

Intrinsic Instability of Adiabatic and Non-adiabatic Premixed Flames at Sufficiently Low Activation Energy

Kaewpradap Amornrat* and Jugjai Sumrerng

Department of Mechanical Engineering, King Mongkut's University of Technology Thonburi, Bang Mod, Thung Khru, Bangkok 10140, Thailand

Abstract

The effects of low activation energy on the intrinsic instability of adiabatic and non-adiabatic cellular premixed flames were studied by using two-dimensional unsteady calculations of reactive flows based on the compressible Navier-Stokes equation. For the Lewis number that was lower than unity ($Le=0.5$), the growth rate and the normalized burning velocity (S_{cf}/S_b) increased when the activation energy was lower for adiabatic premixed flames due to the decrease in the Zeldovich number. When the heat loss increased, the growth rate was lower and the normalized burning velocity was higher. However, the ratio of the cell size to the critical wavelength (D_{cell}/λ_c) was smaller compared to that of adiabatic premixed flames. For the Lewis number that was unity ($Le=1.0$), the growth rate and the normalized burning velocity were almost constant and slightly decreased even at sufficiently low activation energy. Moreover, for the Lewis number was higher unity ($Le=1.5$), the growth rate and the normalized burning velocity were lower. Even at sufficiently low activation energy for adiabatic premixed flames and slightly lower growth rate and lower normalized burning velocity were obtained. The results show that a lower growth rate is obtained at sufficiently low activation energy due to a decrease in the Zeldovich number. Even at low activation energy, the effects of hydrodynamic instability play a more destabilizing role (stabilizing role) for $Le<1.0$ ($Le>1.0$) to obtain a higher (a lower) normalized burning velocity compared to adiabatic cellular premixed flames owing to the heat.

Keywords: Sufficiently low activation energy; Adiabatic premixed flames; Non-adiabatic premixed flames; Navier- Stokes equation; Zeldovich number; Heat loss.

1. Introduction

In the past, the combustion of fossil fuels that emitted the greenhouse gases such as carbon dioxide and nitrogen oxide was studied. Thus, the lean combustion of hydrogen-air was studied to reduce the emission of greenhouse gases. In contrast, since hydrogen is lighter than air, intrinsic

instability plays an important role on cellular flame fronts in hydrogen-air combustion [1]-[2]. Basically, there are three types of effects associated with the intrinsic instability of premixed flames, namely body-force effects, diffusive-thermal effects and hydrodynamic effects [3]. Body-force effects are caused by the difference in density between above and

*Correspondence : amornrat.kae@kmutt.ac.th

below fluids, and are significant only at the sufficiently small burning velocity. Generally, the premixed flames with large burning velocity such as hydrogen-air flames are rarely affected by body-force effects. Diffusive thermal effects, caused by the preferential diffusion of mass versus heat, have a destabilizing (a stabilizing) influence when the Lewis number of the deficient reactant is lower than unity. Hydrodynamic effects are caused by a thermal expansion of reactive gases through the flame front. This type of effects strongly influences the intrinsic instability of premixed flames [4]-[5]. Besides three effects of intrinsic instability, the effects of activation energy on the characteristics of premixed flames were investigated in a previous study. The pulsating instability was found in premixed flames with large activation energy at a high Lewis number [6]. Moreover, the flame propagation affected by activation energy in large scale vertical flows was numerically studied [7]. In a previous study, the effects of medium and high activation energies were studied in terms of the intrinsic instability for adiabatic and non-adiabatic premixed flames [8]. In order to focus on the high-temperature air combustion (HiTAC), the effects of sufficiently low activation energies were studied on the intrinsic instability of premixed flames [9,10]. Especially for practical combustion devices such a micro combustor, the heat loss to the surroundings of premixed flames strongly affects the combustion phenomena e.g. flame quenching and burning velocity. As the heat loss affects premixed flames due to the intrinsic instability, it is important to study the instability of premixed flames with heat loss. In a past investigation, heat loss weakened the hydrodynamic instability because the instability intensity of non-adiabatic flames is lower than that of adiabatic flames. Moreover, unburned-gas temperatures and the effects of heat loss on the diffusive-thermal instability of premixed flames were studied [11]. A decrease in intensity

