Research paper

# Lewis number profiles in propagating flame and DDT process

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Received : November 29, 2011 Accepted : April 11, 2012

## Abstract

In this study Lewis number (Le) for laminar premixed flame in oxy-hydrogen stoichiometric mixture was investigated numerically. This is the first time to analyze values of Le for the whole flow field. It is known from definition that low Le is beneficial in flame propagation and our numerical simulations are a proof for that. On the edge of the flame Le is extremely low, which indicates that the flame accelerates. Flame can propagate with more than a speed of sound in the reactive mixture, which results in deflagration-to-detonation transition (DDT) and detonation. The present paper shows such propagating process with low Le as well as the profiles of Le in the DDT domain.

***Keywords*** : Lewis number, detonation, deflagration, DDT

## 1. Introduction

Lewis number (Le) has caught the attention of researchers for a long time. It defines a ratio of the thermal and mass diffusivities, which is very important in case of combustion of either subsonic or supersonic. Lewis number is considered as an important parameter in detonation, cell bifurcation or a turbulent flame. Nevertheless, it shows an importance in case of a laminar flame, too.

It was postulated by Law[1] that if we consider some control volume for a propagating flame, it can be seen that total energy conservation is maintained for Lewis number of unity and its flame temperature is noted as the adiabatic flame temperature. When Lewis number is less than one, the heat loss exceeds mass gain and the final temperature is lower than adiabatic one. The reverse situation happens for Lewis number greater then unity.

It was shown[2)–7)] that Lewis number is important in a premixed flame propagation. Even a small difference, like 0.2, from unity can show noticeable changes in a flame speed or curvature.

Karlin et al.[8] presented interesting results on Lewis number correlated with temperature, reaction rate, and velocity distribution in flames. They indicated also flame front evolution in the channel with Lewis number set to different values. It was shown that when Lewis number is low and invert flame front is formed, the significant intensification of chemical reactions at its front is accompanied by local temperature incensement. Nayagam and Williams[9] proved that Lewis number different from the unity shows the change in the flame propagation velocity. When it is greater than unity, velocity increases and in the case of values smaller than unity the situation is opposite. This is connected with excess enthalpy. Their numerical study was performed for the steady edge-flame propagation at general Lewis numbers. At the same time Kurdyumov and Fernández-Tarrazo[10] performed two- and three-dimensional numerical analysis on Lewis number for premixed flames in open ducts with a circular cross section. For Lewis number less than unity flame in a case of isothermal wall propagated faster than that for a case with adiabatic wall. It was explained as the effect of the higher flame curvature near a cold wall. The subject of pulsing and hydrodynamic instabilities at large Lewis number was discussed by Yuan et al.[11]. Han and Huh[12] investigated the displacement speed on a flame front density evolution in turbulent premixed combustion respect to Lewis number. They showed that a higher turbulent burning velocity was a result of Lewis number less than unity. Recent study of Lewis number in a premixed flame was discussed in the work of Chakraborty et al.[13] and Kurdyumov[14].

The present paper will show propagation process for laminar premixed flame with low Le as well as the profiles of Le in the DDT domain.

## 2. Numerical model

Our numerical model uses Navier-Stokes equations[15)–18)] and a Peresen and Hanson chemical reaction model with 9 species and 18 reactions. The finite difference schemes used are: a Harten-Yee, non-MUSCL modified-flux TVD method[19] for the convective term, a point-implicit method for the production term, and a Strang-type time splitting method for the time integration term to keep a second order accuracy explicitly. The average values at the cell boundary are computed by the Roe-averaged method. Calculations were performed for stoichiometric H2/O2 mixtures in 2-dimentional channel with 45 mm in width and 2 mm in height. As shown in Figure 1, the right side of the channel is an open end while all other are simulated as adiabatic walls. The grid system is build out of $7.5 \times 10^6$ (500 x15000) points, where the grid size in y-direction changes from 1 μm at the wall to 6 μm on the axis of the symmetry. In x-direction grid size is constant and equals 3 μm. Validation of the code[20] was done by comparing with the one of Urtiew and Oppenheim experiments[21]. A domain is divided into three regions as shown in the Figure 1. The ignition source region (ISR) has high pressure and temperature, while shock region (SR) is set to have 23 times higher pressure (16.997kPa) than ambient region (AR) and temperature of 981 K according to shock conditions. Initial conditions are summarized in the Table 1.

