquid analog in the initial conditions does not produce any significant effect on the final reaction products and flame temperature. As Al_2O_3 does not exist in the gas phase, an equilibrium reaction of decomposition into AlO, Al_2O_2, and AlO_2 sub-oxides was proposed. The constants of 12 reactions of the kinetic scheme of aluminum combustion in oxygen were provided.

Based on the diffusion concepts of aluminum particle combustion, Aita et al. [74] proposed a simple model of single-stage kinetics. Under the assumption of a constant particle size in spherical coordinates, combustion of a single particle was numerically studied. A parametric analysis of the burning rate as a function of the particle size was performed. The boundaries of the diffusion coefficient range were discussed.

Fedorov and Shulgin [75] performed a theoretical study of combustion of a 80-nm aluminum particle on the basis of a semi-empirical model of the Arrhenius-type reduced kinetics. They analyzed the dependences of the pre-exponent, burning time, and reaction activation energy on the ambient temperature. Good agreement with the experimental data [68] was obtained in the considered ranges of temperature and pressure. It was noted that the error of the diffusion model [74] in comparisons with the same date is several times higher.

An idea of a mechanism where the ignition and initial stage of combustion of nanoparticles are induced by the melt-dispersion mechanism was developed in [76–79]. The main principle is based on the fact that thermal expansion of aluminum during its melting due to fast heating (in a high-temperature flow and in shock waves) leads to rupture of the oxide film on the particle surface and to formation of a wave propagating inward the particle. This wave is accumulated at the center and transforms to an unloading wave, resulting in particle fragmentation.

Thus, particle combustion occurs in the regime of oxidation of individual molecules (or clusters) in the gas phase. The presentation of oxide film rupture is consistent with the data that confirm the fact of ignition at temperatures close to the aluminum melting point; however, particle fragmentation has not yet been confirmed in experiments. Observations of the nanoparticle behavior in high-temperature inert media did not reveal aluminum vapors or clusters [80].

Models of combustion of aluminum nanoparticles in various media (within composite propellants and in a water jet) and various issues of particle ignition, melting, etc. were discussed in [81–83]. The presented kinetic schemes mainly refer to oxidation in water media, but they also include oxidation reactions with oxygen [82] and the model of aluminum oxide clusterization in combustion products [83]. In the models [81–83], the nanoparticles are not considered as finite-radius physical bodies, which is consistent with the melt-dispersion mechanism [76–79] where the particle burning time is independent of the particle size. Nevertheless, the calculations display good agreement with experimental data on the laminar flame propagation velocity and with the combustion region structure calculated by other researchers.

2.3. Description of Heat Transfer in Suspensions of Nanoparticles under Dynamic Conditions

Detonation flows are characterized by the presence of regions of thermal and velocity relaxation behind the leading shock wave. For an adequate description of the conditions of suspension ignition under dynamic conditions, one should take into account the specific features of the particle heating process. The widely used relations for convective heat transfer of spherical particles in the continuum regime have the following form [7]:

$$q_2 = (6m_2\lambda_1/d_2^2)\mathrm{Nu}(T_1 - T_2), \tag{3}$$

$$\mathrm{Nu} = 2 + 0.6\mathrm{Re}^{1/2}\mathrm{Pr}^{1/3}, \quad \mathrm{Re} = \frac{\rho_{11} d_2 |u_1 - u_2|}{\mu_1}.$$

Here d_2 is the particle diameter, m_2 is the particle mass, λ_1 and μ_1 are the thermal conductivity and dynamic viscosity of the gas, Nu is the Nusselt number, Pr is the Prandtl number (usually taken to be 0.7), Re is the Reynolds number, T_1 and T_2 are the gas and particle temperatures, u_1 and u_2 are the gas and particle velocities, and ρ_{11} is the own density of the gas. The characteristic time of thermal relaxation is determined by the formula

$$\tau_T^{\mathrm{cont}} = d_2^2\rho_{22}c_{v2}/(6\lambda_1\mathrm{Nu}), \tag{4}$$

where c_{v2} is the specific heat of the particles and ρ_{22} is the own density of the particles. For velocity equilibrium (static heating) conditions, it is usually assumed that Nu = 2. This approach is used for modeling ignition and combustion of micron-sized aluminum particles.

For nano-sized particles, however, the process of heating in a hot gas flow does not correspond to the continuum regime because the mean free path and even the gas molecule size can be comparable with the particle size [84]. The formulas derived in [84] allow one to estimate that the mean free path of molecules of a diatomic gas under standard conditions (1 atm and 280 K) is approximately 200 nm and is inversely proportional to pressure. Therefore, the effects of the free-molecular flow regime should be taken into account in these cases [66].