significantly affects the characteristics of cellular premixed flames. In another study, a simulation of non-adiabatic flames was performed using the compressible Navier-Stokes equation, and the effects of heat loss on the chaotic behavior were estimated [12]-[13]. However, past investigations of the instability of non-adiabatic flames did not precisely treat the effects of low activation energies. This study focuses on the intrinsic instability of adiabatic and non-adiabatic of premixed flames at sufficiently low activation energy. The numerical calculation of two-dimensional reactive flows with one-step irreversible chemical reaction was performed using the compressible Navier-Stokes equation to analyze the unstable behavior of cellular flames generated due to the intrinsic instability.

2. Nomenclatures

A	non-dimensional heat-loss parameter, referred to as κ / δ^2
A_m	non-dimensional heat-loss parameter at quenching point, referred to as κ / δ^2
a_0	non-dimensional initial amplitude of a disturbance, referred to as δ
B	non-dimensional frequency factor of the reaction rate, referred to as S_u / δ
C_p	specific heat at constant pressure
c_u	sound velocity of the unburned gas
D	diffusion coefficient
D_{cell}	cell depth
E	non-dimensional activation energy of the reaction rate, referred to as RT_u
e	non-dimensional stored energy, referred to as p_u
Le	Lewis number ($= \alpha / D$)
M_u	Mach number of the burning velocity of an adiabatic planar flame ($= S_u / c_u$)
N	integer
Pr	Prandtl number ($= \nu / \alpha$)
p	non-dimensional pressure, referred to as p_u
p_u	pressure of the unburned gas

- Q non-dimensional heating value, referred to as $C_p T_u$
- R universal gas constant
- S_{cf} non-dimensional burning velocity of a cellular flame, referred to as S_u
- S_h non-dimensional burning velocity of a planar flame, referred to as S_u
- S_u burning velocity of an adiabatic planar flame
- T non-dimensional temperature, referred to as T_u
- T_u temperature of the unburned gas
- t non-dimensional time, referred to as δ / S_u
- u, v non-dimensional velocities in x - and y -directions, referred to as S_u
- x, y space coordinates
- Y mass fraction of the unburned gas
- α thermal diffusivity
- γ ratio of two specific heats
- δ preheat zone thickness ($= \alpha / S_u$)
- κ thermal conductivity
- λ non-dimensional wavelength of a disturbance, referred to as δ
- λ_c non-dimensional critical wavelength, referred to as δ
- ρ non-dimensional density, referred to as ρ_u
- ρ_u density of the unburned gas
- ω non-dimensional growth rate, referred to as S_u / δ

bulk viscosity, Dufour effects, Soret effects, and pressure gradient diffusion are neglected. Moreover, the acceleration is neglected, because body-force instability is a significant factor only when premixed flames have sufficiently small burning velocities. The flow variables were non-dimensionalized by the preheat zone thickness, the burning velocity of a planar flame, the density, the pressure, and the temperature of the unburned gas. The compressible Navier-Stokes equation was employed to analyze hydrodynamic instability. In the energy equation, the viscous term was disregarded, because it is insignificant in the present problem. The Cartesian coordinates were written as this follows.

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}}{\partial x} + \frac{\partial \mathbf{G}}{\partial y} = \mathbf{S} \tag{1}$$

where

$$\mathbf{U} = \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ e \\ \rho Y \end{pmatrix}$$

$$\mathbf{F} = \begin{pmatrix} \rho u \\ \rho u^2 + \frac{p}{\gamma M_u^2} - \text{Pr} \left(\frac{4}{3} \frac{\partial u}{\partial x} - \frac{2}{3} \frac{\partial v}{\partial y} \right) \\ \rho uv - \text{Pr} \left(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \right) \\ (e + p)u - \frac{\gamma}{\gamma - 1} \frac{\partial T}{\partial x} \\ \rho Yu - \frac{1}{\text{Le}} \frac{\partial Y}{\partial x} \end{pmatrix}$$