Lewis number is calculated for the whole mixture at every grid point using the equation (1):

$$Le_i = \frac{\alpha}{\sum_j D_{ij}} = \frac{\varkappa}{\rho \cdot D_i \cdot Cp} \tag{1}$$

where

$$D_i = \frac{1 - Y_i}{\sum_{j \neq i} \frac{X_{ij}}{D_{ij}}} \text{ for species i} \tag{2}$$

and $\alpha$ is a thermal diffusivity [m$^2$/s], $D_{ij}$ is a binary diffusion coefficient for i-and jth species [m$^2$/s], $\varkappa$ is a thermal conductivity [W/mK], $\rho$ is a density [kg/m$^3$], $Cp$ is a specific heat [J/kgK], $Di$ is the effective diffusion coefficient of ith species, $X_i$ is a mole fraction of ith species, and $Y_i$ is a mass fraction of ith species.

## 3. Results and discussion

We were able to obtain a value of Lewis number for every grid point for a propagating flame, deflagration-to-detonation transition, and detonation process. At the very early stage of flame development Lewis number is up to 0.61. This maximum value is seen on the inner edge of the flame front when the flame is just an ignition sphere. When it develops into a laminar flame which wrinkles on the edges close to the left wall, Lewis number grows to unity. This happens in less than 1 μs. At the time of 1 μs after the ignition, Lewis number becomes 1.10 and the area of the maximum values grows towards the center of the flame. Furthermore, at the stage of development, a region inside the flame, where Lewis number is about 0.60, is created. Figure 2 shows the early stage of the flame development from the time of 0.15 μs through 1.77 μs. The part of the tube (2.00x3.45 mm) presented in Figure 2 shows the left region of the model, where ignition takes place: left, top and bottom sides of the figure are walls. One can observe how the maximum value of Le changes and the flame develops. The reader should pay attention on the scales in that figure, because the minimum and the maximum values slightly changes for each point in time. The right figures in Figure 2 show the value of Le along the center line, which changes from below 1, 10 to unity as time passes.

Once the flame is developed, Lewis number varies between 0.12 and 1.43. Flame propagates with a distance from the precursor shock (about 2.0-2.5 mm) and creates compression waves due to its piston effect, which compresses the reactive mixture in front of it. There are many compression waves propagating between the flame and the precursor shock (Figure 3).They merge into weak shock waves. Even though they are weak they carry enough energy to heat up the region to cause an ignition. The highest value of Le is obtained in the inner part of the

**Table 1** Initial conditions.

| Region | Pressure [kPa] | Temperature [K] |
|---|---|---|
| Ignition source region (ISR) | 2500 | 2000 |
| Shock region (SR) | 16.997 | 981 |
| Ambient region (AR) | 0.739 | 289.15 |

