Benchmark study of combustion model of premixed gas by using LBM

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The propane gas combustion in a combustor was calculated using a two-dimensional LBM method that used pressure, temperature, and the distribution function fp of chemical components: f_T, f_{C3H8}, f_{O2}, f_{CO2}, f_{N2}, and f_{H2O}. WOLFRAM MATHEMATICA was used in the calculation and three cases were calculated— Case1: one dimension combustion flame of a uniform mixed gas (Re = 124) to obtain an average reaction rate omega; Case2: A two-dimensional problem, without the influx, where ignition occurred in the center of the area; and Case3: calculate the combustion of the air-fuel mixture from fuel jets ejected from both upper and lower boundary. The flow field simulation area in the axial symmetry was 1/4. The shape of the flame front consisted of a curved surface, and then a nearly horizontal flame front was formed at the end of the simulation. For the one-dimensional case, the propagation speed was 0.25m/sec, which was larger than the results reported by Huidan Yue [9]. The flame propagation speed roughly matched that of the two-dimensional simulation by Yamamoto [7].

Key Words: LBM, Combustion, Flame Front

Nomenclature

$f_{p,q}$	:	pressure distribution function
$f_{T,\alpha}$	:	temperature distribution function
$f_{Yi,\alpha}$	:	Y^i specy distribution function
τ_V	:	relaxation time for variable
ρ		v=p,T,Y^i
ω	:	density
cp	:	reaction rate
	:	Specific heat coefficient for air
x	:	Cartesian coordinate
y	:	Cartesian coordinate

Subscripts

p	:	pressure
T	:	Temperature
Y^i	:	concentration of species
f	:	distribution

INTRODUCTION

There are several stages in the combustion process in the engines. The problem of atomization of the injected fuel and the problem of vaporization from liquid particles to gas, the problem of mixing of small particles and air, the problem of mixing of fuel gas and air, ignition and detonation problem, stabilization of flames. These are fluid dynamics problems. For the combustion process there are very complicated chemical reactions between interacting species. Although the engine is tested at high pressure (automobile, gas turbine) and low pressure (ramjet engine), the conditions of combustion are required for low NOx generation and low fuel consumption regarding the specification of the engine. These are common requirements of design. However, in practice a large number parameters of thermo-aerodynamics parameters and chemical reaction parameters are needed to be considered.

Although experience has precedence, it takes time and great expense to develop a combustion system. For this reason, in recent years, experiments and numerical simulations of elementary processes are conducted as much as possible; designers use the results, and use high-speed parallel computers as possible as they can.

The high speed simulation is used, not only for the research on elementary process but also the entire simulation of the actual machine. It is desired to develop numerical simulators of fundamental processes with higher accuracy.

Currently three methods are used as high precision numerical simulations: Direct Compressible NS equation, high precision LBM method, and particle method which are performed with accuracy of tertiary or higher order. NS is valid for Kudson Number less than 0.1, and LBM method is valid for less than 10, and can be used Ku, the particle method is not limited.

1. The compressible NS was developed by TVD method and high precision scheme, but the boundary conditions are complicate, thus the code becomes is extremely long.

The reason why LBM has attracted attention in recent years is that it is being said that the simulation algorithm is simple and it is suitable for parallel programming. At the beginning of the development of LBM was from LGA model like particle method used for gas, it was too noisy, and then the distribution function method from Boltzmann equation is set as a basic equation. Most people have used the BGK approximation. This method is common LBM simulation method. Although there

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is no similarity in the form of the NS equation and the Boltzmann equation, it is known that the Euler equation and the NS equation are derived from the Boltzmann equation. Therefore, the LBM simulation must agree with NS for small Knudsen number. The discretization of LBM has two methods:

1) Qian & Zho (1998) streaming and collision method [1],

2) Differential equation method Kataoka (2004) [2],

The Streaming-Collision method is often used in low Mach approximation. The successful direct simulations by He and Doolen [4] and Martin [5]) are known. For research on boundary conditions for small Reynolds number, He and Zou showed samples of boundary settings.

