EFFECT OF TRANSIENT HEAT TRANSFER ON IGNITION OF METAL PARTICLES

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Ignition and combustion of metal particles are the issues of interest for many industrial and aerospace applications. When simulating ignition and combustion of metal particles using available standard models, a number of simplifying assumptions are usually adopted, which are not always justified. The objective of this work is to develop a new particle-heating model with the correction factors to the Newton law taking into account transient heat transfer to a particle and nonuniform temperature distribution inside the particle. The new particle-heating model was shown to correlate much better with detailed numerical calculations than the standard model. The transient heating effects were proved to be important for the problem of solid-particle ignition in the oxidizer gas.

1 Introduction

Dynamics of heating, ignition, and combustion of reactive solid particles are the issues important for various applications, including aerospace and chemical technologies, chemical propulsion, ground transportation, and industrial safety [1]. Modern Computational Fluid Dynamics (CFD) software packages utilize the simplest standard models of particle heating based on the Newton law [2] and particle ignition and combustion based on overall heterogeneous or homogeneous, Arrhenius-type, macrokinetic laws of one or several reactions [3].

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The validity of many assumptions adopted in such standard models remains questionable. First, the Newton law is known to be valid only for steady-state heat transfer and the consequences of its application to intrinsically transient problems of particle heating and ignition are not quite clear. Second, the standard models deal with the mean particle temperature, thus assuming that the thermal conductivity of particle material is infinitely large. However, this assumption can be violated when ignition of a relatively large particle of low-conductivity material is considered or when the chemical reaction rate at a particle surface is sensitive to the surface temperature. In general, the Newton law should operate with the particle surface temperature rather than the mean temperature. Third, application of convective heat transfer correlations of the Ranz–Marshall type [4] for modeling heat fluxes between solid particles and gas under conditions of nonzero velocity slip in two-phase flows is also not fundamentally substantiated. Such correlations were derived from the measurements in steady-state flows and their use in transient two-phase flow conditions is questionable.

Regarding the overall kinetic law of particle ignition, it is usually derived by fitting the measured ignition delays and the results of calculations based on the standard particle ignition model with several unknown Arrhenius parameters (e.g., preexponential factor and activation energy) [5]. The Arrhenius parameters of the overall reaction rate constants are then found by applying the least-square procedure. In view of the above assumptions adopted in the standard model of particle heating, the Arrhenius parameters thus obtained can appear to have little common with the actual values relevant to the problem under consideration. There are many examples in the literature, when the values of preexponential factors and activation energies determined for particular conditions of particle ignition (e.g., large samples of cubic or cylindrical geometry, etc.) were applied for other conditions (fine particles of spherical or flaked shape, thin filaments, etc.). In view of these implications, there is a need in a reliable model of solid-particle heating to provide the basis for improved modeling of particle ignition and combustion.

The objective of this work is to develop a new particle-heating model with the correction factors to the Newton law taking into account transient heat transfer between a particle and the ambient gas and nonuniform temperature distribution inside the particle.

2 Formulation

2.1 Standard Model

The standard model (further referred to as the ST-model) of spherical particle heating in the quiescent gas is written in the form [1]:

$$cm\frac{d\overline{T}}{dt} = \alpha S(T_{g\infty} - \overline{T}) \tag{1}$$

with the initial condition

$$\overline{T}(0) = T_0 \tag{2}$$

where t is time, $\overline{T}$ is the mean particle temperature, $T_{g\infty}$ is the ambient gas temperature, α is the heat transfer coefficient, $S = 4\pi R^2$ is the particle surface area, $m = (4/3)\pi\rho R^3$ is the particle mass, c is the specific heat of particle material, ρ is the particle material density, and R is the particle radius. From now on, index 0 relates to the initial parameters, and index g relates to gas. The heat transfer coefficient α is determined from condition Nu $= 2$, i.e., $\alpha = \lambda_g/R$, where Nu is the Nusselt number and λ is the thermal conductivity. Coefficient λ_g is usually calculated at a certain reference temperature, e.g., $(\overline{T} + T_{g\infty})/2$.

Introducing the characteristic time scale of particle heating, R^2/a ($a = \lambda/(\rho c)$ is the thermal diffusivity of particle material), and characteristic temperature, T_0, the standard model of Eqs. (1) and (2) can be presented in the dimensionless form:

$$\frac{d\overline{\Theta}}{d\text{Fo}} = 3\text{Bi}\left[\Theta_{g\infty} - \overline{\Theta}\right] ; \quad \overline{\Theta}(0) = 1 \tag{3}$$

where $\overline{\Theta} = \overline{T}/T_0$ is the dimensionless mean particle temperature, $\Theta_{g\infty} = T_{g\infty}/T_0$ is the dimensionless gas temperature at a large distance from the particle, Fo $= at/R^2$ is the Fourier number, and Bi $= \alpha R/\lambda$ is the Biot number.