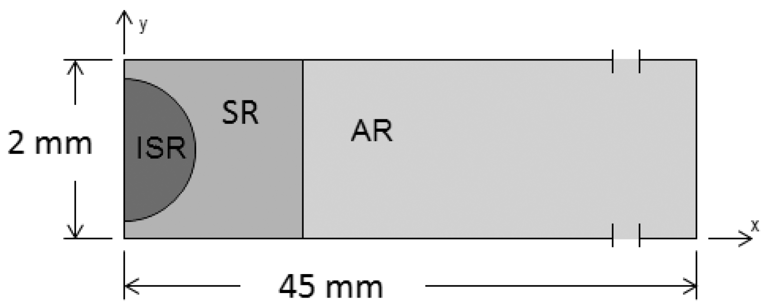


**Figure 1** Numerical model. ISR-ignition source region, SR-shock region, AR-ambient region.

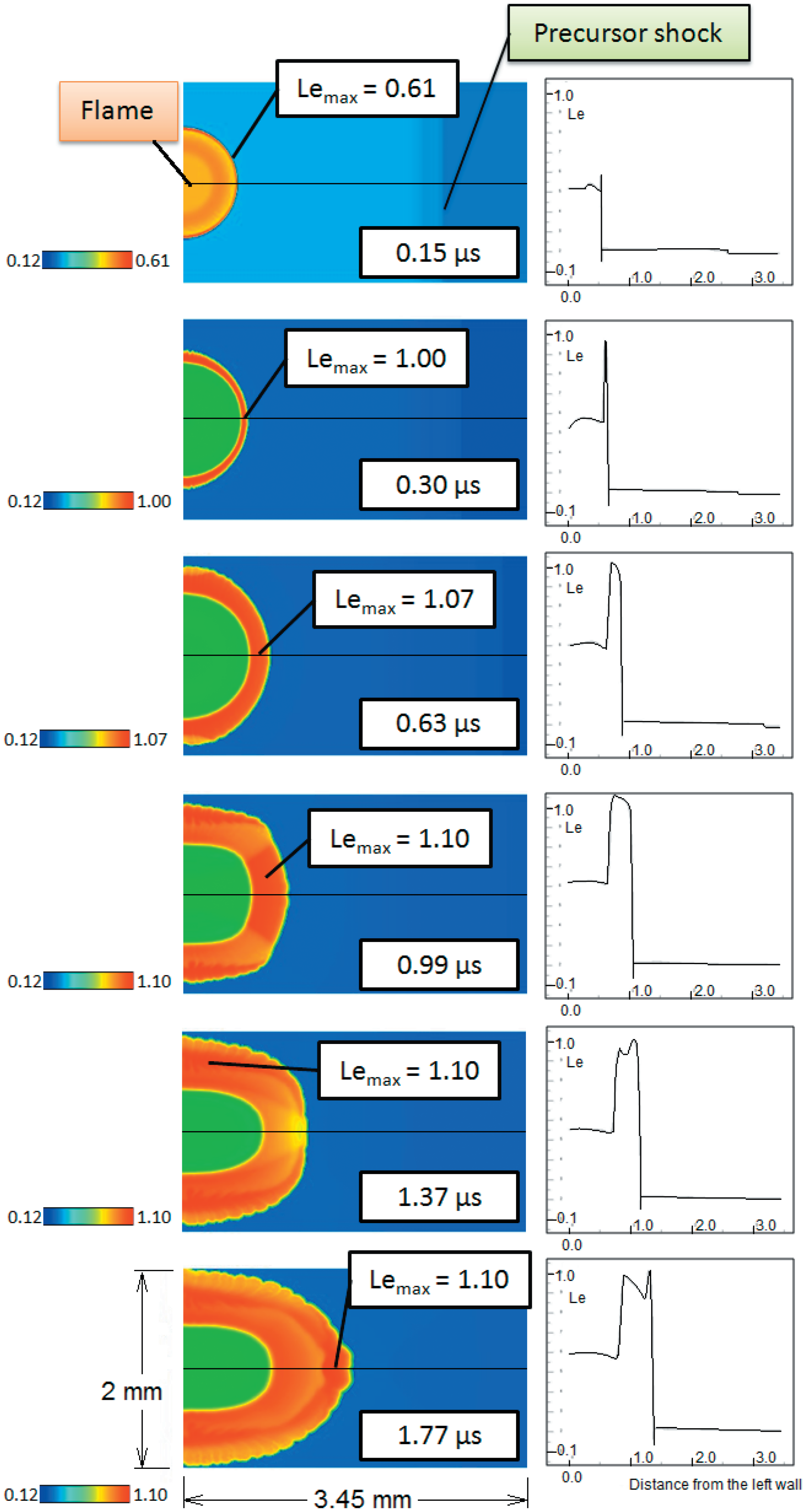


Figure 2 Lewis number at the early stage of a flame development.