The problem of combustion has the following problems;

1. Stability of combustion,
2. High Mach number computation [compressible flow],
3. Computation of flow including variables of various chemical substances (large capacity)
4. Mechanism of ignition

Most engineer compute averaged combustion flames by using RANS with turbulent flow models, but the mechanism of detonation accompanying shock, are omitted, and it is used as post-diction of experimental results.

Apart from the question of whether it is possible to achieve the correct prediction by accumulate the simplified benchmarks. There are many benchmark computations for combustion:

LES[8] was carried out under simplified counter flow combustion with a simpler shape and perfectly premixed gas for verification [8] Legier, JP, Poinsor, T., et al)

The most commonly used LBM in combustion computation is a two dimensional model of low Mach number approximation (incompressible). There is a pioneer work by Yamamoto, He & Doolen:. Their stable simulations were made with this approximation even for thermal expansion and intense change in density since the temperature equation and velocity equations are uncoupled.

Under un-coupling condition, there were undershoot and overshoot pointed by S. Chen et al [10] Therefore, if we use un-coupling system, we need careful consideration to evaluate benchmark simulations. In the present work we use uncoupling method, and will test three benchmark simulations,

The first test is one dimensional tube where we can obtain the spreading speed of the flame-front. For the first two-dimensional problem, the mean flow velocity is zero, and the flame is spread cylindrically. In the next two-dimensional problem, the mixed gas ejects from the upper and lower surfaces at the center of the blowout. Since it is a laminar flow problem, it is expected that the flame side will be steady, but in the experiment it becomes unsteady. In this research, we may know the detail mechanism of the combustion process with the present computation by comparing with the previous work.

METHOD

We use the distribution function f_p of the pressure, though most researchers use the distribution function f_v of the velocity. The representative length is less than 1cm, where the flow is stable from convection by gravity. The functions of temperature f_T and chemical components, f_{C3H8}, f_{O2}, f_{CO2}, f_{N2}, f_{H2O} were used. We use MATHMATICA for checking the equations and performing simulations. Three cases are selected: Case1: The computational domain is in a one-dimensional channel, and initially it is filled with a uniform gas mixture (lean) and the inlet also has a uniform flow of the mixture shown in Fig.1. We calculate the propagation velocity of flame in the region, the peak flame temperature, and the average reaction rate. Case2: The flame is ignited at the center of the domain, and the domain is two-dimensional without the inflow, as shown in Fig. 2. Case3: The configuration is that used in [6],[7]. We use the same parameters of [7]. The mixed gas is ejected from both upper and lower boundaries to the central line, and the air-fuel mixture starts to burn at the center of the domain, spreading horizontally and attaining steady combustion. We compute the ignition to the steady state to determine the overall rate of combustion ω_{ov} shown in Fig.3.

The geometry shown in Fig.1 is similar to [7]. The mesh size is N_x=500 and N_y=3. The computer code was written for two dimensional problems. The initial flow velocity and the concentrations of chemicals are uniform. We expect that the flame surfaces move in the flow-wise direction since the combustion propagation speed is smaller than the speed of flow. So, we will find both front and back of the flame body in the flow wise direction. Figure 2 shows two dimension problem without the mean flow velocity, thus there is no convection U=0 at initial and on boundaries. The frame will spread in radial direction, thus the propagation speed will be slower than one of the plane wave in one dimensional case. Figure 3 shows the configuration of the typical benchmark computations. The mixed fuel springs from both top and bottom, and merges near the center line. The ignition point is at the center of the domain. Though the size is 10mm, it is not clear the gravity effect will be counted or not if

we compare with the high temperature experimental data. The flow is symmetric in x axis and also y axis, thus we need only quarter of the domain. The mixed gas is impinged slow velocity u=0.1m/sec.

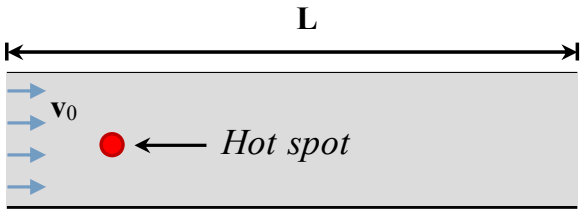


Figure 1. Schematic of 1D simulation.

