Numerical simulations of ignition in turbulent flow

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1 Introduction

Premixed turbulent combustion has been intensively studied due to its fundamental and practical importance. For example, lean premixed turbulent combustion has great potential for increased fuel economy and reduced NOx emissions in spark–ignition engines [1,2] and gas turbines [3]. Minimum ignition energy is an important property for safety standards as well as for the fundamental understanding of the ignition process of combustible mixtures. Furthermore, the deep understanding of ignition processes is crucial for optimization of ignition systems especially when ignition of lean premixed mixtures under turbulent combustion is considered. Despite a number of investigations of ignition process in turbulent flow this important and extensively studied subject still has many unresolved fundamental issues.

Previous experimental investigations [4,5] show that minimum ignition energy increases gradually with turbulent intensity. Then for the turbulent intensity exceeds some critical value the abrupt increase of minimum ignition energy was observed. This transition was associated with different combustion modes. This paper is an attempt to gain inside the physical processes underlying such transition. The main difficulty in modeling turbulent combustion, as in many other turbulence-related problems, is the wide range of spatiotemporal scales involved. Moreover it may be difficult to distinguish the most important physical processes responsible for the flame behavior on the basis of detailed numerical simulations due to coupling influence of many factors such as turbulence, chemical kinetics, hydrodynamics effect and other. As it was demonstrated in paper [6,7] the basic characteristics of flame extinction in multiple-scale flow field may well be described within the framework of reduced thermal-diffusion model coupled with prescribed flow field roughly described the main features of turbulent flow.

In present paper the results of 2D numerical simulations of ignition in time-independent, space-periodic array of large-scale vorticities are presented. The flame initiation in the flow field obtained by numerical simulations of the two-dimensional Euler equation for decaying turbulence was studied too in order to investigate the effect of developed turbulence on ignition process.

2 Mathematical model

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A conventional one-step, constant-density, nonadiabatic, reaction– diffusion–advection model for time-independent periodic vortical flowfield is adopted. In appropriately chosen units the corresponding set of equations for the temperature and the deficient reactant concentration reads,

$$\frac{\partial T}{\partial t} + \vec{V} \cdot \nabla T = \Delta T + (1-\sigma) W(C,T) \tag{1}$$

$$\frac{\partial C}{\partial t} + \vec{V} \cdot \nabla C = Le^{-1} \Delta C - W(C,T) \tag{2}$$

$$W(C,T) = 0.5(1-\sigma)^2 Le^{-1} N^2 C \exp\left(N\left(1 - 1/T\right)\right)$$

$$\vec{V} = \left(A \sin(kx)\cos(ky), -A\cos(kx)\sin(ky)\right)$$

Here T is the scaled temperature in units of T_b, the adiabatic temperature of combustion products; C is the scaled concentration of the deficient reactant in units of C_0, its value in the fresh mixture; x, y is non-dimensional spatial coordinates in units $l_{th}=D_{th}/U_b$, the thermal width of flame, where D_{th} is the thermal diffusivity of the mixture and U_b is the velocity of a planar adiabatic flame in the high activation energy limit; t is the scaled time in units D_{th}/U_b^2; $\sigma = T_0/T_b$ where T_0 is the fresh mixture temperature; $Le=D_{th}/D_{mol}$ is the Lewis number, where D_{mol} is the deficient reactant molecular diffusivity; V is the prescribed flow-field and A is its intensity in units of U_b; k is the periodic flow wave-number in units of l_{th}; $N=T_a/T_b$ is the scaled activation energy, T_a being the activation temperature. It is necessary to notice that the mathematical model was significantly simplified in order to extract the main physical processes governing ignition in the turbulent flow. In particular the radiative heat losses is not taken into account in (1). It may be supposed that radiative heat losses will not affect the qualitative results and will only lead to decreasing of the minimum ignition energy.

Equations (1) and (2) are considered in the domain $0 \leq x \leq 4\pi/k$, $0 \leq y \leq 4\pi/k$ and subjected to the insulating boundary conditions,

$$\partial T/\partial x = \partial C/\partial x = 0 \text{ at } x=0,\ 4\pi/k \tag{3}$$

$$\partial T/\partial y = \partial C/\partial y = 0 \text{ at } y=0,\ 4\pi/k \tag{4}$$

The problem (1)-(4) was solved for N=10, σ=0.2, Le=0.9 that roughly correspond to the methane-air mixture with equivalence ratio equal to 0.5.

The system of equations (1)-(2) with boundary conditions (3)-(4) was solved numerically by explicit finite-difference scheme of the second-order accuracy with respect to the spatial variables and first-order accuracy with respect to time.