3. Governing Equations

In this study, two-dimensional unsteady compressible reactive flows are considered where the abundant reactant is excessive and the chemical reaction is controlled by the deficient reactant. The chemical reaction used in this study is an exothermic one-step irreversible reaction, and the reaction rate obeys the Arrhenius' equation. The burned and unburned gases have the same molecular weights and the same Lewis numbers, and satisfy the ideal gas equation. The specific heats and transport coefficients are constant throughout the whole region. The radiation,

$$\mathbf{G} = \begin{pmatrix} \rho v \\ \rho uv - \text{Pr} \left(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \right) \\ \rho v^2 + \frac{p}{\gamma M_u^2} - \text{Pr} \left(\frac{4}{3} \frac{\partial v}{\partial y} - \frac{2}{3} \frac{\partial u}{\partial x} \right) \\ (e+p)v - \frac{\gamma}{\gamma-1} \frac{\partial T}{\partial y} \\ \rho Y v - \frac{1}{\text{Le}} \frac{\partial Y}{\partial y} \end{pmatrix}$$

$$\mathbf{S} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \frac{\gamma}{\gamma-1} \{QB\rho Y \exp(-E/T) - A(T-1)\} \\ -B\rho Y \exp(-E/T) \end{pmatrix}$$

The ideal gas equation of state is

$$p = \rho T \quad (2)$$

4. Numerical Simulations

The physical parameter of adiabatic flame temperature was general for hydrogen-air or methane-air premixed flames as $T_u = 7.0$ at room temperature and atmospheric pressure. The non-dimensional parameters were $Q = 6.0$, $\gamma = 1.4$, and $\text{Pr} = 1.0$. The burning velocity was sufficiently small compared with the velocity of sound, $M_u = 1.0 \times 10^{-2}$. The used Lewis numbers were 0.5, 1.0 and 1.5 with the heat loss being $A=0$ and maximum heat loss being $A=A_m$. In this study, the low activation energies $E=14$ and 35 were studied. The effects of activation energy are follow the Zeldovich equation (Eq.3)

$$\beta = E \frac{T_f - 1}{T_f^2} \quad (3)$$

The initial conditions were provided by the solution of a stationary plane flame, on which a disturbance periodic in the y direction was superimposed. The

displacement of the flame front in the x direction due to the superimposed disturbance was

$$a_0 \sin(2\pi y / \lambda) \quad (4)$$

The initial amplitude a_0 was set to 0.1 for the calculation of the dispersion relation. For cellular flames, a_0 was set to 1.0. The simulation domain is 100 and 800 times the preheat zone thickness in the x -direction and the critical wavelength in the y -direction. In the y -direction, a uniformly spaced grid is used as the grid size of $\lambda_c / 64$. The time-step interval was set to 5×10^{-5} to satisfy the CFL condition. This study is calculated using IBM system X iDataPlex dx360 M3 at National e-Science Infrastructure Consortium.

5. Results and Discussion

5.1 Dispersion relation

As a sufficiently small sinusoidal disturbance was superimposed on a planar flame, it grew exponentially with time. The growth rate of a disturbance depended on the wavelength as a wave number. The relation between the wave number and the growth rate is referred to as the dispersion relation. Figs.1-3 illustrate the dispersion relations at $\text{Le}=0.5$, 1.0 and 1.5 with small activation energy $E=14$ and 35 for adiabatic and non-adiabatic flames. These relations show that the growth rates increase (decrease) and that the unstable range is wide (narrow) when $\text{Le}=0.5$ (1.5) compared with $\text{Le}=1.0$ because of a destabilizing (stabilizing) influence from the diffusive-thermal effects. The linearly most unstable wave number specified in dispersion relation, is called the critical wave number corresponding to the critical wavelength. The critical wavelength is the space between cells. We refer to this space as the cell size of a cellular flame. The critical wavelengths at $\text{Le}=0.5$, 1.0 and 1.5 with sufficiently small activation energy $E=14$ for adiabatic flames are 23.87, 37.25 and 43.68, respectively (see Table 1).