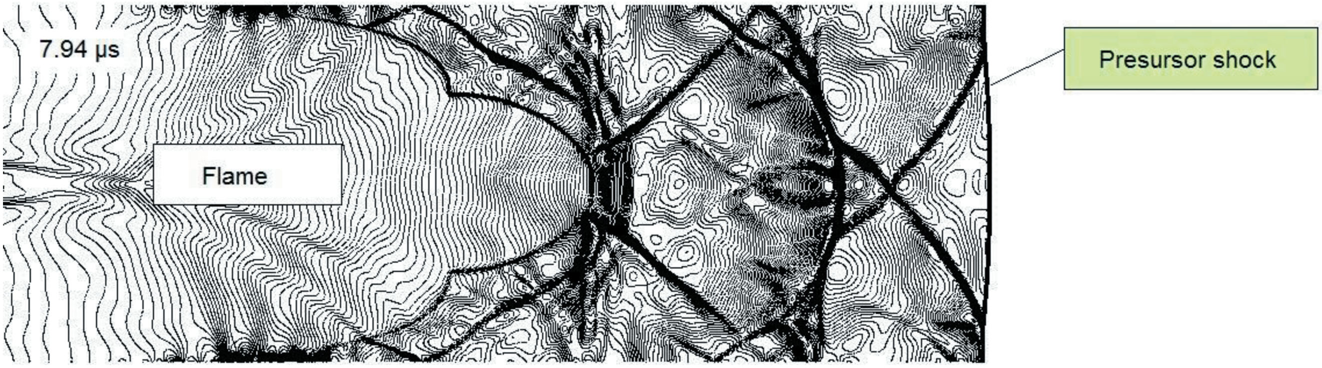


Figure 3 Shock waves propagating behind the precursor shock and in front of the propagating flame at 7.94µs.

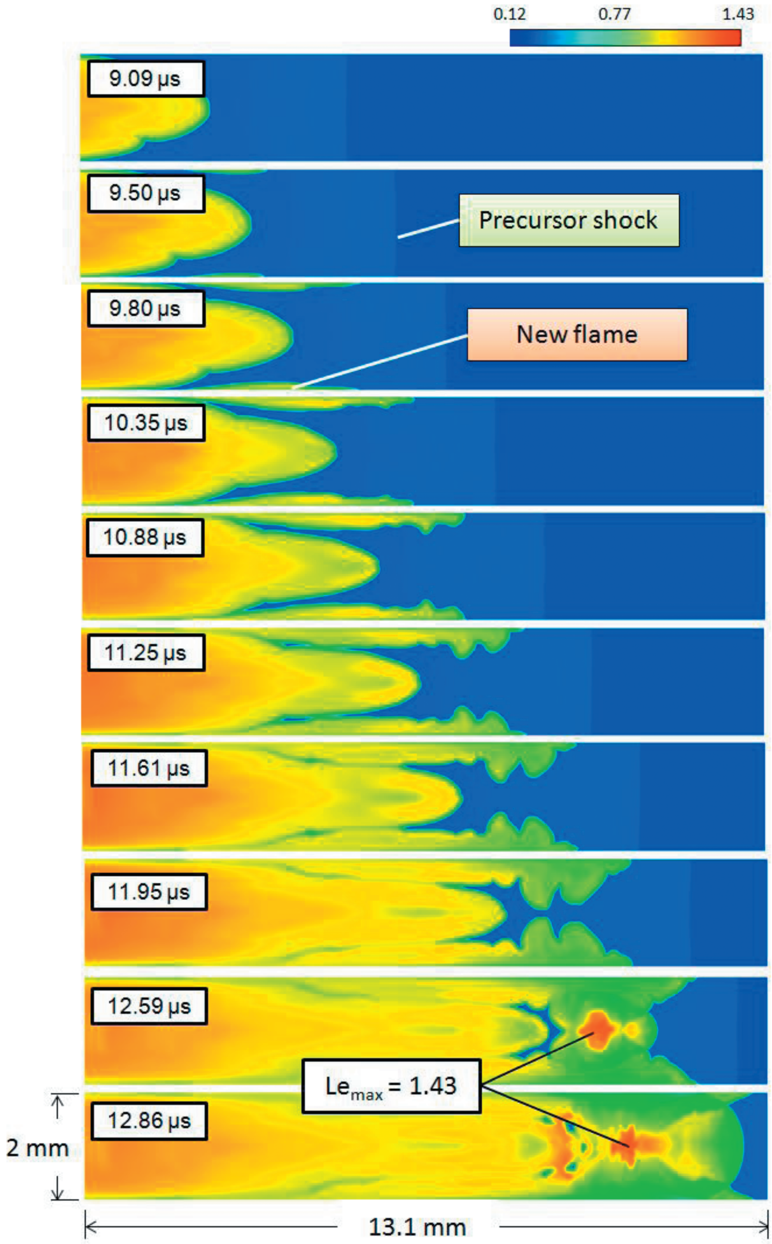


Figure 4 Lewis number profile and the maximum Lewis number for the moment of detonation.