2.2 New Model

Generally speaking, the Newton law used in Eqs. (1) and (2) is valid only for the steady-state conditions. In transient conditions, the coefficient

α will be a function of time, e.i., $\alpha = \alpha_{\text{eff}} = \alpha(t)$. Moreover, Eq. (1) implies that the mean particle temperature $\overline{T}$ is equal to the particle surface temperature T_i, which is not true, in particular, at the initial stage of the particle heating process.

Thus, Eq. (1) should be replaced by equation:

$$cm\frac{d\overline{T}}{dt} = \alpha_{\text{eff}}S(T_{g\infty} - T_i) \tag{4}$$

which is also subjected to the initial condition of Eq. (2). To complete the statement of the problem, one has to determine parameters α_{eff} and T_i as functions of time t, mean particle temperature $\overline{T}$, and thermophysical parameters of the problem. The new particle-heating model based on Eq. (4) will be further referred to as the NEW-model.

In the dimensionless form, Eq. (4) can be written as:

$$\frac{d\overline{\Theta}}{d\text{Fo}} = 3\text{Bi}_{\text{eff}}[\Theta_{g\infty} - \Theta_i]; \quad \overline{\Theta}(0) = 1 \tag{5}$$

where $\Theta_i = T_i/T_0$ is the dimensionless particle surface temperature and $\text{Bi}_{\text{eff}} = \alpha_{\text{eff}}R/\lambda$ is the effective Biot number.

The approximate relationship for the coefficient α_{eff} entering Bi_{eff} can be obtained using the analytical solution of the transient heat transfer problem between a spherical particle and ambient gas at constant particle temperature ($\overline{T} = T_i = const$) [6]:

$$\alpha_{\text{eff}} \approx \lambda_{\text{eff}}R^{-1} = \lambda_g\left(1 + \sqrt{\frac{R^2}{\pi a_g t}}\right)R^{-1} \tag{6}$$

where $a_g = \lambda_g/(\rho_g c_p)$ is the gas thermal diffusivity and c_p is the specific heat of gas at constant pressure. Equation (6) was obtained from the comparison of two relationships for the heat flux to/from the particle surface, namely, the Newton law,

$$q = \alpha_{\text{eff}}(T_{g\infty} - T_i)$$

and the relationship derived from the analytical solution,

$$q = \frac{\lambda_g(T_{g\infty} - T_i)}{R}\left(1 + \frac{R}{\sqrt{\pi a_g t}}\right)$$

To determine the dimensionless particle surface temperature Θ_i entering Eq. (5), the following approach was used. The temperature Θ_i was assumed to be a polynomial function of the mean particle temperature $\overline{\Theta}$:

$$\Theta_i = \sum_{j=0}^{n} b_j \overline{\Theta}^j \qquad (7)$$

where n is the polynomial order and b_j are the polynomial coefficients. To determine n and b_j, a detailed problem of particle heating described in the next subsection was formulated and solved.

2.3 Detailed Model

The detailed problem of transient heat transfer between gas and a particle was formulated based on the following governing equations:

$$\frac{\partial T_g}{\partial t} - a_g \frac{\partial^2 T_g}{\partial r^2} - \left(\frac{2a_g}{r} \right) \frac{\partial T_g}{\partial r} = 0 \qquad (8)$$

$$\frac{\partial T}{\partial t} - a \frac{\partial^2 T}{\partial r^2} - \left(\frac{2a}{r} \right) \frac{\partial T}{\partial r} = 0 \qquad (9)$$

subjected to the initial conditions:

$$t = 0 : \quad T_g = T_{g\infty}; \quad T = T_0 \qquad (10)$$

and boundary conditions:

$$r = 0 : \quad \frac{\partial T}{\partial r} = 0$$
$$r = R : \quad T = T_g = T_i , \quad \lambda \frac{\partial T}{\partial r} = \lambda_g \frac{\partial T_g}{\partial r} \qquad (11)$$
$$r \to \infty : \quad \frac{\partial T_g}{\partial r} = 0$$

where r is the radial coordinate. The particle-heating model based on Eqs. (8) and (9) and conditions (10) and (11) will be further referred to as the D-model (abbreviation of "detailed").