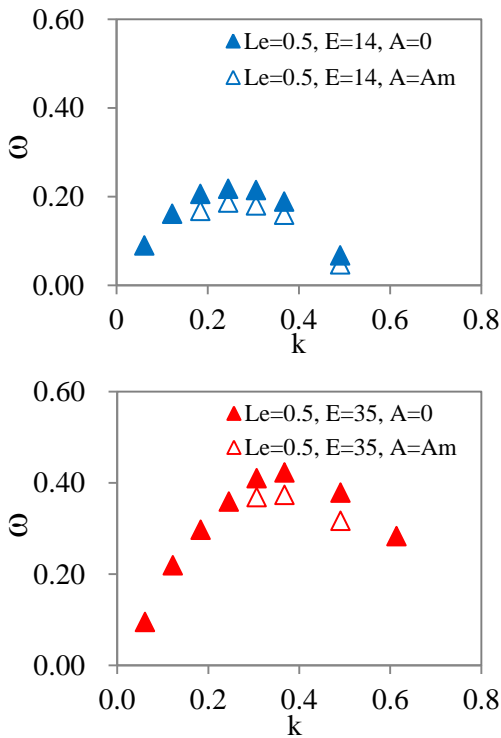


Fig.1. Dispersion relation at $Le=0.5$ for $A=0$ and $A=Am$, (a) $E=14$, (b) $E=35$.

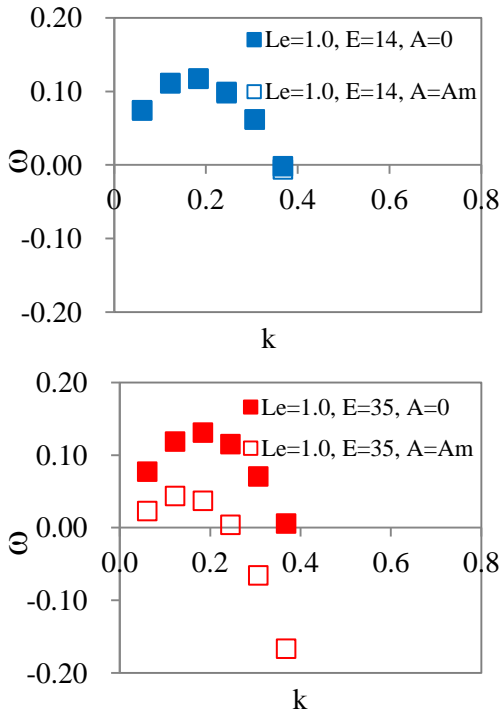


Fig.2. Dispersion relation at $Le=1.0$ for $A=0$ and $A=Am$, (a) $E=14$, (b) $E=35$.

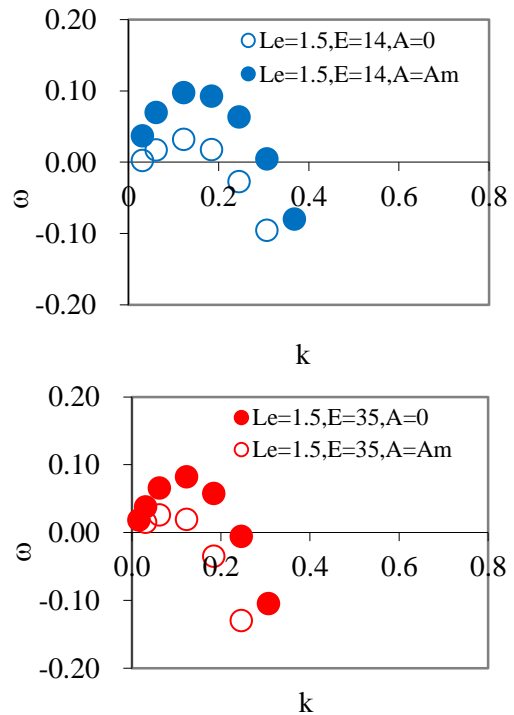


Fig.3. Dispersion relation at $Le=1.5$ for $A=0$ and $A=Am$, (a) $E=14$, (b) $E=35$.

