

“Particle” Approach for Flame Front Propagation Fast Modeling in the Given Premixed Gas Flow Field

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Abstract

The objectives of the present study are the formulation of the models of flame front evolution capturing the effects of flame propagation in the prescribed non-stationary premixed gas flow field. The algorithm of real time simulations of flame evolution within frame of “flamelet” approach is offered to model shape of flame front propagating in the given non stationary gas flow fields. The algorithm is based on “particles” method and representation of the burned and unburned gases by a two sets of different particles, moving on the fixed trajectories, corresponding to the given flow field.

Keywords: flame modeling, numerical simulation.

1. INTRODUCTION

Nowadays the development of effective algorithms of simulations of the premixed flame evolution in the practical devices having complex geometry and nonstationary gas flows is issue of the day. As numerical modeling of gas combustion with detailed chemical kinetics and real gas flows demands huge computing expenses there is a necessity to apply more simple, but not losing the physical meaning, the simplified models of flame evolution. In a case when characteristic scale of internal structure of a combustion wave much less than characteristic size of gas flow perturbations it is reasonable to use the simplified representation of a flame as an interface between unburned and burned gasses. This model assumes that flame surface moves along its normal with given velocity called a burning velocity. The value of burning velocity may be estimated by preliminary simulation of 1D combustion wave taking into account detailed kinetics of chemical reactions. In this approximation the gas flow is determined by equations free of effects introducing by combustion. This approximation is known as “flamelet” model [1] and it is widely used in engineering simulations. In the simplest case one can assumes that the burning velocity is constant and it is determined by mixture content only. In the present work the algorithm of real time simulations of flame evolution within frame of “flamelet” approach is offered to model shape of flame front propagating in the given non stationary gas flow fields appearing in the combustion chambers with complex geometry. The algorithm is based on representation of the continuous media as set of a large number of elementary particles, moving on the fixed trajectories, corresponding to given flow field. Each particle is characterized by spatial coordinates and two states corresponding to burned and unburned gases, respectively. The flame front is considered as a boundary dividing two sorts of the particles. The formulation of the model and the algorithm of the calculations is described in the next section. The figure 1 shows results of the method.

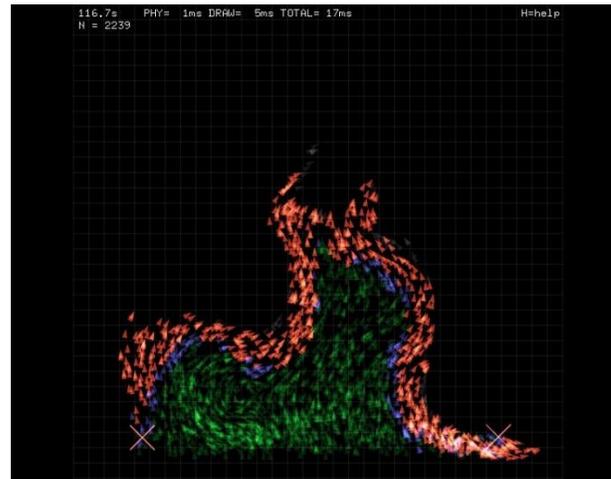


Fig. 1: Turbulent flame touch simulated by particles based real time algorithm. Green and red particles correspond to the unburned and burned mixture, blue particles marks the flame

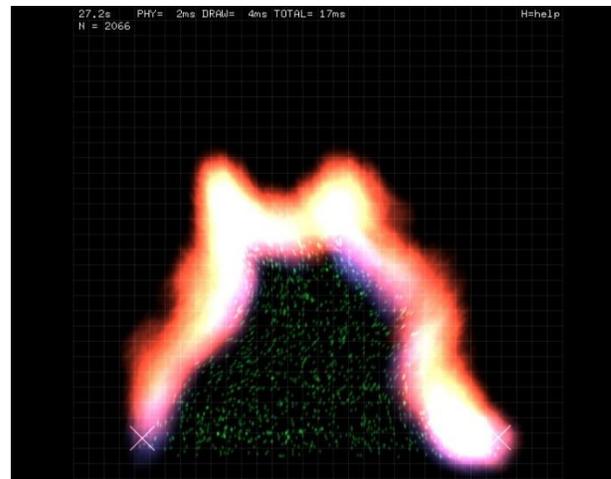


Fig. 2: Real time post effect flame simulation.

In many practical devices with gas combustion the flame thermal thickness is small in comparison with the sizes of the combustion room. Therefore flame may be considered as a surface dividing unburned and burned mixtures. This surface is characterized by ability to move on unburned mixture with constant burning velocity U_b [5]. The burning velocity is considered to be known from theoretical evaluations or experimental data. Writing the flame front equation in the form $F(x, t) = 0$ and assuming that flame front propagates in the unburned gas with given flow

velocity field $V(x, t)$ one can obtain the flame front evolution equation in the form

$$\frac{\partial F}{\partial t} - \left(\vec{V}, \vec{\nabla} F \right) = U_b \left| \vec{\nabla} F \right| \quad (1)$$

In the particular case of flame front equation $z = f(x, y, t)$ and velocity vector $V = (0, 0, W(x, y))$ equation (1) has a form

$$\frac{\partial f}{\partial t} - W = U_b \left(\left(\frac{\partial f}{\partial x} \right)^2 + \left(\frac{\partial f}{\partial y} \right)^2 + 1 \right)^{1/2} \quad (2)$$