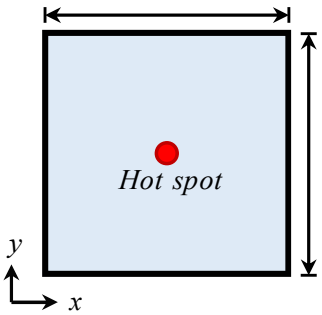


Figure 2. Schematic of 2D simulation.

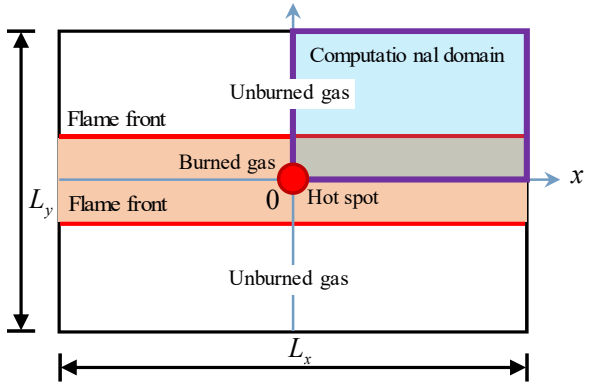


Figure 3. Schematic of symmetric burner flow, Mesh (80x48).

GOVERNING EQUATION FOR D2Q9

The governing equation is based on D2Q9 Lattice Boltzmann model [1]. Flow field equation for distribution function:

$$f_{p,\alpha}(x+e_\alpha\delta t,t+\delta t)-f_{p,\alpha}(x,t)=-\frac{1}{\tau_u}[f_{p,\alpha}(x,t)-f^{eq}_{p,\alpha}(x,t)] \quad (1)$$

Temperature field equation:

$$f_{T,\alpha}(x+e_\alpha\delta t,t+\delta t)-f_{T,\alpha}(x,t)=-\frac{1}{\tau_T}[f_{T,\alpha}(x,t)-f^{eq}_{T,\alpha}(x,t)]+w_\alpha Q_T \quad (2)$$

Species equations are:

$$f_{Y^i,\alpha}(x+e_\alpha\delta t,t+\delta t)-f_{Y^i,\alpha}(x,t)=-\frac{1}{\tau_u}[f_{Y^i,\alpha}(x,t)-f^{eq}_{Y^i,\alpha}(x,t)]+w_\alpha Q_{Y^i} \quad (3)$$

w_α, Q_T is the reaction rate and heat energy by combustion.

The pressure p, temperature T and the species fractions Yi can be found by summation of the corresponding distribution functions on α.

$$p=\sum_\alpha f_{p,\alpha},\quad T=\sum_\alpha f_{T,\alpha},\quad Y^i=\sum_\alpha f_{Y^i,\alpha} \quad (4)$$

The overall chemical reaction rate depends on species fractions and gas density, is defined as follows;

$$\omega_{ov}=k_{ov}\rho^2\frac{Y_{C_3H_8}}{M_{C_3H_8}}\frac{Y_{O_2}}{M_{O_2}}e^{-\frac{E}{RT}} \quad (5)$$

The source term due to heat production is given as

$$Q_T=\frac{Q\delta t}{\rho C_p T_0}\omega_{ov} \quad (6)$$

where T_0=300K is the reference temperature unit. The heat source terms due to chemical reactions are

$$Q_{Y^i}=a_i\frac{M_i\delta t}{\rho}\omega_{ov} \quad (7)$$

where T_0 =300K is the reference temperature unit. The heat source terms due to chemical reactions are $Q_Y{}^i$. The stoichiometric coefficients are: a_{C3H8} = -1, a_{O2}= -5. It's worth noting that, the reaction product of species does not give contributions to simulation, so their field equations may be dropped for reducing CPU time.

BENCHMARK COMPUTATION RESULTS

For the case1, one dimensional uniform mixed gas flow problem is following. We set the equilibrium distribution with the given velocity u_0 on the boundary conditions for both the inlet and the outlet, and also set periodic conditions on the sidewalls boundary shown in Fig.1. The results in Fig.4 shows that the spike of the flame is shown at t=7, and the spike split in to two at t=200 since the flame spread out from the ignition point to both the upstream and downstream directions with the burning velocity. The inlet velocity of a propane/air mixture is U_0 =1 m/s, the temperature T_0=300K and the equivalence ratio is 0.6. The length L=16.7 mm and the Reynolds number Re=124 as same as one of [7]. The present simulation yields the front speed of the combustion flame, the resultant burning velocity is 0.25 m/s that is greater than the result of [7].

