On Mathematical Modeling of Spherical Non-adiabatic Diffusion Microflames

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1 Introduction

Recent development of silicon technologies and occurrence of new materials has led to an opportunity of creating highly effective small-sized thermoelectric and photovoltaic power generators. Their use opens new prospects in creation of microscale energy-supply devices. Micro combustion systems may be used as source of heat and infra red radiation in such kind of devices. Therefore, detailed investigation of characteristics of microscale combustion is important problem.

One-dimensional flames are very attractive for fundamental studies of the flame structure. Such investigations can provide deep understanding of the basic mechanisms of instability, flame stabilization and flame quenching. This paper addressed to the theoretical analysis of a non-adiabatic spherical diffusion microflame.

Heat-diffusion model with one-stage global chemical reaction, representing combustion processes of burner-generated spherical diffusion flame, has been proposed in [1]. Exact analytical solutions of this problem cannot be obtained because of strong nonlinear term of equations regarding to chemical reaction rate. The authors of the works [1, 2] used asymptotic expansion method [3] for finding of approximate solutions. An alternative method of obtaining approximate solutions is to use localized reaction zone assumption [4]. Nowadays this method is advanced for premixed gas combustion only.

The main goal of the present work is to develop an appropriate mathematical model of spherical non-adiabatic diffusion microflame including effects of incomplete consumption of fuel and oxidizer [5]. The current analytical approaches [1, 2, 6] encounter the difficulties in modeling of stationary regimes of diffusion gas combustion under strong non-adiabatic conditions or near the flammability limits because these approaches are incapable of describing incomplete reactant consumption effects.

In additional to analytical results, the numerical simulations of spherical micro flames under assumption of global chemical kinetics have been carried out. Analytical and numerical results of the present study are compared with some results of the previous theoretical approaches.

2 Theoretical Model

The configuration of the investigated problem is shown in Fig.1. Fuel is supplied radially through a porous sphere of radius a, with mass flow rate $\dot{m}$. The surrounding atmosphere contains oxidant only. The chemical activity modeled by a one step irreversible reaction. Present theoretical analysis and numerical simulations was carried out in the frame of heat-diffusion model have been proposed in [1]. Governing equations describe gas temperature distribution and mass fraction distribution of fuel and oxidizer. The differential equations are

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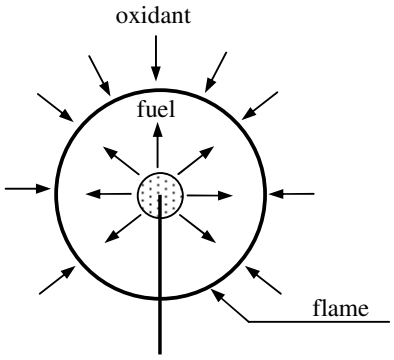

Fig. 1. Schematic representation of the spherical burner.

supplemented by boundary conditions at the porous sphere surface and far downstream. These boundary conditions same as in previous studies [1,2] except the boundary conditions for gas temperature. There are two possible ways to assign the boundary conditions for temperature at sphere surface depending on physical situation including

$$\frac{dT}{dr} = M(T-1), \text{ or} \qquad \text{(a)}$$

$$T = T_0 \qquad \text{(b)}$$

The first case (a) represents the adiabatic condition assuming absence of any heat sources or sinks at the surface of the porous sphere. The boundary condition (b) means that the emergent gas temperature is maintained on the constant level and it is equal to T_0.

Direct analytical investigation of spherical diffusion flame in the frame of heat-diffusion model meets with significant difficulties because of strong nonlinear term of equations regarding to chemical reaction rate. In present study we approximated chemical reaction rate by the step function. It was shown what substitution of the approximate solution in the original formulation gives a remainder in the right-hand side of the equations proportional to $1/\theta$, where $\theta >> 1$ is the dimensionless activation energy. Smallness of the remainder is necessary condition of closeness between approximate solution and the solution of the initial problem. The further rigorous proof of such closeness is beyond the scope of this article. In this paper we restrict ourselves by comparison of the theoretical results obtained in the frame of the approximate model with the results of numerical simulations.