It is interesting to note that this equation is similar to the Hamilton-Jacobi equation describing propagation of the relativistic particle in the field with potential $U(x, y)$ [4]:

$$\frac{1}{c_0^2} \left(\frac{\partial S}{\partial t} + U \right)^2 - \left(\frac{\partial S}{\partial x} \right)^2 - \left(\frac{\partial S}{\partial y} \right)^2 = m^2 c_0^2 \quad (3)$$

Flame front evolution in the case of resting gas may be described on the base of the Huygens principle applying in the ray optics. Let us suppose that flame front shape is known at some moment, for instance at $t = 0$. In order to find the flame front shape at subsequent time moment $t = dt$ according to the Huygens principle the set of spheres of radius $U_b dt$ with its centers belonging to the initial surface should be plotted. The envelope curve of this set of spheres represents the flame shape at $t = dt$. Applying this principle for subsequent time intervals the flame front evolution can be tracked. In the case of the moving fluid

with given velocity field $\vec{V}(\vec{x}, t)$ the technique based on the Huygens principle can be applied too. The only difference is that all points of initial surface must be previously shifted on vector $\vec{V}(\vec{x}, t) dt$. Proposed algorithm assumes that continuum is filled by the finite number of randomly distributed particles moving with velocity equal to the local velocity in corresponding 2-D point. Each particle is characterized by spatial coordinates and value describing the state of the corresponding elementary gas volume, namely unburned or burned. Flame front defines as the interface separating the regions field by unburned and burned gases. More specifically, the flame front may be defines in the following manner. Let us divide the calculation domain on uniform cells so that each cell comprises at least two particles. Lets calculate difference between numbers of unburned and burned particles for each cell. Finally, lets single out the cells for which this difference is less than some fixed number. The flame front may be described by any surface passing through these cells. If the average distance between neighboring particles is δ the size of the square in 2D case must be not less than 2δ and the accuracy of determination of the flame front position depends on the cells size. The following algorithm is proposed for numerical simulations of the flame front evolution. On each time step all unburned particles located inside the circles centered at the burned particles are replaced by the burning particles. The procedure of particles properties changing is applied at every fixed time step τ and the circles radius is $U_b \tau$. From physical point of view, this algorithm models ignition of the fresh mixture volumes by hot burned gas. Dependency of the velocity of self-propagating wave of ignition on average distance between neighboring particles is discussed in the next section. Calculation of one algorithm iteration for system of N particles demands implementation of $O(N^2)$ operations for checking the particles belonging to the igniting circles. However, usage of the particle spatial coordinates

sorting method allows to reduce calculation cost to $N \cdot \log N$ operation per one time step.

This acceleration is achieved by sorting of the particles in cells and neglecting certainly far located particles during the search of the particles belonging to the ignition circle. The sorting results are also useful in determination of the flame front surface. Utilization of the memory pool for data structures describing particles also leads to the calculations acceleration.

2. RESULTS

Flame front burning velocity on the non-uniform grid of particles depends on average distance between particles. For simplicity, we consider the 1D grid case. The fluctuation of average distance between two neighbor particles d can cause the decrease of value of burning velocity in numerical simulations. Numerical experiments demonstrated that, for example, error value of 1% of burning velocity corresponds to 50 particles placed into the "ignition" radius $U_b \tau$. We also carried out a numerical experiment to measure the velocity of the outward propagating cylindrical flame to investigate the influence of fluctuation of partial density on flame characteristics. Numerical experiments shown that flame front speed did not depend on its radius and the proposed algorithm keeps the spatial isotropy.

This algorithm was applied to simulate the flame propagating in non-uniform non-stationary flows. The implemented algorithm allows interactively change number of the particles, the velocity field, and gives possibility for interactive ignition and quenching of flame in the real-time. The figure 1 shows results of simulations of flame front propagating in constant Poiseuille flow with randomly distributed non-stationary point vortices. This configuration roughly corresponds to a turbulent flame torch. The proposed algorithm provides 25 fps on the one core of Pentium Dual-Core 2.5GHz with particles number $N = 20000$. The figure 2 shows the result of real time post computation for more clear flame presentation.

3. CONCLUSION

In the paper the numerical algorithm describing flame front evolution within frame of "flamelet" model is suggested. This algorithm assumes the representation of the continuous medium by set of discrete particles. The developed algorithm can be generalized in future to the model that takes into account self-ignition and flame quenching mechanism. For this aim one can apply the flame front model that incorporates flame front inertial effects and the dependency of flame front velocity on the local flame front curvature [3]. The work was partially supported by cooperative grants of Siberian Branch of the Russian Academy of Sciences and Collaborative Research Project J11028 IFS Tohoku University.

4. REFERENCES

- [1] K.N.C. Bray, Turbulent Reacting Flows. Topics in applied physics, 44, (1980), pp.115-183.
- [2] R. Hockney, J. Eastwood, Computer simulation using particles, Mir, Moscow, (1987).
- [3] S. Minaev, K. Maruta, R. Fursenko, Combustion Theory Modelling, 11(2), (2007), 187
- [4] G. Sivashinsky, Lett. Nuovo Cimento, 77A(1), (1983), pp.21-38.
- [5] Ya.B. Zeldovich et al., Mathematical theory of combustion and explosions, Nauka, Moscow, (1980).

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