(a)

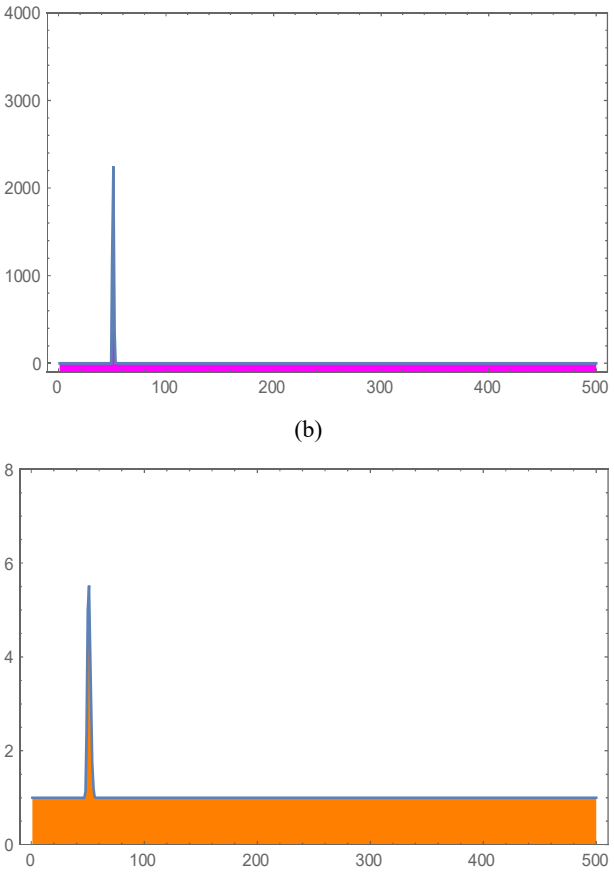
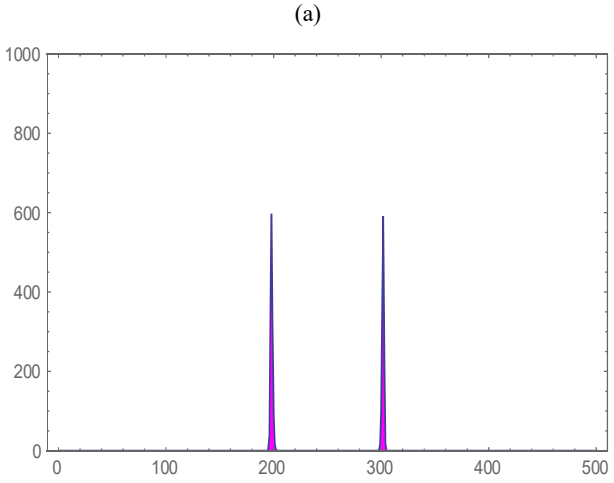


Figure 4. (a) The combustion rate and the temperature at the moment of ignition one dim problem. I.e. 7 times iteration. Combustion rate, at t=7. (b) The combustion rate and the temperature at the moment of ignition one dim problem. I.e. 7 times iteration. Temperature at t=7.

For the case2, two dimensional uniform mixed gas problem with no inlet is following. We took N_x=60, N_y=60 in 2D case. The physical parameters are the same as the 1D case. It is clear that the flame has a circular front, and propagates with the burning velocity S_L = 0.1 m/s that agrees with [7] in Fig.5.