For determination of ignition energy the following initial conditions were applied,

$$C=0,\ T=T_{ini},\ \text{for } 2\pi/k-\delta/2 \leq x \leq 2\pi/k+\delta/2,\ 2\pi/k \leq y \leq 2\pi/k+\delta$$

$$C=1,\ T=\sigma,\ \text{otherwise}$$

To simulate the spark ignition the parameter δ was fixed and chosen small enough namely equal to 3.0. The spark duration is not taken into account. Investigations of the spark duration effect on minimum ignition energy is the subject of further research. The numerical simulations start with respectively low initial temperature T_{ini} knowingly less than ignition temperature. After the flame extinguish the initial temperature increased by constant increment and the calculations with new initial conditions are performed. This procedure repeats until the flame ignition occurs at some initial temperature T_{ini}. This temperature is referred ignition temperature.

Three sets of the orthogonal grids provides 5, 10 and 15 grid points per thermal thickness were employed. Convergence tests showed that the results of calculations for the two last-named finer grids are qualitatively the same and quantity difference in ignition temperature T_{ini} is less than 1%.

3 Results and discussion

Dependencies of ignition temperature T_{ini} on flow-intensity A calculated for different wave numbers k are shown in Fig.1. Since the size of initial high-temperature domain is constant the ignition temperature is proportional to the ignition energy. For the prescribed flow field applied in present simulations parameter A is proportional to the non-dimensional turbulent intensity. As it is seen from Fig.1 the ignition temperature grows almost linearly with A for moderate wave-numbers (see curves k=0.2, k=0.4 in Fig.1). For large wave numbers which correspond to the respectively small eddies size the growth rate of $T_{ini}(A)$ dependencies slows down with increase of flow intensity (see curves k=0.6, k=1.0 in Fig.1). In the case of ignition in the large-scale eddies flow the ignition temperature is almost constant until the turbulent intensity A exceeds some critical value, then the abrupt linear increase of ignition energy is observed. This behavior resemble experimental results presented in [4,5].

The ignition occurs only if the maximal temperature exceeds some critical value during characteristic ignition time t_{ign}. The maximal temperature decrease in time is due to two factors: thermal conductivity and convective diffusion which consists in capturing of the portions of hot gas by neighboring eddies accompanied by spreading high temperature zone in space. Increasing of flow-intensity leads to the intensification of convective diffusion and therefore to the increasing of the ignition temperature up to the level provides by the criterion $T(t_{ign})>T_c$.

At small A the distortion of initial hot spots by flow is low and the ignition energy mainly determines by thermal conductivity and almost equals to the ignition energy in the quiescent gas (see curves k=0.025, k=0.05 in Fig.1). The increase of flow intensity A for large-scale eddy flow (k=0.025, k=0.05) leads to the abrupt increase of ignition temperature. Such a drastic change in the ignition temperature may be related with peculiarities of cooling of the warm jets have formed by vortical flow. At small flow intensity the cooling is mainly caused by the diffusion heat dissipation. Increasing of the flow intensity entails the flow convergence leading to the narrowing of the jet and to the intensification of

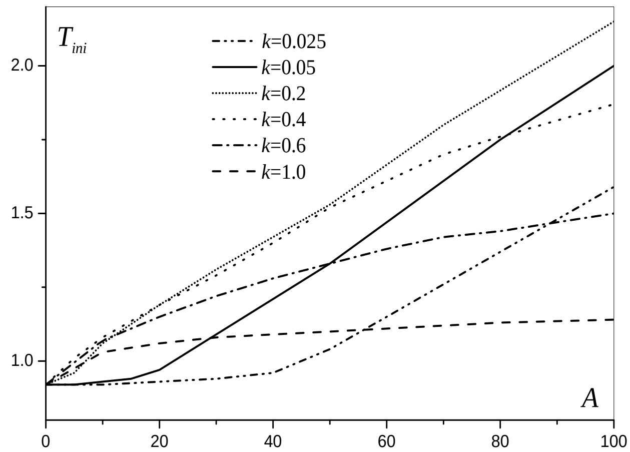

Figure 1. Dependencies of ignition temperature on flow-intensity calculated for different wave numbers