Various heat transfer aspects were considered in the review [85] in addition to the general issues of modeling the processes in aerosols of nano-sized particles (transport, clusterization, etc.). The problems in the description of thermal interaction of a gas and nano-sized particles were also considered in [86–89].

Kuhlmann et al. [86] derived the formulas for convective heat transfer in the continuum and free-molecular regimes. These formulas yield the expressions for the characteristic times of thermal relaxation. In particular, the formula for the free-molecular gas flow around the particle is

$$\tau_T^{fm} = \frac{d_2\rho_{22}c_{v2}}{6\alpha p}\sqrt{\frac{8\pi m_g T_1}{k_{\mathrm{B}}}}\left(\frac{\gamma_1 - 1}{\gamma_1 + 1}\right),$$
$$\mathrm{Kn} = \frac{RT_1}{\sqrt{2}\pi d_g^2 N_{\mathrm{A}} p d_2}. \tag{5}$$

Here d_g and m_g are the size and mass of the ambient gas molecule, k_{B} is the Boltzmann constant, α is the accommodation coefficient, γ_1 is the parameter of the adiabat for the gas, and N_{A} is the Avogadro number. The influence of the choice of the accommodation coefficient presentation on the results of modeling the heat transfer dynamics was analyzed in [86]. It was found from the comparison with the experimental data in [86] that $\alpha \approx 0.43$ for an individual spherical particle; for particle aggregates, the effective value of this coefficient was found to be $\alpha_{\mathrm{eff}} = 0.25$.

Liu et al. [87] and Mohan et al. [88] discussed the limits of applicability of the continuum and free-molecular regimes: an adequate option was assumed to be the continuum regime for Knudsen numbers smaller than 0.01 and the free-molecular regime for Knudsen numbers greater than 10. A transition from one regime to the other is observed in the interval 0.01–10 [66]. Kuhlmann et al. [86] proposed the following simple expression for the transitional regime:

$$\tau_T^{\mathrm{tr}} = \tau_T^{fm} + \tau_T^{\mathrm{cont}}. \tag{6}$$

This expression was discussed in [87] together with other approximation formulas. As was noted in [88], a more precise description has to be based on numerical calculations.

Daun and Huberman [89] made an attempt to take into account the curvature of the nanoparticle surface and the Knudsen boundary layer in the thermal dynamics of the free-molecular and transitional regimes of heating. It was noted that the proposed approach improves the estimate of the Knudsen boundary layer thickness. However, this improvement produces a minor effect on the overall rate of heat transfer; moreover, there are other sources of uncertainty (non-unique determination of the mean free path and transport properties). Possibly, the effect of curvature will be more important for fractal-like aggregates. Identification of the boundary layer in the analysis of thermal dynamics in the transitional regime was performed in the theoretical study [90]. An explicit formula was proposed for the dependence of the heat transfer coefficient of a spherical particle on the Knudsen number, which was compared with the results of the Monte Carlo simulations based on the Boltzmann equation. This method can be used under high-temperature conditions for arbitrary dependences of the specific heat and thermal conductivity on temperature.

It is also necessary to mention the paper of Allen et al. [91], who performed a theoretical analysis of heat transfer for an aluminum nanoparticle with allowance for the correction of the accommodation coefficient in the distribution of the heat release energy during particle combustion.

The estimates show that the time τ_T^{fm} for individual particles 1 μm in size at atmospheric pressure or particles 100 nm in size in shock waves can exceed $\tau_T^{\rm cont}$ by an order of magnitude or more. Formula (5) also allows one to estimate the length of the thermal relaxation region in shock and detonation waves. It turned out that the length of this region even for 1-nm particles in shock waves is greater by two or three orders of magnitude than the thickness of a real shock wave, which reaches up to four mean free paths of gas molecules [92, 93]. Owing to this fact, in the description of the dynamics of heating, ignition, and combustion of nanoparticles in shock waves, one can neglect the effects of viscosity and heat conduction in the shock wave structure and consider the latter as an ideal shock in accordance with the Euler approach.

