Burning of fuel droplets incorporating solid carbon particles

V.F. Nikitin^{a,b}, V.V. Tyurenkova^{a,b}, N.N. Smirnov^{a,b}

^a Federal Science Center Scientific Research Institute for System Analysis of Russian Academy

of Sciences

36-1, Nakhimovskiy pr., Moscow, Russia, 117218
^b Moscow M.V. Lomonosov State University
GSP-1, Leninskie Gory, Moscow, Russia, 119991

1 Abstract

In the present paper the development of physical and mathematical models, allowing to consider the effect of multiphase fuel (hydrocarbon liquid + solid combustible material) on the conditions of ignition and modes of propagation of combustion in polydisperse nonuniform mixtures. In this case, the combustion of different droplet fractions occurs in different modes: the volatile fraction evaporates and burns in the gasphase mode, and the solid fuel fraction reacts with the oxidizer in the heterogeneous mode. The effect of the presence of a solid fraction in droplets reacting in a heterogeneous regime on the evaporation rate of the volatile fuel component is studied. The effect of tightness due to the presence of other drops on the evaporation rate of each drop is taken into account. The results of computational modeling of flame propagation during ignition of polydisperse mixture of liquid hydrocarbon fuel droplets with solid fine carbon particles are presented.

2 Introduction

Most of liquid fuels are being injected into the combustion chamber in the form of liquid sprays, and then evaporation of liquid fuel brings to formation of the combustible mixture of fuel vapor with gaseous oxidant. Solid carbon or metallic fuels being injected in the form of a powder in the gaseous oxidant atmosphere burn, mostly, in heterogeneous reacting regime. In both combustion mechanisms: gas phase reaction and heterogeneous reaction, - diffusion plays predominant role. The mechanisms of burning and models for combustion of such droplets and/or particles are well developed and are being used successfully in main combustion simulators [1,2]. One of the methods to improve thermal efficiency carbon or metallic powder could be mixed with liquid fuel. This mixture being injected into combustion chamber forms two-phase droplets, containing both liquid phase and solid particles. Experimental measurements of the laminar flame velocity in droplet gas mixtures and its dependence on the medium parameters are presented in [3, 4] Numerical simulation of ignition and combustion of a jet of liquid fuel

Correspondence to: vfnikster@gmail.com

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during injection into the combustion chamber is presented in [5]. Micro models of single droplet combustion have been developed taking into account non-equilibrium surface evaporation and the presence of several independent reactions in the gas phase [6]. The present research is aimed at developing model of two-phase droplets burning.

3 Mathematical model of particle interaction with the surrounding flow

Consider the simulation of the motion of a single particle. It is reduced first of all to the algorithm of transformation of a vector of characteristics of a particle over time, where for each model particle: C is the number of real particles represented by the model particle, m_f - mass of liquid hydrocarbon component of the drop, m_s - mass of solid reagent particles forming the skeleton in the drop, m_t - mass of condensed oxide, r - coordinates of the particle (radius-vector), u - particle velocity, w - stochastic component of the velocity of the surrounding gas particle, ϕ - the volume of the particle, T_s - the temperature of the particle.

The law of motion and heat exchange of particles

For each model particle the law of motion looks like:

$$(m_{fi} + m_{si} + m_{ti})\frac{du_i}{dt} = (m_{fi} + m_{si} + m_{ti})g - \frac{m_{fi} + m_{si} + m_{ti}}{\rho}\Delta p + f_{ri}, \qquad \frac{dr_i}{dt} = u_i$$
(1)

where the forces acting on the particle are: gravity, Archimedes force, resistance force and force taking into account the influence of stochastic gas pulsations (it is modeled together with the resistance force).

The internal thermal energy of the i -th model particle is

$$E_{si} = m_{si}(c_s T_{si}) + m_{fi}(c_f T_{si}) + m_{ti}(c_t T_{si})$$

where c_s , c_f , c_t -specific heat of the solid reagent, condensed hydrocarbon component and nonvolatile oxide residue, respectively. To model the balance of internal energy we will use the following equation:

$$\frac{dE_{si}}{dt} = q_i + Q_{si} + \dot{e}_{ei} - \dot{m}_{si}(c_s T_{wi}) - \dot{m}_{fi}(c_f T_{wi}) + \dot{m}_{ti}(c_t T_{wi})$$
(2)

where T_{wi} is the surface temperature of the particle; q_i - heat flow from gas to particle, modeled by the formula, taking into account the correction for the flow around the particle gas.

