Turbulence, Heat and Mass Transfer 5
K. Hanjaliœ, Y. Nagano and S. Jakirlic (Editors)

Effect of Transient Heat Transfer on Metal Particle Ignition

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Abstract - 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 in turbulent flows are the issues important for various applications, including aerospace and chemical technologies, chemical propulsion, ground transportation, and industrial safety [1]. Modern CFD software packages utilize the simplest standard models of particle heating based on the Newton law and particle ignition and combustion based on overall heterogeneous or homogeneous, Arrhenius-type, macrokinetic laws of several reactions [2].

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. Third, application of convective heat transfer correlations of the Ranz–Marshall type [3] for modeling heat fluxes between solid particles and gas in two-phase turbulent flows is also not fundamentally substantiated. Such correlations were derived from the measurements in steady-state flows and their use in transient conditions is questionable.

Regarding the overall kinetic law of particle ignition, it is usually derived by fitting measured ignition delays and the results of calculations by the standard particle ignition model with several unknown Arrhenius parameters [4]. These parameters 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.

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. 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]:

$$cm\frac{d\overline{T}}{dt} = aS(T_{g\infty} - \overline{T})\,, \quad \overline{T}(0) = T_0 \tag{1}$$

where the notations are self-explanatory. From now on, index 0 relates to the initial parameters, and index g relates to gas. The heat transfer coefficient a is determined from condition Nu = 2, i.e., $a = l_g / R$, where R is the particle radius.

3. New Model

Generally speaking, the Newton law used in Eq. (1) is valid only for the steady-state conditions. In transient conditions, the coefficient a will be a function of time, e.i., $a = a_{eff}$ = a (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:

$$cm\frac{d\overline{T}}{dt} = a_{eff} S(T_{g\infty} - T_i)\,, \quad \overline{T}(0) = T_0 \tag{2}$$

The new heating model based on Eq. (2) will be further referred to as the NEW-model.

The approximate relationship for the coefficient a_{eff} was 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) [5]:

$$a_{eff} \approx l_{eff} R^{-1} = l_g \left(1 + \sqrt{\frac{R^2}{p\, a_g\, t}}\right) R^{-1} \tag{3}$$

where a_g is the gas thermal diffusivity. The dimensionless surface temperature $\Theta_i = T_i / T_0$ was assumed to be a polynomial function of the mean dimensionless particle temperature $\overline{\Theta} = \overline{T} / T_0$:

$$\Theta_i = \sum_{j=0}^{n} b_j \overline{\Theta}^{\,j}\ ; \tag{4}$$

To determine n and b_j, a detailed problem of particle heating was solved.

4. Detailed Model

The problem of transient heat transfer between gas and a particle was based on equations:

$$\frac{\partial T_g}{\partial t} - a_g \frac{\partial^2 T_g}{\partial r^2} - \left(\frac{2a_g}{r}\right)\frac{\partial T_g}{\partial r} = 0\,, \quad \frac{\partial T}{\partial t} - a\frac{\partial^2 T}{\partial r^2} - \left(\frac{2a}{r}\right)\frac{\partial T}{\partial r} = 0 \tag{5}$$

subjected to the initial conditions: $t = 0$: $T_g = T_{g\infty}$; $T = T_0$, and boundary conditions:

$$r = 0\text{: } \frac{\partial T}{\partial r} = 0\,;\ r = R\text{: } T = T_g = T_i\,,\ l\frac{\partial T}{\partial r} = l_g \frac{\partial T_g}{\partial r}\,;\ r \to \infty\text{: } \frac{\partial T_g}{\partial r} = 0$$

where r is the radial coordinate. The particle heating model based on Eqs. (5) will be further referred to as the D-model (abbreviation of “detailed”).

Equations (5) with the initial and boundary conditions were solved numerically using the implicit finite-difference scheme [6] and validated against analytical solutions [7]. The governing equations of the model were also integrated with regard for the dependence of the material density on temperature. The effect of thermal expansion was insignificant.