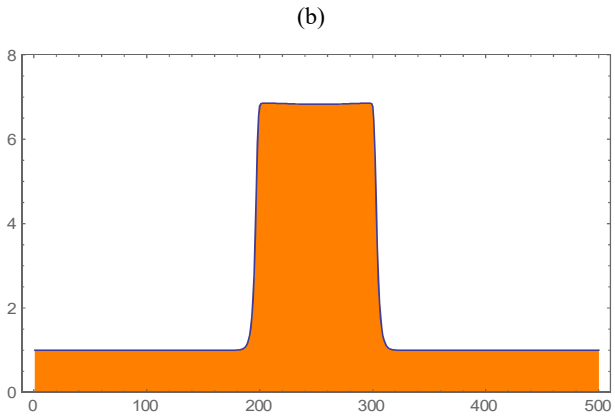


Figure.5. (a) The combustion rate at t = 2000 (one dim problem). (b) Temperature at t = 2000 (one dim problem).

We used Cartesian coordinate, so the solution does not depend on the geometry. It is not clear there is a similarity law of the combustion. The speed of propagation will depend on the ignition point and distance from the ignition point.

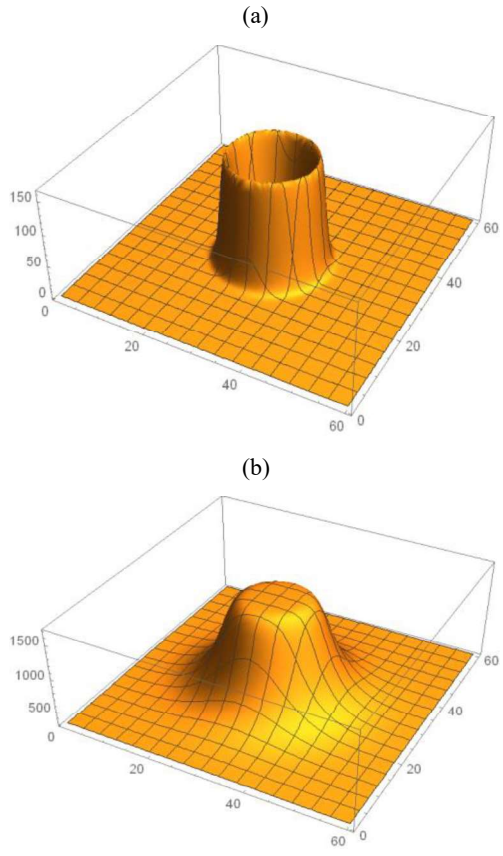
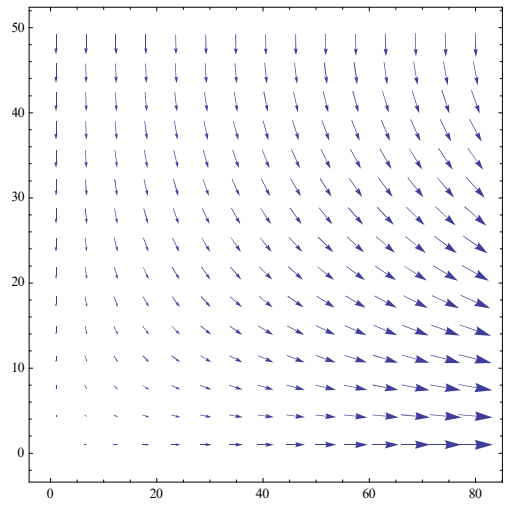


Figure 6. (a) The combustion rate at t = 1000 for case 2. (b) The temperature at t = 1000 for case 2.

For the case3, two dimensional uniform symmetry mixed gas combustor problem is following. The configuration is shown in Fig.3. The computational results show the detail flame propagation process clearly. It started from the center of the domain, and first formed an oblong around the center and was getting flat flame front in Fig.6, and formed nearly two dimensional flame body. The reaction rate

became zero near the center line (y=0), and the temperature remained constant around the centerline. The remained oxygen was 11% that is slightly larger than 9% of [7]. The temperature on the centerline was about 1990K that is larger than 1910K of [7]. The present computation results almost agree with [7] within CFD errors.

