

# Numerical Simulation of Ignition in ABC – Flow Modeling 3D Turbulence using a GPU – based approach

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## 1 Introduction

Flame initiation in turbulent flow is one of the most important problems in combustion theory. It plays an important role in the performance of various energy conversion devices with gas combustion. Investigation of ignition processes have not only fundamental importance but also essential for a better control of fuel efficiency, exhaust emission, and idle stability of the engine operation. For example, lean premixed turbulent combustion has great potential for increased fuel economy and reduced NO<sub>x</sub> emissions in spark – ignition engines [1,2] and gas turbines [3]. Most practical combustion devices require combustion events to be initiated at a predetermined location and time. 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 conditions 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.

The main difficulty in turbulent combustion modeling, 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 ignition on the basis of detailed numerical simulations due to coupling influence of turbulence, chemical kinetics, transport processes and other. As it was demonstrated in paper [4,5] the basic characteristics of flame extinction and ignition in turbulent flows may be well described within the framework of reduced thermal – diffusion model coupled with prescribed flow field roughly describing the main features of turbulent flow.

In our previous studies [6] in the frame of thermal – diffusion model, we investigated the ignition process in two prescribed 2D flow fields: Taylor Green vortex flow and the flow field, which is pre – calculated in the frame of the two – dimensional Euler equation for freely decaying turbulence. However, turbulence is essentially 3D phenomenon, and 2D turbulence is not the simplified model of 3D turbulence. In the present paper, the results of 3D numerical simulations of ignition in time – independent ABC – flow modeling turbulence are presented. The influence of velocity amplitude, vortex size and Lewis number on minimum ignition energy are investigated. The main goal of this work is gain inside the physical processes governing the ignition in turbulent flow. Reduced

mathematical model allows us to decouple thermal – diffusive and hydrodynamic processes for better understanding of flame dynamics after its initiation by hot spot.

## 2 Mathematical model

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

$$\partial T / \partial t + \vec{V} \cdot \nabla T = \Delta T + (1 - \sigma)W(Y, T) \quad (1)$$

$$\partial Y / \partial t + \vec{V} \cdot \nabla Y = Le^{-1} \Delta Y - W(Y, T) \quad (2)$$

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

$$V_x = U(A \sin(kz) + C \cos(ky))$$

$$V_y = U(B \sin(kx) + A \cos(kz))$$

$$V_z = U(C \sin(ky) + B \cos(kx))$$

Here  $T$  is the scaled temperature in units of  $T_b$ , the adiabatic temperature of combustion products;  $Y$  is the scaled concentration of the deficient reactant in units of  $Y_0$ , the value in the fresh mixture;  $x, y, z$  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;  $\sigma = T_0/T_b$  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;  $N = T_a/T_b$  is the scaled activation energy,  $T_a$  being the activation temperature;  $V = (V_x, V_y, V_z)$  is the dimensionless prescribed velocity vector that is exact solution of the Euler equations,  $U$  is its intensity in units of  $U_b$  and  $A, B, C$  is constants;  $k$  is the periodic flow wave – numbers in units of  $1/l_{th}$ .

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 loss is not taken into account in equation (1). It may be supposed that radiative heat loss will not affect the qualitative results and will only lead to decreasing of the ignition energy.

Equations (1) and (2) are considered in the cube:  $-20\pi \leq x \leq 20\pi, -20\pi \leq y \leq 20\pi, -20\pi \leq z \leq 20\pi$  and subjected to the periodic boundary conditions along all coordinates.

The problem (1) – (2) was solved numerically for  $N = 8.65, \sigma = 0.17, A = B = C = 1$  that roughly correspond to the lean methane – air mixture.

The system of equations (1) – (2) with boundary conditions 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. Implementation of the difference scheme has been performed on the graphics accelerator NVIDIA TESLA M2090 on the grid  $1024 \times 1024 \times 1024$  using parallel computing platform and programming model CUDA. Investigation of the convergence of the algorithm is performed by comparing the simulation results on the sequence of the grid refinement.

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

$$T = E / (\sqrt{4\pi t})^3 \cdot e^{-\frac{r^2}{4t}} + \sigma \quad Y = 1 - e^{-\frac{r^2}{4t}}$$

which correspond to the temperature distribution from point source after time  $t$ . Parameter  $t$  characterizes the size of igniting hot spot and should be small enough ( $\sim 3$ ) to simulate spark ignition,  $E$  – dimensionless energy of point source. The numerical simulations start with respectively low initial energy  $E_{ini}$  knowingly less than minimum ignition energy  $E_{ign}$ . After the flame extinguish the initial energy increased by constant increment and the calculations with new initial conditions are performed. This procedure repeats until the flame ignition occurs at some initial energy. This energy is referred minimum ignition energy in the center  $E_{ign}$ .