flame and for the DDT process. The Precursor shock heats up the medium behind it and creates boundary layer, which thickness in this case is about 21 µm. Multiple shocks keep on heating up both walls and finally one can observe an auto-ignition triggered by a shock-boundary layer interaction at both walls (Figure 4).This is the origin for new flames, which propagate with more than local sonic speed along both walls, change its shape, and grow towards the center of the tube. After a short time they collide at the center of the tube and at some distance from of the propagating flame. From this point detonation starts and Lewis number reaches its maximum value of 1.43.

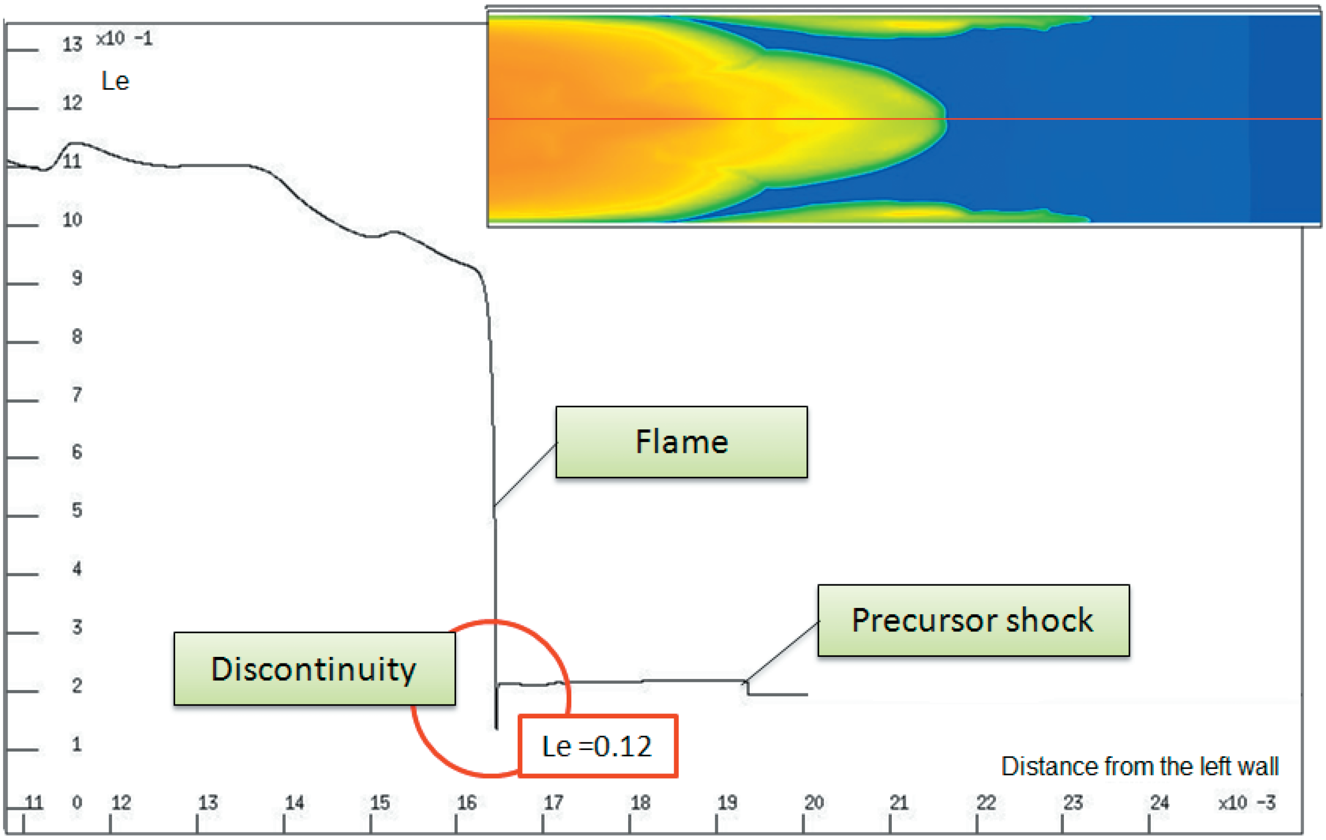


Figure 5 Discontinuity at the edge of a flame seen in the Lewis number profile.