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In the dimensionless form, the D-model can be represented as:

$$\beta \frac{\partial \Theta_g}{\partial \mathrm{Fo}} - \frac{\partial^2 \Theta_g}{\partial \xi^2} - \frac{2}{\xi} \frac{\partial \Theta_g}{\partial \xi} = 0$$

$$\frac{\partial \Theta}{\partial \mathrm{Fo}} - \frac{\partial^2 \Theta}{\partial \xi^2} - \frac{2}{\xi} \frac{\partial \Theta}{\partial \xi} = 0$$

$$\mathrm{Fo} = 0: \quad \Theta_g = \Theta_{g\infty} ; \quad \Theta = 1 \tag{13}$$

$$\xi = 0: \qquad \frac{\partial \Theta}{\partial \xi} = 0$$

$$\xi = 1: \qquad \Theta = \Theta_g = \Theta_i , \quad \frac{\partial \Theta}{\partial \xi} = \delta \frac{\partial \Theta_g}{\partial \xi} \tag{14}$$

$$\xi \to \infty: \quad \frac{\partial \Theta_g}{\partial \xi} = 0$$

where $\beta = a/a_g$ and $\delta = \lambda_g/\lambda$.

The set of Eqs. (12) with the initial and boundary conditions of Eqs. (13) and (14) was solved numerically using the implicit finite-difference scheme and the procedure described in [7] and validated against known analytical solutions [8]. To take into account thermal expansion of particle material due to transient particle heating, the governing equations of the D-model were also integrated with regard for the dependence of the material density on temperature. The effect of thermal expansion was shown to be insignificant. Therefore, to simplify the calculations, thermal expansion of the materials was neglected.

The values of b_j in Eq. (7) were determined by statistical processing of numerical solutions for spherical particles of steel, silver, and mercury 70 μm in diameter at different initial conditions (Table 1). The calculations indicated that the polynomial of the third order ($n = 3$) was sufficient for attaining a reasonable agreement of Eq. (7) with the results of numerical solution. For example, for steel and silver particles heated in air at normal pressure, the error of the polynomial approximation of Eq. (7) did not exceed $\varepsilon_{\max} \approx 0.5\%$–2.6% up to mean particle temperatures of $\overline{\Theta} = 4.3$ ($T \approx 1250.15$ K). The error ε was defined as

$$\varepsilon = \left(1 - \frac{\overline{\Theta}}{\overline{\Theta}_D} \right) \cdot 100\%$$

Table 1 Recommended values of n and b_j in the polynomial of Eq. (7)

n	b_0	b_1	b_2	b_3
3	0.0469521	0.931	0.03682	$-6.129 \cdot 10^{-3}$

where index D relates to the D-model. The recommended values of b_j are presented in Table 1.

3 Results of Calculations

To study the comparative performance of the models described above, a set of calculations was made. Table 2 shows the list of particle materials analyzed, as well as relevant thermophysical properties used in the calculations. In all cases, the particle diameter was taken equal to 70 μm. In the calculations, temporal variation of particle mean temperature $\overline{\Theta}$ in hot air with temperature $\Theta_{g\infty}$ at atmospheric pressure was monitored. Table 3 and Fig. 1 show the results of calculations in terms of the maximal discrepancy, $\varepsilon_{\max}$, of $\overline{\Theta}$ from the mean temperature predicted by the D-model, $\overline{\Theta}_D$, and the mean temperature itself predicted by ST-, NEW- and D-models. For the sake of convenience, Table 3 shows the dimensional values of the corresponding temperatures. It is seen from Table 3 and Fig. 1 that contrary to the ST-model, the NEW-model correlates well with the D-model.

Table 2 Thermophysical properties of particle materials

Particle material	λ, W/(m·K)	c, J/(kg·K)	ρ, kg/m^3
Steel (at 293.15 K)	45.0	461.0	7900
Silver (at 273.15 K)	458.0	234.0	10500
Mercury (at 273.15 K)	7.9	138.0	13600

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Table 3 Results of calculations for steel, silver, and mercury particles at $\overline{\Theta}(0) = 1$ ($T_0 = 293.15$ K)