Generally, for combustion problems dimensionless activation energy is large quantity $\theta >> 1$. For the infinity large value of dimensionless activation energy, the reaction zone width tends to zero, therefore, the formulation of the approximate problem admits further simplification. Proceeding in the approximation solutions to the limit of infinity thin chemical reaction zone one can obtain approximate piecewise-linear formulation including nonlinear boundary conditions at the flame front. Stationary temperature and reactant mass fraction distributions in the frame of this approximate model can be found analytically and they depends on fuel mass flow rate, flame front position and other parameters. From the boundary conditions at the flame front surface one can obtain the implicit algebraic equation for defining dependency of flame radius on mass flow rate. Gas temperature and mass fraction of the fuel and oxidizer at the flame front are also defined from the algebraic equations.

In contrast to the previous theoretical approaches [1,2], which implied numerical calculation of first order non-linear differential equations, the presented model is reduced to solution of implicit algebraic equations.

3 Results and Discussion

Figure 2 illustrates the typical dimensionless dependencies of flame radius r_f (Fig. 2a), flame temperature T_f (Fig. 2b), gas velocity on flame front V_f (Fig. 2c) and oxidizer mass fraction β (Fig. 2d) on mass flow rate M. Gas flow velocity at the flame front is defined by formula $V_f = M / r_f^2$. These curves have been calculated for the case of non-adiabatic boundary conditions (b) at the porous sphere surface. The marked lines correspond to the dependencies obtained in the frame of the Burke-Shuman model [6]. This model assumes the complete reactant consumption in the reaction zone.

As one can see from Fig. 2, there are two possible flame front positions for the given mass flow rate. Based on physical consideration and results of numerical simulations we suppose that solution with larger value of gas flow velocity (marked by solid line) at the flame front is stable.

In the case of large values of dimensionless mass flow rate M, the solution with larger gas velocity at the flame front coincides with Burke-Shuman solution. The oxidizer and fuel are completely consumed (see Fig 2d) at large M. Stationary solutions exist only if mass flow rate exceeds some critical value M_{cr}. The heat losses from the reaction zone to the burner gradually intensify with decreasing of the flame radius. For M close to M_{cr}, the flame is stabilized at radius which is larger than value followed from Burke-Shuman theory. Such increase of flame radius leads to incomplete consumption of the oxidizer at the flame front due to effects of flows stretch (Fig. 2c). The incomplete consumption of the oxidizer leads, in turn, to the flame temperature decreasing. The competition between decreasing of heat losses and the effects of flame temperature reduction results in the flame stabilization at larger radius than predicted by Burke-Shuman model (Fig. 2a,b). For $M = M_{cr}$ the heat losses reach its critical value and further removal of the flame front from the burner cannot compensate reduction of the temperature due to incomplete oxidizer consumption.

The dimensionless numerical dependencies of flame radius, flame temperature and gas velocity at the flame front on mass flow rate are represented in Fig. 2 a, b,c by open circles. These figures illustrate good agreement between theoretical results obtained under localized reaction zone assumption and the results of numerical simulations. Numerical simulations also indicate that oxidizer consume incompletely in the reaction zone for small values of fuel mass flow rate.

Numerical simulations for the adiabatic boundary condition (a) were also carried out. It was found that in this case numerical data and theoretical results obtained in the frame of proposed model coincide with Burke-Shuman prediction for all values of mass flow rate.