Figure 4 shows Lewis number profile in the time sequence from 8.87 to 11.25 μs. One can observe an auto-ignition in the boundary layer. Figure 4 also shows the maximum value of Lewis number for deflagration-to-detonation transition and expresses the exact moment of collision.

In Figure 5 the Lewis number profile at the center line and a discontinuity at the edge of the flame are shown, where the lowest Le is 0.12. There are at least 5 grid points at the very edge of the flame to resolve this problem. The jump at the discontinuity is connected with the stoichiometric condition, which indicates a switch in the deficient reactant. Such a low Lewis number implies that thermal diffusivity goes down. Figure 6 presents close look at the Lewis number profile at the edge of the flame. 50 μm represents about 16 grid points.

With the stoichiometric conditions, which postulated before[22–24], it is clear according to our results and definition that the greater Le indicates more heat loss and less reactant species diffusion, while the relatively low values are favorable for the flame propagation. When flame accelerates faster, it reaches a speed of sound for the reactive mixture, accelerates even more, and finally transits to detonation.

Figure 7 presents the local Mach number values versus time in three points ; the center of the tube and two locations in the boundary layer. The first one, Boundary layer 1, is measured 1.0 μm from the bottom wall, while the second one, Boundary layer 2, 10.5 μm also from the bottom wall. The flame velocity relative to the flow just behind the precursor shock is about 1946 m/s.

One should not forget that the whole mixture is responsible for the conductive heat losses. Nevertheless, the flame propagation is limited by diffusivity in the species transport.

## 4. Conclusions

We were able to show the local values of Lewis number for a premixed laminar flame propagation, deflagration-to-detonation transition (DDT), and detonation process. In our case auto-ignition occurs in the boundary layer triggered by the shock-boundary layer interaction. The ignition in the boundary layer does not depend on a Lewis number. Once flame is developed, the highest value of Lewis number is calculated inside of the propagating flame and at the moment of flames collision (Le = 1.43), which is the origin for DDT and detonation. The lowest value obtained is 0.12 and it is at the edge of the flame, which is connected with the discontinuity in the medium. There are at least 5 grid points exist at the edge of the flame. This means the profile of Lewis number is well resolved. The flame accelerates faster in stoichiometric conditions for low Le. The flame propagates faster than the speed of sound and transits to detonation.

Lewis number actually does not influence DDT or detonation, but its values at certain places helps to understand the physics.

## Acknowledgements

This simulation was performed using Osaka University Cyber Media Center.