Particle material	$\Theta_{g\infty}$ ($T_{g\infty}$, K)	$\varepsilon_{\max}$, %		$\overline{T}$, K	
		NEW	ST	NEW/D	ST/D
Steel	1.2388 (363.15)	-0.069	-0.380	307.48/307.26	315.64/314.45
	2.2622 (663.15)	-0.580	-7.200	363.81/361.71	451.18/420.87
	3.2855 (963.15)	-0.574	-15.700	329.70/327.92	561.38/485.20
	4.3089 (1263.15)	-2.014	-23.730	706.85/721.37	645.01/521.30
Silver	1.2388 (363.15)	-0.044	0.045	295.96/295.83	294.30/294.43
	2.2622 (663.15)	-0.460	-1.450	308.69/307.28	311.72/307.28
	3.2855 (963.15)	-0.740	-4.890	321.78/319.42	335.03/319.42
	4.2066 (1233.15)	-0.800	-9.140	328.00/325.39	361.52/331.24
Mercury	1.2388 (363.15)	0.264	-0.473	354.24/355.18	335.52/333.95
	1.5799 (463.15)	-0.600	-2.150	365.54/363.37	380.37/372.38
	1.9210 (563.15)	-0.870	-4.470	394.75/391.36	419.94/401.95
	2.2622 (663.15)	-0.980	-7.129	401.28/397.37	457.80/427.34
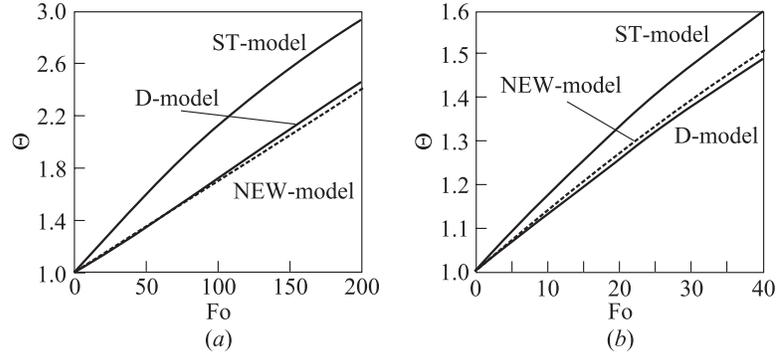
Figure 1 Time history of the mean temperature of a steel particle at $T_{g\infty} = 1263$ K (a), and mercury particle at $T_{g\infty} = 663$ K (b)

4 Model Generality

To demonstrate the generality of the NEW-model, it was applied to the problem of aluminum, magnesium, and boron particles heating in hot

Table 4 Thermophysical properties of aluminum, magnesium, and boron at $T_0 = 293.15$ K

Particle material	λ, W/(m·K)	c, J/(kg·K)	ρ, kg/m^3
Aluminum	225.0	900.0	2700
Magnesium	139.0	1020.0	1740
Boron (cristal.)	27.0	1026.0	2340

Table 5 Results of calculations for magnesium, aluminum, and boron particles at $\overline{\Theta}(0) = 1$ ($T_0 = 293.15$ K)

Particle material	T_∞, K	ε_{max}, %		$\overline{T}$, K	
		NEW	ST	NEW/D	ST/D
Magnesium	930.15	−1.04	−12.43	363.00/359.77	446.30/397.00
	1600.15	1.42	−31.25	536.18/543.89	713.87/543.89
Aluminum	930.15	−0.98	−12.80	371.25/368.44	440.18/391.93
	1600.15	2.01	−31.37	529.35/540.19	709.63/540.19
Boron	930.15	−0.79	−13.65	347.48/344.75	475.22/418.14
	1600.15	2.63	−31.36	592.95/608.97	727.68/553.95

air at atmospheric pressure using the data of Table 1. Particles of these materials are widely used as energetic additives to propellants. Table 4 shows the corresponding thermophysical properties of these materials. Table 5 and Fig. 2 show the results of calculations at $T_{g\infty} = 1600.15$ K. The initial particle diameter was taken equal to 70 μm.

Comparison between the D-, ST-, and NEW-models indicates that the NEW-model correlates much better with the D-model than the ST-model. The maximal error in the predicted mean temperature inherent in the NEW-model is only 1%–3%, while the error of the ST-model reaches the value of up to 30%. The higher error is attained at higher gas temperatures.