Droplet mass transfer model

In this paper, it is assumed that, along with the process of evaporation of the liquid, irreversible heterogeneous chemical oxidation reactions of the solid reagent can take place on the surface of the particle, as a result of which condensed and gaseous oxides can be formed

$$nMe + mO_2 \rightarrow \alpha Me_n O_{2m}^{(s)} + \beta Me_n O_{2m}^{(g)}, \alpha + \beta = 1$$

To calculate the evaporation rate of the condensed volatile component and the combustion rates of the solid reagent due to the action of oxygen on the skeleton, the formulas obtained from the solution of the problem of heterogeneous combustion in the vicinity of a spherical particle are used. The system of equations for the case when all chemical transformations occur on the surface has the form:

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$$\frac{d}{dr}r^{2}\rho v = 0, \qquad \frac{d}{dr}(r^{2}\rho vY_{i}) = \frac{d}{dr}r^{2}\rho D\frac{dY_{i}}{dr}, \qquad \frac{d}{dr}(r^{2}\rho v\hat{c}_{p}T) = \frac{d}{dr}r^{2}\frac{\lambda}{\hat{c}_{p}}\frac{d\hat{c}_{p}T}{dr}$$
(3)

where *r* - radial co-ordinate from the center of the particle, ρ, v, T - density, radial velocity and temperature of surrounding gas, $Y = \rho_i / \rho_r$ mass concentration of the *i* -th component, i=1 stands for O_2 ; $i=2 - CO_2$; i=3- CO; $i=4 - N_2$; $i=5 - H_2O$; $i=6 - H_2$; $i=7 - Me_nO_{2m}$; ... $i=N - C_kH_l$ - hudrocarbon vapors; λ, D - heat conductivity and diffusion coefficients; \hat{c}_p - mean heat capacity of the mixture.

The total mass flow from the particle consists of the mass flow of the evaporated hydrocarbon and gaseous products of the reaction of the solid reagent with oxygen:

$$\dot{m} = \dot{m}_t + \dot{m}_s - \dot{m}_t \tag{4}$$

The boundary conditions on the surface have the following form:

$$(\rho v)_{w}Y_{iw} - (\rho D)_{w}\frac{dY_{i}}{dr}\Big|_{w} = g_{iw} = -\frac{\Phi_{i}}{\Phi_{Me}}k_{1}(T_{w})s_{Me}Y_{1w}, \ (\rho v)_{w}Y_{Nw} - (\rho D)_{w}\frac{dY_{N}}{dr}\Big|_{w} = \frac{m_{N}}{\pi d_{0}^{2}} = (\rho v)_{w}y_{N}$$

$$(\rho v)_{w}Y_{4w} - (\rho D)_{w}\frac{dY_{4}}{dr}\Big|_{w} = 0, \qquad \lambda_{f}\frac{dT}{dr}\Big|_{f} + (\rho v)_{w}y_{N}h_{L} = \lambda\frac{dT}{dr}\Big|_{w} - g_{Me}Q_{pw}(T_{w})$$
(5)

The boundary conditions in the outer domain $(r \rightarrow \infty)$ for the homobaric problem (p=const) are as follows: $Y_{Ne}=0$, $Y_1=Y_{1e}$, $Y_2=Y_{2e}$, $T=T_e$, $Y_i=Y_{ie}$. We assume that reactions in the gas do not exist in the neighborhood of the particles and all the chemical transformations take place only on the surface of the particle in the pure heterogeneous regime, that is, pairs of fuel can not be outside the surface, having not entered into reaction with the oxidizer on the surface: $Y_{Me}\equiv 0$ for $r=r_0$ taking into account the input of a new variable and assuming surface temperature to be equal to the equilibrium evaporation temperature allow to obtain the following relations :

$$\xi_{0} = \frac{\lambda}{\rho D c} \frac{N u_{i}}{2} \frac{T_{e} - T_{w}}{T_{w} - T_{si} + \frac{h_{L}}{c}} + \frac{k_{1}(T_{w}) s_{Me} r_{0}}{\rho D} \cdot \left(\frac{Q_{\rho w}}{c(T_{w} - T_{si}) + h_{L}} - \alpha \phi_{1} - \beta \phi_{7} \right) Y_{1w}, \qquad Y_{1w} = \frac{Y_{1e} e^{-\xi_{0}}}{1 + s_{Me} \alpha \phi_{1}^{2} V e \frac{1 - e^{-\xi_{0}}}{\xi_{0}}}, Ve = \frac{k_{1}(T_{w}) r_{0}}{\rho D}$$

In the process of droplet heating its temperature increases $(T_w-T_{si})\rightarrow 0$, and the rate of mass transfer also increases.