It should be noted that all publications dealing with the behavior of nanoparticles in the gas flow refer to conditions of usual heating, i.e., to static conditions (Nu = 2). However, heating of particles behind the shock wave proceeds under velocity nonequilibrium conditions. For the continuum flow regime, this is manifested as the dependence of the heat transfer rate and, correspondingly, of the characteristic time of thermal relaxation on the Nusselt number. For nano-sized particles, it is usually assumed that the Reynolds number is very low, and the Nusselt number is equal to 2. However, in shock waves, where the characteristic velocities are of the order of 10^3 m/s, the Reynolds number can reach ≈50, while the Nusselt number is approximately 5 for 1-μm particles, 3 for 100-nm particles, and 2.5 for 10-nm particles. The influence of this factor on heat transfer under free-molecular conditions is one of the uncertainties noted in [89].

2.4. Thermophysical and Transport Properties of Aluminum Nanoparticles under Dynamic Conditions

To describe velocity relaxation of suspensions of particles whose size is comparable with the mean free path of gas molecules, one has to take into account the Cunningham correction coefficient $C_{\rm C}$ in the drag force of the phases [85, 94]:

$$f_2 = \frac{\rho_2}{\tau_u}(u_1 - u_2), \quad \tau_u = \frac{4 d_2 \rho_{22} C_{\rm C}}{3 c_D \rho_{11} |u_1 - u_2|}, \qquad (7)$$

$$C_{\rm C} = 1 + 2{\rm Kn}[1.257 + 0.4\exp(-1.1/2{\rm Kn})].$$

The existing dependences of the drag coefficient on the Reynolds number, which are used for micron-sized particles, are usually extended to the range of nano-sized particles. In [13, 44, 45, 48, 49], the drag coefficient c_D was determined with allowance for the supersonic flow in the detonation structure:

$$c_D({\rm Re}, {\rm M}_{12}) = [1 + \exp(-0.43/{\rm M}_{12}^{4.67})] \times (0.38 + 24/{\rm Re} + 4/\sqrt{\rm Re}), \qquad (8)$$

$${\rm Re} = \frac{\rho_{11} d_2 |u_1 - u_2|}{\mu_1}, \quad {\rm M}_{12} = \frac{|u_1 - u_2|\sqrt{\rho_{11}}}{\sqrt{\gamma_1 p}}.$$

A specific feature of nanoparticles is the dependence of their thermophysical properties on the particle size. Some publications on this topic were reviewed in [66]. Experimental data on the melting temperature of nano-sized aluminum particles were reported in [66, 95]. The melting temperature starts to deviate significantly from the basic value of 933 K corresponding to the continuous medium at particle sizes smaller than 10 nm and reaches 673 K for 3-nm particles. This behavior was confirmed in the experimental investigations [96] and theoretical calculations by molecular dynamics methods [97, 98]. The influence of pressure and internal defects of the structure of the interparticle space in a powder of aluminum nanoparticles of bulk density was also analyzed in [98]. No significant effect of pressure in the range of 1–300 atm on particle melting was observed.

Investigations of specific features of melting of aluminum particles by various methods, including molecular dynamics, were performed in [99–103]. Fedorov and Shulgin [99] discussed various approximations for the dependence of the melting temperature on the particle size. Based on solving the Stefan problem and analyzing the velocity of melting front propagation, they obtained data on the dependence of the melting time of aluminum nanoparticles on the particle size and ambient temperature. In [100], Fedorov and Shulgin reported the data on the dependences of the specific heat and phase transition heat on the initial size and temperature of aluminum particles. Those investigations were performed within the framework of the semi-empirical model of molecular dynamics, which was verified on the basis of the dependence of the melting temperature on the nanoparticle size. A nonmonotonic dependence of the specific heat on temperature, an increase in the peak values of the specific heat, and a decrease in the specific heat of melting with reduction of the particle size from 10 to 3 nm were noted. As the particle size increases above 10 nm, the dependences of these thermophysical parameters tend to limiting values corresponding to the volume phase. A comparison of the aluminum nanoparticle melting characteristics calculated by the molecular dynamics and phenomenological models revealed their good agreement in terms of the melting time. Similar results were obtained in [101] by the method of molecular dynamics, DL POLY software package, and two types of parametrization of the embedded atom potential. Significant scatter of available experimental and numerical data (dependences of the melting temperature on the nanoparticle size) was noted. Based on comparisons of data obtained by different methods, the validity of the semi-empirical model of molecular dynamics proposed in [100] for the description of the thermal history of the aluminum nanoparticle was confirmed. Fedorov and Shulgin [102] performed molecular dynamic modeling of melting of aluminum nanoparticles with the use of the DL POLY software package and embedded atom potential for determining the heat transfer coefficient. Analytical approximations of the derived dependences of the thermal conductivity and specific heat on the particle temperature and size were provided. Fedorov et al. [103] proposed a new physicomathematical model of melting of nano-sized aluminum samples, which takes into account the dependences of thermophysical variables on the particle temperature and size found by the molecular dynamics method. The melting times of nano-sized aluminum samples were found as functions of the particle size and ambient temperature for spherical, cylindrical, and plane symmetries.