(a)



(b)

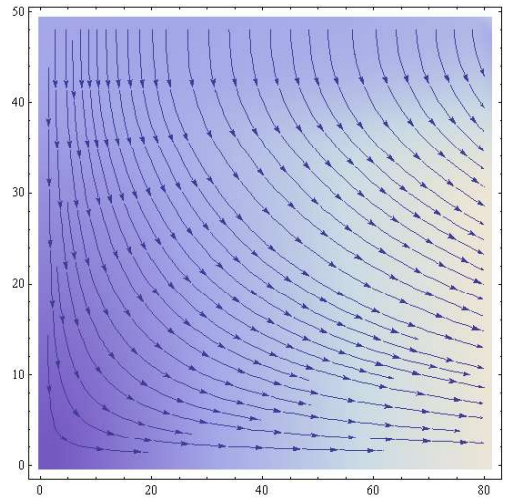
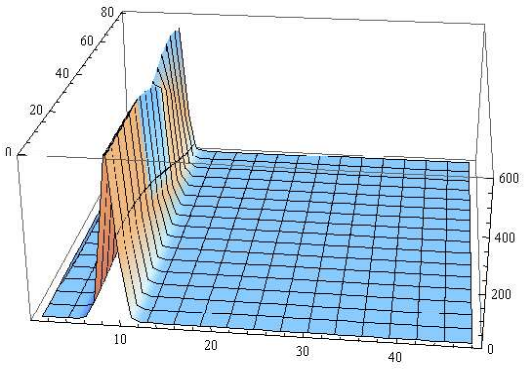


Figure 7. Converged Velocity vectors (a) and Streamline (b).

(a)



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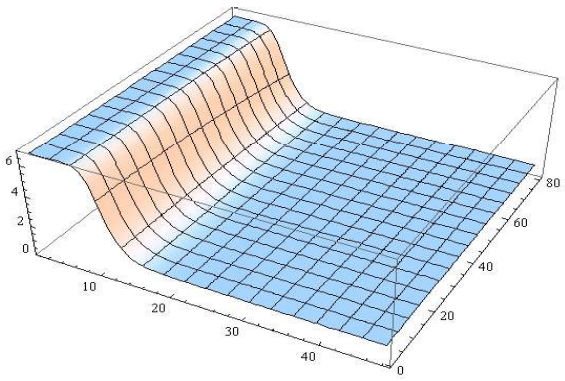
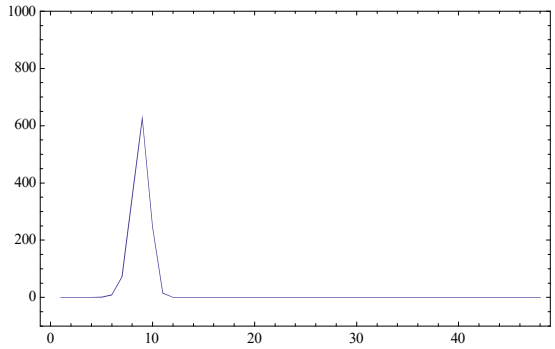


Figure 8. (a) Converged reaction rate. (b) Converged temperature.

(a)



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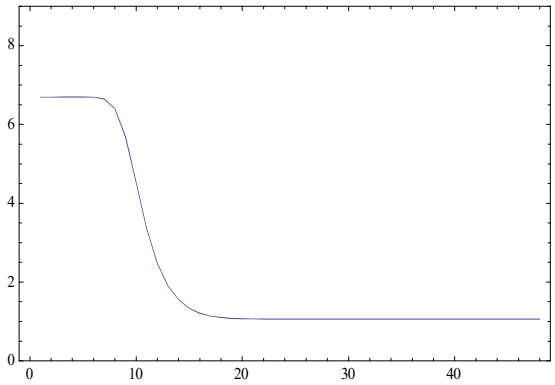

(c)

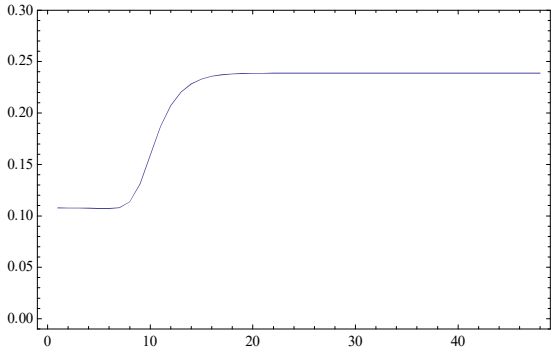

Figure 9. Reaction rate (a), Temperature (b), and Oxygen (c).