4 Solution of the model problem of droplet evaporation.

To solve the model problem of evaporation of a single drop, we consider the case when there is $(T_w-T_s)\rightarrow o$, $\alpha=0$, (a mixed mode of chemical reaction). To calculate the change in droplet volume, we obtain the formula for the evolution of radius

$$\frac{dr_0}{dt} = \frac{\dot{m}}{4\pi r_0^2 \rho_i} = \frac{\rho D \xi_{fs0}}{r_0 \rho_i}$$
(6)

Introducing new notations $z = \frac{r_0}{r_*}$, $\tau = \frac{t}{t_*}$, $t_* = \frac{\rho_i r_*^2}{\rho D \xi_*}$ and, assuming the Lewis number close to one, and Reynolds number small, convert to the following form:

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$$z\frac{dz}{d\tau} = 1 + s_{Me} Ve\left(\frac{Q_{pw}}{c(T_e - T_w)} + \frac{h_L}{c(T_e - T_w)}\right) Y_{1e}, \tau = 0, z = 1$$
(7)

Note that the formula (7) is valid only in the presence of a liquid fraction. After evaporation of the liquid fraction completely, the temperature of the surface of the particles begins to increase along with the speed of a heterogeneous reaction. Further reducing the radius is calculated by the known models of heterogeneous combustion.

In Fig. 1 the results of calculation of the combined droplet radius decrease with time depending on the initial content of condensed fuel in it are presented. For simplicity, we consider the case when the specific heat flux to the particle, the specific energy release in a heterogeneous reaction and the specific heat of evaporation of the liquid from the surface are of the same order of magnitude. In the case when there is no condensed fuel in the drop ($S_{Me}=0$), the solution has the form: $z = \sqrt{1-\tau}$, $0 \le \tau \le 1$. In the presence of condensed fuel, the evaporation of the liquid is faster due to additional energy release. When only the solid residue remains, the rate of mass consumption decreases abruptly, but then increases rapidly due to an increase in the temperature of the condensed residue.



Figure 1. Changing the radius of the combined droplet with time depending on the initial content of condensed fuel in it : $1 - s_{Me}^0 = 0.$; $2 - s_{Me}^0 = 0.04$; $3 - s_{Me}^0 = 0.5$.

5 Combustion of a polydisperse mixture of hydrocarbon droplets with small particles of solid carbon

Ignition of a mixture of dispersed hydrocarbon fuel with fine dispersed solid carbon was calculated in a closed cylindrical volume of 1.25 m3. A model of ignition is used in which energy without a shock mechanism is introduced during exposure to a small volume of medium [4]. The boundaries of the flame front were determined along the five Central rays (horizontally, vertically and at an angle of 45 degrees to the horizon) as the position of the maximum rate of oxidation of volatile components. The boundaries of the flame zone were also determined where the reaction rate was 1/10 of the intensity maximum.

Below (Fig. 2) the illustration of the evolution of fields of temperature in the problem of combustion of a dispersed hydrocarbon-carbon fuel in the air. The figures show the temperature of the gas, the temperature image is superimposed on the velocity field in the form of segments. In Figs. 3 the following integral combustion parameters are shown depending on the time: the mass of the condensed (liquid+solid) dispersed phase $M_p(t)$, the average pressure P(t) in the chamber and the position of the flame front $R_f(t)$. Graphs P(t) and $M_p(t)$ strongly correlate: the pressure in the chamber increases primarily with a decrease in the mass of the condensed phase, which passes into the gas. The maximum pressure rise occurs after the passage of the flame front, at times 70-80 MS.. After t = 80 MS, the pressure increase stops very sharply, and the mass of the condensed phase approaches a value corresponding to the mass of the non-volatile non-combustible component. From the graphs of the flame fronts propagation (Fig. 3c) one can see the following. The blue and red lines (almost identical) correspond to the flame front position according to the

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maximum oxidizer gradient and temperature. The difference between these lines is noticeable only at the ignition stage due to the energy source.