### 3 Results and discussion

Fig. 1 demonstrates the typical evolution of the temperature isosurface  $T = 0.9$  colored according to the absolute value of the gas velocity, which shows the successful ignition with the following parameters:  $U = 2.0$ ,  $Le = 1.0$ ,  $k = 0.1$  and  $E_{ign} = 176$ . The initial hot spot is stretched along the streamlines and the gas temperature is increased, that finally leads to the ignition of the mixture in the entire domain. In the case of smaller ignition energy, the spread of the initial hot spot is almost the same, but the temperature cannot increase to the required level and after a short period of temperature magnification it begins to fall and ignition does not occur.

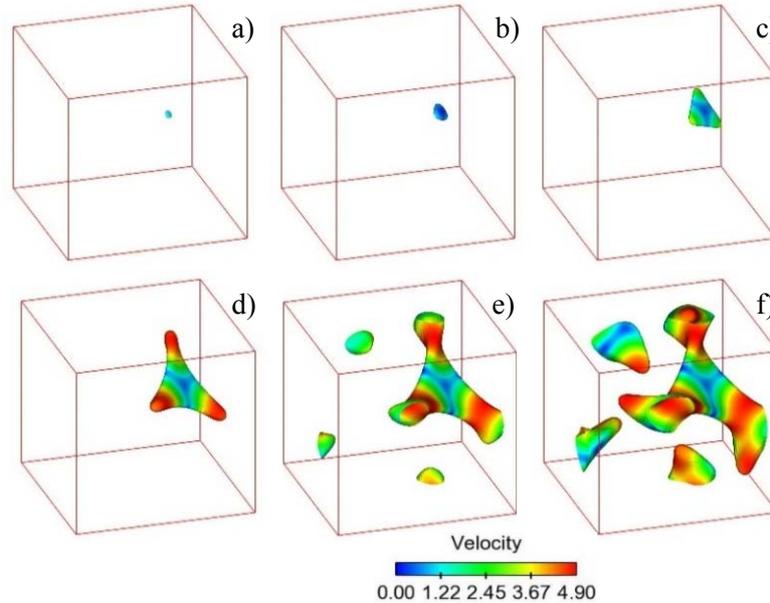


Figure 1. Temporal evolution of the temperature isosurface  $T = 0.9$  at  $U = 2.0$ ,  $Le = 1.0$ ,  $k = 0.1$  and  $Q_{ign} = 176$

Dependencies of the ignition energy for ignition in the center on wave number calculated for different flow intensities and Lewis numbers are shown in Fig. 2. For the prescribed flow field applied parameter  $U$  is proportional to the non – dimensional turbulent intensity. It was found that for the fixed value of flow intensity there is a critical wave number corresponding to the maximal ignition energy. In contrast with our previous result that predicted existence of constant critical wave number in 2D flow [6], in 3D flow the critical wave number depends on flow intensity and Lewis number. As it is seen from Fig. 2 the dependence of ignition energy near the critical wave number become stronger with increase the flow intensity and in the figure, it looks like the formation of a sharp peak. At large  $k$  the dependency of ignition energy on flow intensity is weak because in this case the vortices size is comparable with the diameter of initial hot spot. For small values of  $k$ , corresponding to large vortices, the variation of the ignition energy with increase of flow intensity is also slight. This is due to sufficiently smaller size of the igniting hot spot compared with the vortex size. Therefore, the flow velocity is almost constant in the hot spot region and does not change much in the course of the ignition. Thus, the process in both cases is mainly determined by the thermal conductivity. For moderate values of  $k$ , the significant variation of the velocity field around the hot spot plays an important role in ignition. Non uniformity of the flow field leads to the stretching of the initial hot spot (see. Fig. 1d.) and the higher energy is necessary for ignition.

Fig. 3 shows dependencies of ignition energy on flow intensity calculated for different wave numbers and Lewis numbers. The numerical results shows that in large – scale eddies flow (see Fig. 3  $k = 0.1$  for all Lewis numbers), the minimum ignition energy 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 [7,8] and our numerical results obtained earlier for the