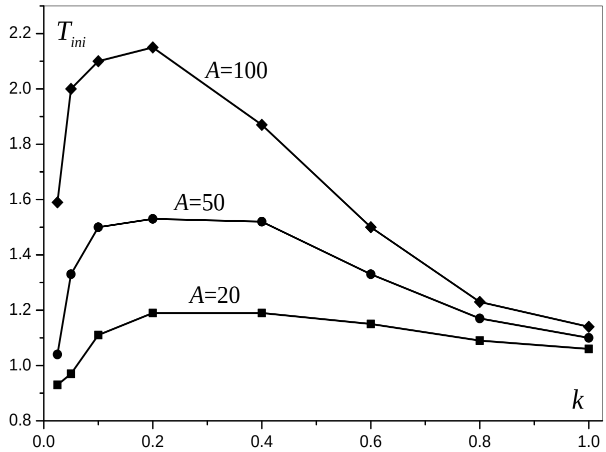

Figure 2. Dependencies of ignition temperature on wave number calculated for different flow-intensities

the jet cooling. Therefore enlarged ignition temperature of initial hot spot is necessary for the flame initiation. Notice that the same mechanism of combustion regimes change related with flow convergence was observed in the case of flame propagating in the large-scale spatially-periodic vortical flow [7]. On the contrary with large-eddies case, the heat diffusivity from small-scale warm jets to the unburned mixture is dominate over the flow convergence effect for small-size eddies flow with characteristic eddies sizes close to the flame heat width. In this case the effect of flow intensification is manifested as simple increase of total heat diffusion from initial hot spot to the unburned mixture at the expense of convective diffusion component. As result, the ignition temperature dependencies on the flow intensity are monotone increasing functions. (see curves k=0.6, k=1.0 in Fig.1).

Figure 2. shows dependencies of ignition temperature T_{ini} on wave number k calculated for different flow-intensities *A*. In the case of fixed value of flow-intensity A there is a critical wave number corresponding to the maximal ignition temperature. This critical wave number is almost independent on flow-intensity and corresponds to the eddy size about 15-30 thermal thicknesses. Numerical simulations show that this non-dimensional critical wave number remains almost constant for mixtures with equivalence ratios 0.5-0.9. It was found that decreasing of the size of initial high-temperature domain δ leads to the significant increase of minimal ignition temperature, at the same time qualitative behavior of the $T_{ini}(A)$ and $T_{ini}(k)$ curves remain the same as well as critical wave number.
In order to investigate the effect of developed turbulence on ignition process the model (1)-(4) with prescribed flow field obtained by numerical simulations of the two-dimensional Euler equation for

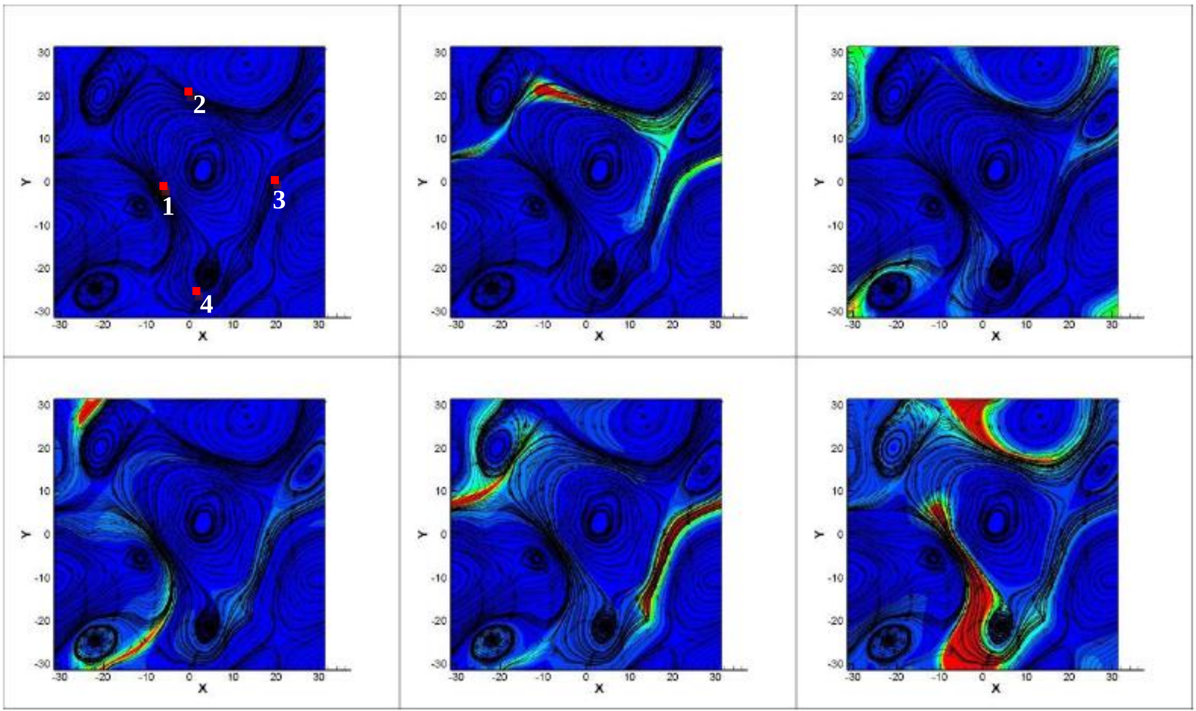

Figure 3. Consecutive configurations of the temperature-field.