Figure 2. Evolution of temperature fields in the combustion problem of dispersed hydrocarbon fuel with solid carbon inclusions in the air (time specified in seconds).



Figure 3. a) Dependence of the total mass of condensed droplets and particles on time. b) The trajectory of the flame front. Black solid lines correspond to the position 1/10 of the reaction intensity maximum thus bounding the flame zone from both sides. The blue and red lines correspond to the flame front position according to the maximum oxidizer and temperature gradients. c) Dependence of mean pressure in the chamber on time.

By the time t = 65 MS front front comes to the wall of the camera. Up to the time t < 57 MS, the front width remains approximately constant. After that, there is a kind of reverse movement to the center of the chamber, and after t = 65 MS its position is unstable, since the approach of the flame to the walls of the chamber, the flame width increases rapidly, the total intensity also increases, but the peak of this intensity decreases. As a result, the position 1/10 of the intensity maximum is shifted back. It is also seen that at first the flame propagates at a speed of 9.6 m/ s, then as it approaches the walls, its speed decreases to 5.8 m / s. The average flame propagation velocity at the selected parameters is 7.9 m/s. Visual instability of the boundaries is due to the presence of large vertexes, which were obtained in numerical simulations due

to discrete particles method describing condensed phase. This numerical effect, nevertheless, qualitatively corresponds to physical instability due to large eddies.

6. Conclusions

When creating physical and mathematical models of the combustion of the agglomerates of the droplets, the study of the effect of multi-phase fuel (hydrocarbon liquid + solid combustible material) on the conditions of ignition and modes of propagation of the combustion of a polydisperse non-uniform mixtures. Introduced dimensionless parameters have important physical meaning: $-\xi_0$ the ratio of speeds mass transfer through the surface of the droplet and the average speed of diffusion from the surface into the gas; V_e the ratio of the speed of heterogeneous reactions on the surface unit to the speed of gas diffusion to the surface. In the presence of condensed fuel in the droplet, the evaporation of the liquid is faster due to the additional energy release because of a heterogeneous reaction on the surface. When only the solid residue remains, the rate of mass consumption decreases abruptly, but then increases rapidly due to an increase in the temperature of the condensed residue due to energy release in heterogeneous reaction.

When the flame propagates in a polydisperse mixture, the thickness of the front reaches a dozen centimeters and at first when propagating from the center of the chamber, where ignition occurs, it remains constant. Then, as the flame approaches the walls of the chamber, the thickness of the front increases, the size of the zone is unstable and varies depending on the direction, the total intensity of the reaction increases, while the maximum intensity decreases.

References

[1] D.L. Dietrich, V. Nayagam, M.C. Hicks, P.V. Ferkul, F.L. Dryer, T.I. Farouk, B.D. Shaw, H.K. Suh, M.Y. Choi, Y.C. Liu, C.T. Avedisian, F.A. Williams, Droplet combustion experiments aboard the International Space Station, Microgravity Sci. Technol. 26 (2) (2014) 65–76.

[2] W.A Sirignano, Fuel droplet vaporization and spray combustion, Prog. Energy Comb. Sci. 9 (1983) 291-322.

[3] H. Burgoyne, L. Cohen, The effect of drop size on flame propagation in liquid aerosol, Proc. Roy. Soc. A225 (1954) 357-392

[4] K. Kikucyi, Y. Otomo, L. Sitzki, K. Maruta, H. Kobayshi, T. Nioka, T. Sakuraya, Flame propagation characteristics of n-decane spray in microgravity, Drop tower days 1998 in Hokkaido. International workshop on short-term experiments under strongly reduced gravity conditions . October 11-14, 1998, 82-84.

[5] V.B. Betelin, V.F. Nikitin, V.R. Dushin, A.G. Kushnirenko, V.A. Nerchenko, Evaporation and ignition of droplets in combustion chambers modeling and simulation, Acta Astronaut. 70 (2012) 23–35.

[6] V.M. Guendugov, N.N. Smirnov, V.V. Tyurenkova, Solving the problem of diffusion combustion of a droplet with allowance for several independent reactions, Combust. Explos. Shock Waves 49 (6) (2013) 648–656.