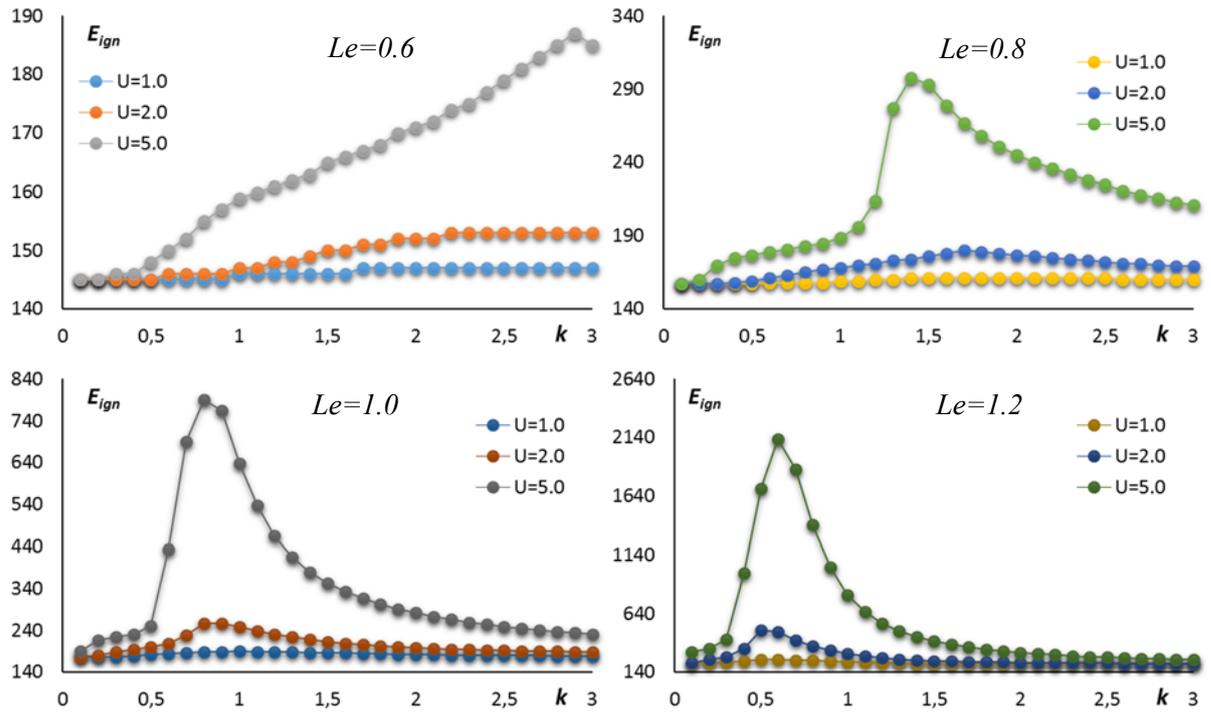


Figure 2. Dependencies of ignition energy  $E_{ign}$  on wave number  $k$  calculated for different flow intensities  $U$  and Lewis numbers  $Le$

2D case[6]. For large wave numbers correspond to the respectively small eddies size the growth rate of  $E_{ign}(U)$  dependencies slows down with increase of flow intensity (see curves  $k=0.5$   $Le=0.6$  and  $0.8$  in Fig. 3). For moderate wave numbers, the ignition energy slowly grows with  $U$ . There are two factors that effected on these dependencies: thermal conductivity and convective diffusion which consists in