Thus, the results of the above-mentioned investigations show that the thermophysical properties of nanoparticles experience changes in the particle size interval below 10 nm. On the other hand, for particles of this size, the ratio of the characteristic times of heating and melting (correspondingly, the ignition delay times) and the burning time is very small. The burning time depends on the particle diameter as $d^{0.3}$ (and becomes independent of the particle diameter for particles smaller than 10 nm), and the duration of the processes proceeding at the stage of ignition decreases in proportion to $d^{1.5} - d^2$ because of the decrease in the melting temperature. Therefore, the stage of melting of nanoparticles smaller than 10 nm is negligibly short, and one can avoid identifying this stage as a separate process.

2.5. Clusterization and Formation of Nanoparticles in the Process of Aluminum Combustion

Studying the detonation combustion of gas suspensions involves some associated problems: clusterization and agglomeration of particles, formation of nanoparticles (of aluminum oxide) in detonation products, etc. Some issues of agglomeration of aluminum nanoparticles in combustion processes were discussed in the review [66]. In particular, clusterization of particles was considered as one of the stages of combustion of aluminum nanoparticles in accordance with the melt-dispersion mechanism [76–79]. The agglomeration processes were mainly considered in the literature in studying combustion of solid propellant compositions containing aluminum [104, 105]. Agglomeration of particles during the combustion of exploded clouds of micron-sized aluminum particles (up to 10 μm) was investigated in [106]. The main reasons for clusterization of particles, which are loosely packed at the initial time, were assumed to be the hydrodynamic features of the flow in the course of dispersion, in particular, the development of the Richtmyer–Meshkov instability of the cloud surface and formation of vortex rings.

The formation of aluminum oxide nanoparticles in aluminum combustion products was considered only in a few papers. Attention to these processes is paid because of the problem of stability of aluminum combustion as part of composite propellants. The experiments of Karasev et al. [107] were performed to study slow low-temperature combustion of aluminum particles 5–15 μm in size under standard atmospheric conditions; the formation of aggregates of aluminum oxide particles approximately 1 μm in size from primary particles of several tens of nanometers was observed. Detonation of the suspension of aluminum particles is characterized by high temperatures of the mixture in the combustion region and detonation products, which reach the aluminum oxide decomposition temperature and may exceed the latter. Though the data on the fractal composition of the products of detonation combustion of aluminum are not available, the thermodynamic calculations of aluminum detonation products reveal the presence of sub-oxides [17]. Thus, parallel to the formation of aluminum oxide nanoparticles, their evaporation and oxide decomposition into sub-oxides occur. In the majority of the theoretical models of detonation of micron-sized aluminum particles, the oxide particles being formed are described as a gas-phase component, and the reactions of decomposition into sub-oxides are ignored.

An attempt to provide a theoretical description of the process of formation and growth of aluminum oxide nuclei in the course of detonation was made in [108]. The theoretical calculations predicted unstable regimes with jumps of condensation, though there is no experimental validation of these phenomena as far as we are aware. The semi-empirical model of nanoparticle formation in metal combustion products within the framework of the continuum description of the processes was considered in [109], but the possibility of applying this model for detonation combustion of aluminum is not obvious. Starik et al. [83] presented a physically grounded model of oxide nanoparticle formation in aluminum combustion products, which is based on the principles of intermolecular interactions and clusterization mechanisms. The model provides a discrete description of formation and growth of nuclei through a sequence of chain reactions; for this reason, integrating it to the model of detonation of gas suspensions within the framework of continuum concepts of mechanics of continuous media is rather difficult. As a whole, many aspects of modeling the formation and growth of solid nanoparticles of aluminum oxide with allowance for its decomposition into sub-oxides in products of detonation of the gas suspension of aluminum particles (under conditions of high temperatures and pressures) are still open.