In the summary of the computational results, first regarding physical point of view we found the clear movements of two flame fronts in one dimensional case. The results are different from the results from 7) and 10) that has single flame front. In the second simulation when the gas is at rest and the flame forms a ring in the radial direction like a spherical wave: the cross section has two peaks like one dimensional case. From this computation we estimated the burning velocity correctly which to the close to the experiment [10]. Third case, counter flow combustion problem, as the extension of the second computation since the ignition point is fixed, so it reduces to the second problem at initial time where the blowing velocity is zero. The results show that it had also a ring at the initial stage. When the flow was stationary, the velocity at the combustion line was 0.25m/sec at the line where vertical velocity is 0.25m/sec as the same flame velocity of the one dimensional case (U=0.25m/sec). Regarding software we used WOLFRAM MATHEMATICA, miscalculations would be small.

Regarding the numerical simulation, the overall computations were steady with this set of parameters. However, a negative reaction rate was observed in the early stage of the computation and the small oscillation of the solutions remained until the end of the computation. More challenging attempt was done: used 1) larger Reynolds number, and used 2) a coupled-viscosity to temperature and found these attempts always caused instability problems.

CONCLUSION

We obtained a similar combustion flame speed to the results to [9], but obtained two combustion flame fronts which are different from [7] and [10]. We need to develop compressible LBM method that is stable at higher Reynolds number and stronger detonation and shockwave.

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REFERENCES

[1] Qian, Y.H., Zhon, Y., “Comple Calilean-invariant Lattice BGK Models for the Navier-Stokes Equation”, NASA/CR-1998-208701, ICASE Report No.98-38, 1998.

[2] Kataoka, T. and Tsutahara, M., “Lattice Boltzmann Model for the compressible Navier Stokes equations with flexible specific-heat ratio”, Physical Review E, 69(3):035701 R, 2004-03.

[3] Meng, J and Zhang, Y., “Gauss-Hermite quadrature and accuracy of lattice Boltzmann models for non-equilibrium gas flows”, Physical Review. E, Statistical physics, Plasmas, fluids, and related interdisciplinary topics, 83(3). Article 0367.ISSN 1063-651X, 2011.

[4] Chikatanmaria, S.S., and Karlin, I., “Entropy and Galilean Invariance of Lattice Boltzmann Theories”, Physical Review Letters, PRL 97, 190601 (2006), 10 Nov, 2006.

[5] Lui, L., “Theory of the Lattice Bolzmann Method :Lattice Bolzmann Models for Non--ideal Gas”, NASA/CR-2001-210858, ICASE Report No. 2001-8.

[6] Bennett, S., “A Lattice Boltzmann Model for Diffusion Binary Gas Mixtures”, University of Cambridge, Ph.D. Dissertation, King’s College, 2010.

[7] Yamamoto. K, He. X, and Doolen. G.D., “Simulation of combustion field with lattice Boltzmann, method”, J. Stat. Phys., 107 (2002), 367-3838).

[8] Legier, J.P., Poinsot, T., and Veynante, D., “Dynamically thickened flame LES model for premixed and non-premixed turbulent combustion”, Center for turbulence research, Proceedings of the Summer Program 2000, pp157-168, 2000.

[9] Yu, H., Luo, L., and Grimanji, S.S.. “Scalar Mixing and Chemical Reaction Simulations using Lattice Boltzmann Metthod”, Imperial College Press, International Jounal of Computational Engineering Science, Vol.3, No.1(2002) 73-87.

[10] Chen, S, Liu, Z, Tian, Z, Shi, B, and Zheng, “A Simple Lattice Boltzmann Scheme for Combustion Simulation”, Computers and Mathematics with Applications 55(2008)1423-1432.

[11] Gao, Y, and Chow, W.K., “A Review on Combustion Modeling”, International Journal on Architechural Science, Volumr 6, Number 2, p38-69,2005.

[12] Obikane, Y, and Khenmedekh, L., “Direct Simulation of the Instability of the Pilot Flame in a Turbo-Engine Combustor”, AIAA paper, July, 2015 Propulsion Conference, Orlando, FL.