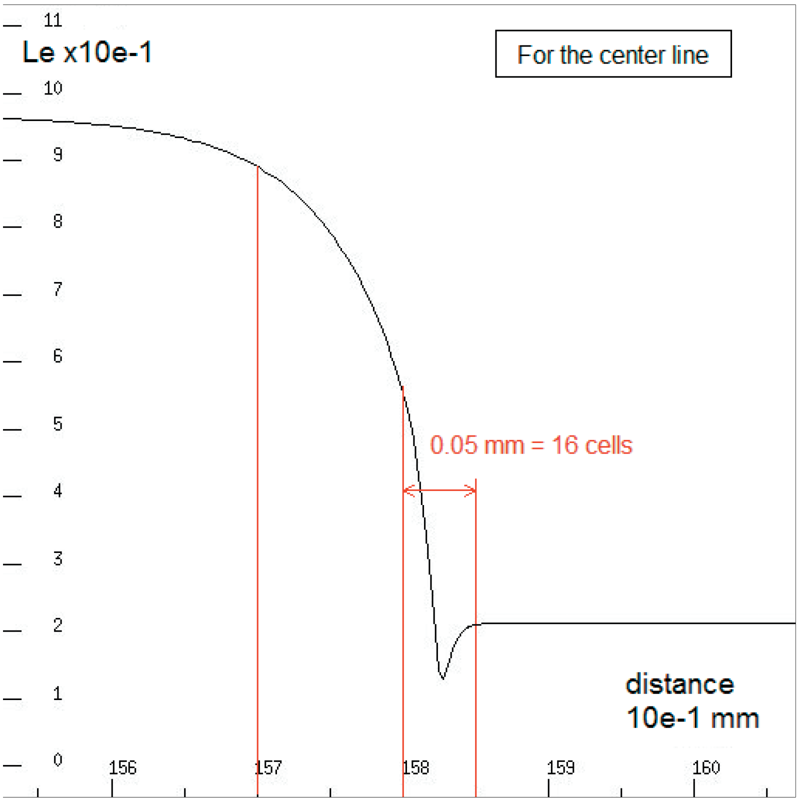


**Figure 6** Close look into discontinuity at the edge of the flame.

## References

1) C. K. Law, Symp. (Int.) on Combust., Vol. 22, Issue 1, 1381-1402 (1989)
2) J. L. McGreevy and M. Matalon, Combust. Flame, 91, 213-225 (1992).
3) D. C. Haworth and T. J. Poinsot, J. Fluid Mech., 244, 405-436 (1992).
4) C. J. Rutland and A. Trouvé, Combust. Flame, 94, 41-57 (1993).
5) A. Trouvé and T. Poinsot, J. Fluid Mech., 278,1-31 (1994).
6) N. Chakraborty and R. S. Cant, Phys. Fluids, 17 (105105) 1-20 (2005).
7) N. Swaminathan and R. W. Grout, Phys. Fluids, 18 (045102) 1-9(2006).
8) V. Karlin, G. Makhviladze, J. Roberts, and V. I. Melikhov, Combust. Flame, 120, 173-187 (2000)
9) V. Nayagam and F. A. Williams, J. Fluid Mech., 458, 219-228 (2002).
10) V. N. Kurdyumov and E. Fernández-Tarrazo, Combust. Flame, 128, 381-394 (2002).
11) J. Yuan, Y. Ju, and C. K. Law, Combust. Flame, 144, 386-397 (2006).
12) I. Han and K. Y. Huh, Combust. Flame, 152, 194-205 (2008).
13) N. Chakraborty, M. Klein, and N. Swaminathan, Proc. Combust. Inst. 32, 1409-1417 (2009).
14) V. N. Kurdyumov, Combust. Flame, 158, 1307-1317 (2011).
15) T. Ito, N. Tsuboi, and H. Miyajima, *Trans. Jap. Soc. for Aeronautics and Space Sci*., Vol. 53, no 172, 86-92 (2008).
16) N. Tsuboi, T. Ito, and H. Miyajima, *Trans. Jap. Soc. for Aeronautics and Space Sci*., Vol. 51, no. 179, 63-70 (2010).
17) N. Tsuboi, Y. Morii, A. K. Hayashi, and M. Koshi, ICDERS 23rd, July 24-29, Irvine, USA (2011).
18) E. Yamada, N. Kitabayashi, A. K. Hayashi, and N. Tsuboi, *Int. J. Hydrogen Energy*, Vol. 36, no.3, 2560-2566 (2011).
19) H. C. Yee, Upwind and Symmetric Shock-Capturing Schemes, NASA TM-89464 (1987).
20) E. Dzieminska, M. Fukuda, A. K. Hayashi, N. Tsuboi, and E. Yamada, Archivum Combustionis, 31, no 3 (2011).
21) P. A. Urtiew and A. K. Oppenheim, Proc. of Royal Soc., A, 295, 13-28 (1966).
22) S. R. Turns, An Introduction to Combustion, 2nd edition, McGraw Hill (2006).
23) E. Schultz, E. Witenberger, J. Shepherd, Proceedings of 16th JANNAF Propulsion Symposium, Cocoa Beach, FL October 8 (1999).
24) F. P. Incropera, D. P. DeWitt, T. L. Bergman, A. S. Lavine, Fundaments of Heat and Mass Transfer, 6th edition, John Wiley and Sons (2007).