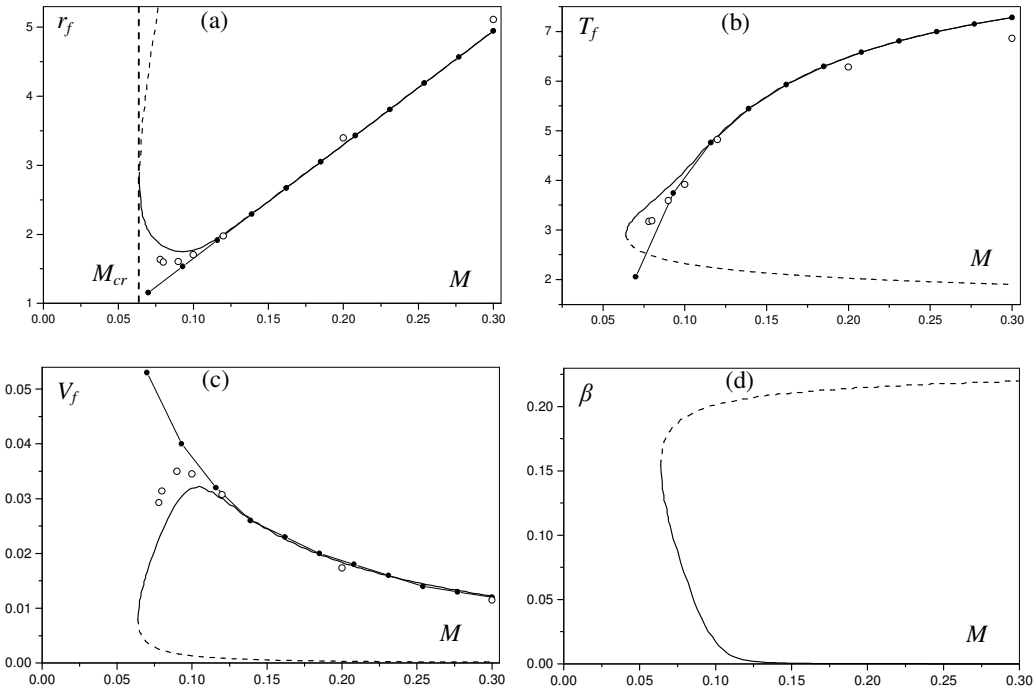

Fig. 2. Typical dimensionless dependencies of flame radius (Fig. 2a), flame temperature (Fig. 2b), gas velocity (Fig. 2c) and oxygen concentration (Fig. 2d) at the flame front on mass flow rate evaluated for the case of non-adiabatic boundary condition (b), $T_0=1$.
Solid and dashed lines correspond to the theoretical results, marked line corresponds to the Burke-Shuman model and the circles correspond to numerical simulations.

4 Conclusions

The model of spherical diffusion microflame presented in this paper is simple enough for analytical analysis and at the same time it is enable to capture the basic features of combustion in non-adiabatic conditions. The proposed model considers effects of incomplete consumption of reactants and their influence on the stationary regimes of combustion. Note, that in the works [1,2], the reactants leakage through the reaction zone was considered as first order correction of the asymptotic expansion method [3]. This approach yields do created difficulties in explanation of flame radius dependency on value of the reactants leakage because the flame radius was determined from the leading order of asymptotic expansion i.e. from the Burke-Shuman model.

Stationary solutions and flammability limits were found in the frame of proposed model. The numerical simulations of spherical micro flames under the assumption of global chemical kinetics were performed too. The theoretical and numerical results are in good agreement with each other. Comparison between previous asymptotic models [1,6] and present model shows that these models give identical results under the conditions close to the adiabatic one. Under the strong non-adiabatic conditions the model developed in the present study predicts the characteristics of the diffusion combustion more precisely than the previous models [1,6].

The theoretical methods and approaches described in this work may be also applied to analytical description of different aspects of diffusion and premixed gas combustion in the cases when incomplete consumption of the reactants may have a vital importance.

4 Acknowledgment

This work was partially supported by the Russian Foundation for Basic Research under Grants RFBR 05-02-16408, 05-08-50278 and Integration project ITPM SB RAS – NCKU, N 2.16.

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