The values of b_j in Eq. (4) were determined by statistical processing of numerical solutions for spherical particles of steel and silver 70 *m*m in diameter at different initial conditions. The polynomial of the third order (n = 3) was sufficient for attaining a reasonable agreement of Eq. (4) with the numerical solution. The recommended values of b_j are: b_0 = 0.0469521, b_1=0.931, b_2 = 0.03682, and b_3 = – 6.129e–3.

5. Results and Discussion

To study the comparative performance of the models, a set of calculations was made for steel, silver and mercury particles. The particle diameter was taken equal to 70 *m*m. In the calculations, temporal variation of particle mean temperature $\overline{\Theta}$ in hot air with temperature $\Theta_{g\infty}$ at atmospheric pressure was monitored. Figures 1 and 2 show the predicted results in terms of the mean temperature histories in the ST-, NEW-, and D-models. It is seen from Figs. 1 and 2 that contrary to the ST-model, the NEW-model correlates well with the D-model. To demonstrate the generality of the NEW-model, it was applied to the problem of aluminum, magnesium and boron particles heating in hot air at atmospheric pressure.

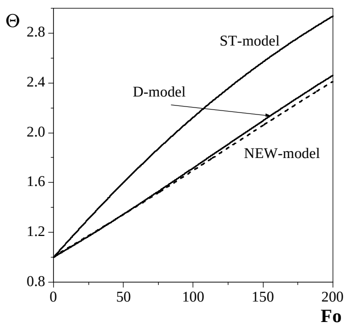

Fig. 1: Time history of the mean temperature of a steel particle at T_{g_∞} = 1263 K

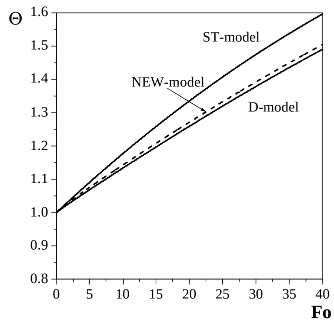

Fig. 2: Time history of the mean temperature of a mercury particle at T_{g_∞} = 663 K

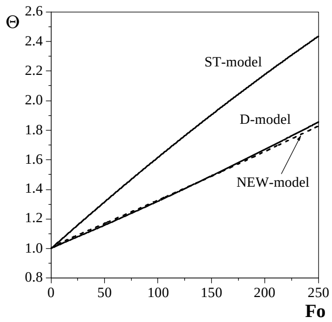

Fig. 3: Time history of the mean temperature of a magnesium particle at T_{g_∞} = 1600 K

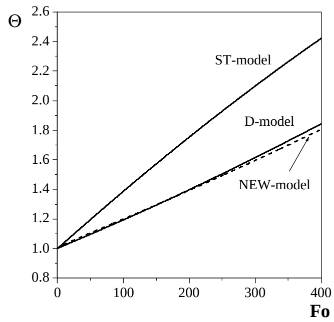

Fig. 4: Time history of the mean temperature of aluminum particle at T_{g_∞} = 1600 K

Particles of these materials are widely used as energetic additives to propellants. Figures 3 and 4 show the results of calculations at different air temperatures. The particle diameter was 70 mm. 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 maximal error is attained at high gas temperatures.

The results of calculations provide important implications for the problem of metal particle ignition in the oxidizing atmosphere. For example, the standard model often used in relevant studies of particle ignition predicts that the mean temperature of boron particle 70 mm in diameter attains a mean temperature of 727.68 K at 5.5 ms, when it is placed in hot air with a temperature of 1600.15 K. This temperature (728 K) exceeds the melting temperature of the 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.

Concluding Remarks

The dynamics of solid particle heating in a hot quiescent air was calculated using three models: (1) detailed model, (2) approximate standard, and (3) 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. Comparison of the computational results provided by the three models for metal particles showed that the new model correlates much better with the detailed model than the standard model. The other important advantage of the new model is that it contains the particle surface temperature, which is important for ignition problems turbulent two-phase flows.

Acknowledgements

The work was partly supported by the Russian Foundation for Basic Research (grants 05-08-18200, 05-08-50115) and AVL LIST GmbH.

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