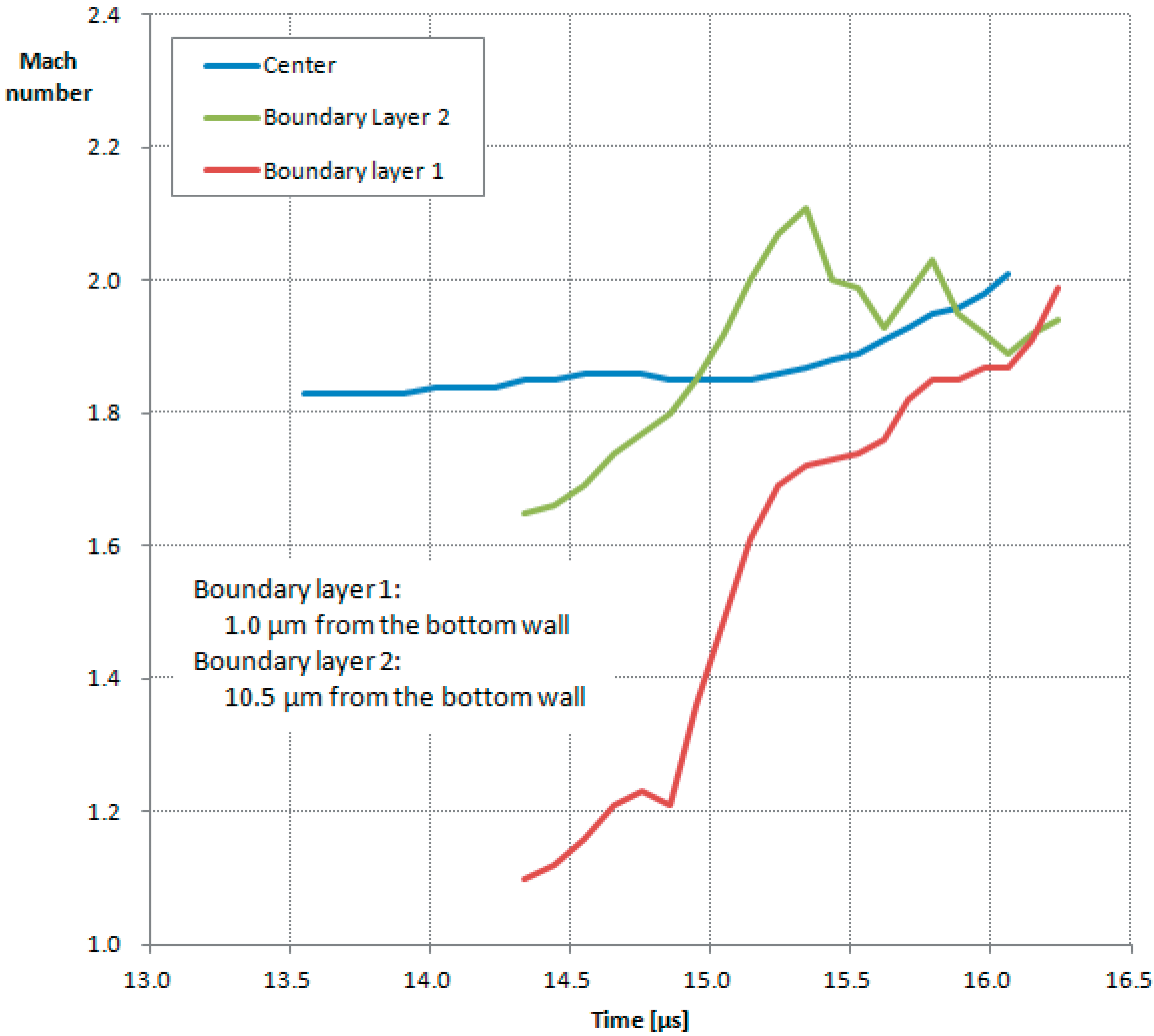


**Figure 7** Mach number versus time in the boundary layer and at the center of the tube. 'Boundary layer 1'and 'Boundary layer 2' are measured 1.0 µm from the bottom wall and 10.5 µm from the bottom wall respectively.