2.6. Modeling of Detonation Processes in Suspensions of Aluminum Nanoparticles

The model of detonation of a stoichiometric suspension of aluminum nanoparticles in oxygen was presented in [110]; it is based on the description of the flow dynamics by the equations of mechanics of continuous media and by the equation of reduced kinetics of chemical reactions [Eqs. (1)–(9)]. In view of the transitional character of heat transfer in a wide range of variation of the flow parameters, it was decided to calculate the thermal dynamics of submicron and nano-sized particles by using the logarithmic interpolation composed of formulas (4) and (5):

$$\tau_T^{\rm tr} = [(\log {\rm Kn} + 2)\tau_T^{fm} + (1 - \log {\rm Kn})\tau_T^{\rm cont}]/3. \quad (9)$$

The description of ignition and combustion of submicron and nano-sized particles is based on the empirical data reported in [66, 68–70]. The ignition criterion is the rupture of the oxide film due to aluminum melting $T_{\rm ign} = T_{melt} = 930$ K, which corresponds to the ignition mechanism proposed in [78, 79]. In the reduced kinetics equation (2), the dependence of the characteristic burning time on the flow parameters and particle size was taken in the form

$$\tau_\xi = \tau_0 (d/d_0)^{0.3} (p/p_*)^{-m}. \quad (10)$$

The activation energy and the exponent in the dependence on pressure were determined in accordance with the experimental data [68] as $E_a = 60$ kJ/mol and $m = 0.5$. The integral heat release in the reduced chemical reaction was determined on the basis of the empirical data for the Chapman–Jouguet detonation velocity [51]. As was demonstrated in the experiments [52] and theoretical calculations [41], the detonation velocity in suspensions of particles smaller than 10 μm depends on the composition and is independent of the particle size.

Khmel and Fedorov [111] analyzed steady Chapman–Jouguet detonation structures, overdriven detonation waves, and attenuated detonation waves (in the quasi-steady approach). It was noted that the scale of the combustion region is significantly greater than the scales of the thermal and velocity relaxation regions of nano-sized particles. The change in the combustion region length due to a change in the amplitude of the leading shock wave was found to be much sharper, which is responsible for the irregular character of cellular detonation in two-dimensional calculations. It was demonstrated that the effects of the free-molecular flow and heat transfer are manifested for particle sizes up to 300 nm; therefore, in modeling detonation of gas suspensions of coarser (submicron) particles, it is possible to use the continuum approximation of small Knudsen numbers.

Numerical simulations of two-dimensional flows of cellular detonation in a plane channel were performed with the use of the model in [112, 113]. The results revealed an increase in the cell size and its irregular character, which is apparently caused by the fact that the activation energy of reduced kinetics of combustion is almost twice the value $E_a = 32$ kJ/mol used in [43–46] to describe the detonation combustion of suspensions of micron-sized particles. In this case, the peak values of pressure at triple points (amplitudes of oscillations) are significantly higher than those in the case of the cellular detonation of micron-sized particle suspensions, which is qualitatively consistent with the experimental data [52]. Thus, the transition from the diffusion-controlled combustion regime (for micron-sized particles) to the kinetic regime (for nano-sized particles) is responsible for qualitatively different properties and characteristics of cellular detonation in gas suspensions of aluminum particles.

CONCLUSIONS

Theoretical and experimental investigations of processes in detonation combustion of suspensions of aluminum particles in gaseous oxidizing media are reviewed. The basic goal of the present review is to describe various approaches and concepts used to construct the detonation model of detonation of gas suspensions of micron- and nano-sized aluminum particles with allowance for the recent data on regimes of particle heating, ignition, and combustion.

Closing relations are derived for the equations of mechanics of heterogeneous media, which describe the

detonation processes in suspensions of nano-sized aluminum particles, in particular, the following features:
—in the description of the dynamic properties and heat transfer of nano-sized particles, one should take into account the transition from the continuum regime of the gas flow around the particle to the free-molecular regime;
—ignition of nano-sized aluminum particles occurs at temperatures corresponding to the aluminum melting point;
—the description of particle combustion is characterized by the transition from the concept of the diffusion-controlled regime to the kinetic regime (Arrhenius reaction) of combustion;
—models of reduced kinetics for the diffusion-controlled regime of combustion of coarse particles and Arrhenius kinetics of combustion of micron-sized and nano-sized aluminum particles, which were developed on the basis of empirical data, are analyzed;
—experimentally observed properties of detonation are noted: the detonation velocity in gas suspensions of micron- and nano-sized particles depends on the particle concentration and oxidizing media and does not depend on the particle size.

The issues of clusterization of solid aluminum oxide particles in detonation products, aluminum oxide decomposition, and formation of underoxidized products (sub-oxides) during the detonation combustion of aluminum have been poorly studied yet. There is a lack of experimental data in this field, and the few available theoretical models require further analysis and improvement.

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