5 Discussion

The results of calculations provide important implications for the problem of metal particle ignition in the oxidizing atmosphere. For example,
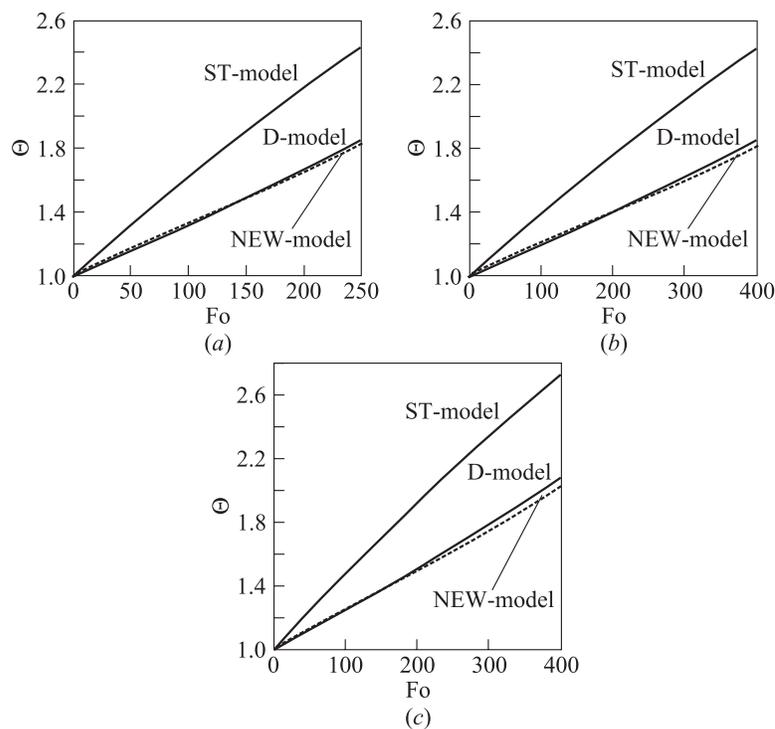
Figure 2 Time history of the mean temperature of a magnesium (a), aluminum (b), and boron (c) particles at $T_{g\infty} = 1600$ K

the standard model often used in relevant studies of particle ignition predicts that the mean temperature of boron particle 70 μm in diameter attains a value of 728 K at 5.5 ms (Fo = 50.4), when it is placed in hot air with a temperature of 1600.15 K (see Fig. 2c). This temperature exceeds the melting temperature of boron oxide film (≈ 723 K), which is often used as a critical temperature of boron particle ignition. According to the NEW-model, during the time of 5.5 ms, the boron particle heats only up to 542 K, other conditions being equal. This mean temperature value correlates well with the prediction provided by the D-model. Clearly, the arising difference in the mean temperature

(about 185 K!) can exert a pronounced effect on the particle ignition timing.

The other important implication of the results is as follows. The macrokinetic Arrhenius parameters of the reaction rate constant relevant to metal particle ignition are often obtained based on fitting the experimental measurements of the particle ignition delay with the standard model similar to the model of Eq. (3) supplemented with the corresponding chemical source term. In view of the significant error associated with the use of the standard heating model, the corresponding Arrhenius parameters obtained by the least-square method could be incorrect. In any case, their applicability to the problems of ignition of particles possessing different size and shape should be properly substantiated.

An important advantage of the NEW-model is that it incorporates a particle surface temperature T_i, which can differ from the mean particle temperature. When solving the problem of particle ignition, this issue can manifest itself in the modification of the particle ignition timing, as the surface reaction rates are very sensitive to temperature.

Concluding Remarks

The dynamics of solid particle heating in a hot quiescent air was calculated using three models: (i) detailed model based on the conjugate equations of thermal conductivity in gas and particle, (ii) approximate standard model based on the ordinary differential equation for the mean particle temperature and the Newton law, and (iii) new approximate model, based on the ordinary differential equation for the mean particle temperature and the Newton law applying the effective heat transfer coefficient and the particle surface temperature. The approximate dependence of the effective heat transfer coefficient on governing parameters and time was derived from the analytical solution for a particle with constant surface temperature. The dependence of the particle surface temperature on its mean temperature was found by generalizing the results of numerical solution of the conjugate problem.

Comparison of the computational results provided by the three models for steel, silver, mercury, aluminum, magnesium, and boron particles showed that the new model correlates much better with the

detailed model than the standard model. The maximal deviations of the predicted mean particle temperature from the solution of the conjugate problem were less than 1%–3% for the new model and up to 30% for the standard model. The largest deviations were obtained for high air temperatures. The latter is particularly important for the problem of metal particle ignition in oxidizer gas. The other important advantage of the new model is that it contains the particle surface temperature, which differs from the particle mean temperature. When solving a problem of particle ignition, the use of the particle surface temperature may affect the process evolution in view of the strong dependence of the rate of heterogeneous reactions on temperature. This implication has been demonstrated on the example of boron particle ignition.

Acknowledgments

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