decaying turbulence [8] were examined. The periodic boundary conditions were assumed. The flow streamlines are presented in Fig.3. The turbulent intensity in numerical simulations was varied by scaling the velocity vector of the obtained flow field. The ignition temperature was calculated for different igniting hotspot locations as depicted in Fig.3a. The dependencies of ignition temperature on velocity scaling factor which is proportional to the nondimensional turbulence intensity are presented in Fig.4. The different curve numbers correspond to different locations of ignition point. It may be seen that ignition temperature strongly depends on location of igniting hotspot. This difference may be explained by different convective diffusion along the igniting hotspot propagation path. The behavior of curves 2-4 resemble the dependencies obtained in the case of space-periodic array of large-scale vortexes (see Fig.1). For some ignition points (see curve 1 in Fig.4) the ignition temperature gradually increase with turbulent intensity. Then for the turbulent intensity exceeds some critical value the abrupt increase of ignition temperature is observed. This behavior qualitatively coincides with experimental results [4,5]. Figure 3 demonstrate consecutive configurations of the temperature-field calculated for the case when the ignition hot spot is located at point 1 and for A=75.0, T_{ini}=1.45. It may be seen that for the large turbulent intensity the distributed combustion regime is observed. This result also coincides with experiments [4,5].

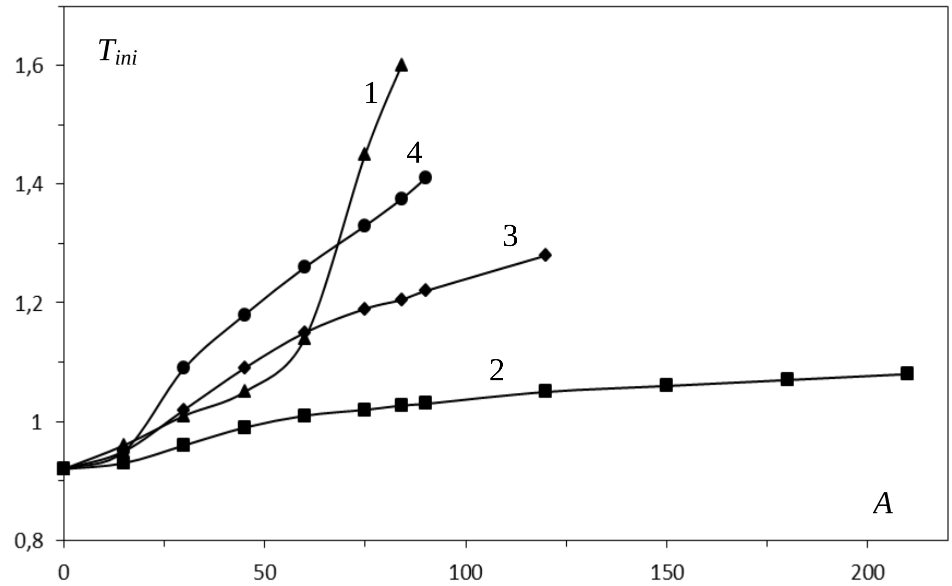

Figure 4. Dependencies of ignition temperature on velocity scaling factor calculated for different igniting hotspot arrangements

4 Conclusions

The ignition process in prescribed flow field modeling turbulent flow was investigated in the frame of 2D thermal-diffusion model. The dependencies of ignition temperature on turbulence intensity and eddies size in the flow field consists of time-independent, space-periodic array of large-scale vorticities were obtained. Analysis of time-dependency of maximal gas temperature allows us to give qualitative explanation of ignition temperature behavior under variation of different parameters. It was found that in the case of fixed value of flow-intensity there is a critical eddies size corresponding to the maximal ignition temperature. This critical wave number is almost independent on flow-intensity and corresponds to the eddy size about 15-30 thermal thicknesses for mixtures with equivalence ratios 0.5-0.9. The numerical results shows that in large-scale eddies flow the ignition temperature is almost constant until the turbulent intensity exceeds some critical value, then the abrupt linear increase of ignition energy is observed. Such behavior resembles previous experimental observations [4,5]. The ignition process in the flow field pre-calculated in the frame of the two-dimensional Euler equation for decaying turbulence was also studied. It was found that behavior of the ignition temperature/turbulent intensity curves strongly depends on the location of the igniting hotspot. At some initial conditions these curves resemble the dependencies previously obtained within the model with spatially-periodic vertical flow. It may be concluded that the reduced thermal-diffusion model combined with prescribed flow field is reasonable for qualitative investigations of the ignition in the turbulent flow. At the same time the further investigations directed toward the adequate description of the turbulent flow field during the spark ignition is necessary.

5 Acknowledgments

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