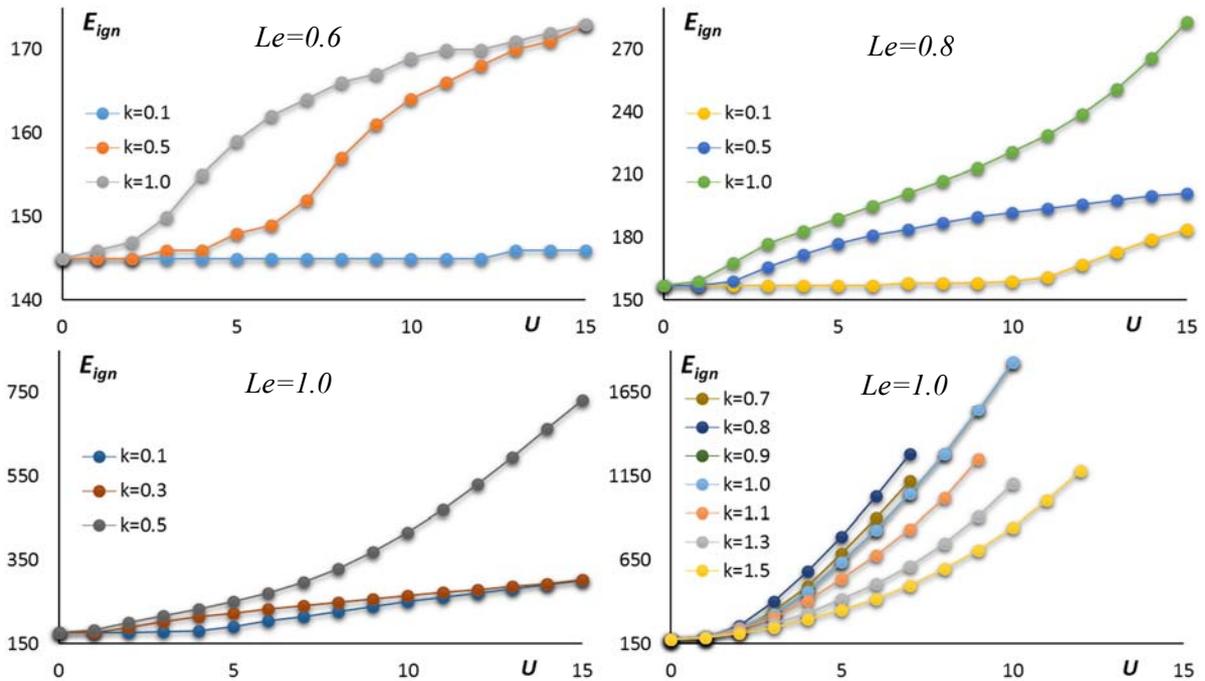


Figure 3. Dependencies of ignition energy  $E_{ign}$  on flow intensity  $U$  calculated for different wave numbers  $k$  and Lewis numbers  $Le$ .

capturing of the portions of hot gas by neighboring eddies accompanied by spreading high temperature zone in space. At small flow intensity the cooling is mainly caused by the diffusion heat dissipation. Increasing of flow intensity leads to the intensification of convective diffusion and therefore to the increasing of the ignition energy.

Besides the dependencies of the ignition energy on flow intensity and wave number the dependencies of the ignition energy on Lewis number were obtained numerically. Fig. 4 shows the dependencies of ignition energy on Lewis number, calculated for  $k = 0.5$  and different values of flow intensity. As seen from Fig. 4, the ignition energy is changing very slowly in the range of Lewis numbers from 0.3 to 1.1, and rapidly increases for Lewis numbers large of 1.2. Such behavior resembles previous results obtained in [9,10] for the spherical flame initiation in the quiescent mixtures with high Lewis numbers. As it was shown in [9,10] the critical value of Lewis number corresponding to the abrupt increase of ignition energy is determined by formula  $N(Le^* - 1) = 1$ . For parameters adopted in the present study, this value is equal to 1.12.

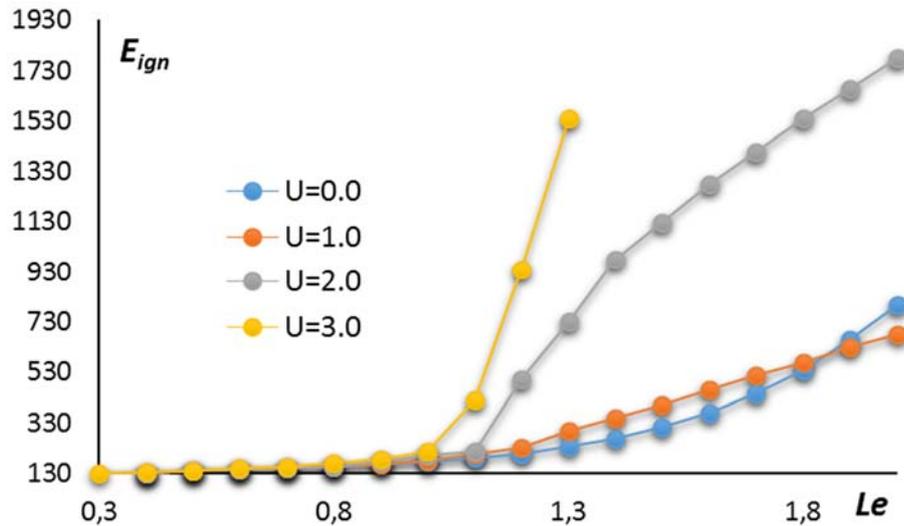


Figure 4. Dependencies of ignition energy  $E_{ign}$  on Lewis numbers  $Le$  calculated for different flow intensity  $U$  and wave numbers  $k = 0.5$ .

Numerical simulations show that these types of dependencies remains almost the same for mixtures with equivalence ratios 0.6 – 0.9

## 4 Conclusions

The influence of premixed gases properties on ignition energy in the ABC – Flow modeling 3D turbulent flow in the frame of thermal – diffusion model was investigated numerically using GPU computing processor. The effect of Lewis number, vortexes size and flow intensity on ignition energy have been studied. Analysis of time – dependency of maximal gas temperature allows us to give qualitative explanation of minimum ignition energy behavior under variation of different parameters. It was found that in large – scale vortexes flow, the ignition energy is almost constant until the turbulent intensity exceeds some critical value, then the rapidly increase of ignition energy is observed. Such behavior resembles previous experimental observations [7,8] and our numerical results obtained earlier for the 2D case[6]. The numerical results shows that in the case of fixed value of flow intensity, there is a critical vortexes size corresponding to the maximal ignition energy. Unlike the two – dimensional case [6], this critical wave number depends on flow intensity and the Lewis number. 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.

## 5 Acknowledgments

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