Table 1. Critical wavelengths (λ_c) of cellular flames at $Le=0.5, 1.0$ and $1.5, E=14$ and 35 for $A=0$.

Le	λ_c	
	E=14	E=35
0.5	23.87	16.92
1.0	37.25	34.60
1.5	43.68	53.99

Table 2. Critical wavelengths (λ_c) of cellular flames at $Le=0.5, 1.0$ and $1.5, E=14$ and 35 for $A=Am$.

Le	λ_c	
	E=14	E=35
0.5	24.12	17.88
1.0	37.45	45.35
1.5	51.12	77.33

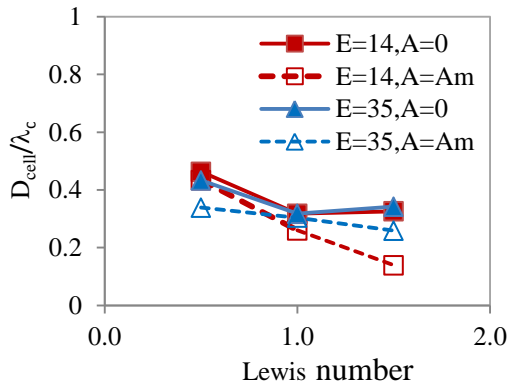


Fig.4. Relation between Lewis number and $D_{\text{cell}}/\lambda_c$ at $E=14$ and 35 for $A=0$ and $A=Am$.

In order to study the effects of heat loss at sufficiently small activation energy, we studied the dispersion relation for non-adiabatic premixed flames at $E=14$ and 35 . For $Le=0.5$ with small activation energy, $E=35$ shown in Fig.1, when the heat loss increases, the growth rate decreases in comparison to that of adiabatic flame. For the sufficiently small activation energy $E=14$ corresponding to the decrease of the Zeldovich effect, the heat loss still leads to a decrease of growth rate owing to the thermal expansion. For $Le=1.5$ flames, the growth rate is small, and the unstable range is narrow for both $E=35$ and 14 due to stabilizing effects because the diffusive-thermal instability appears at $Le>1.0$ (Fig.3). When the heat loss increases, the growth rate obviously decreases, and the unstable range is narrow due to the heat expansion. Even though the Zeldovich effect is lower at sufficiently low activation energy, the growth rate still decreases due to the strengthening hydrodynamic effects in non-adiabatic flames.

Fig.4 shows the relation between the Lewis number and $D_{\text{cell}}/\lambda_c$. At $Le=0.5$, $D_{\text{cell}}/\lambda_c$ significantly increases because λ_c decreases due to the destabilization of diffusive-thermal instability appeared when $Le<1.0$. In addition, for $Le=1.5$, $D_{\text{cell}}/\lambda_c$ slightly decreases because λ_c increases due to the

stabilization of diffusive-thermal instability appeared when $Le>1.0$. Moreover, $D_{\text{cell}}/\lambda_c$ is lower when the heat loss affects the critical wavelength owing to the enhancement of hydrodynamic instability. As a result, the intensity of the intrinsic instability decreases due to the heat loss.

5.2 Cellular flame

Essentially the cellular flame is generated due to the intrinsic instability and is superimposed with the finite disturbance ($a_0=1.0$) with the critical wavelength on a planar flame. The cellular flame front is defined as the position with a maximum reaction rate. The unburned gas flows in from the left at the burning velocity of a planar flame, and the burned gas flows out to the right. The superimposed disturbance appears due to hydrodynamic instability and then the cellular flame front forms. The increase in the burning velocity is indicated by the upstream movement of the cellular flame.

For $Le=1.0$ flames, the cellular flame fronts at $E=14$ and 35 for adiabatic and non-adiabatic flames were considered. The cellular flame fronts of $E=14$ and 35 are almost the same for adiabatic and non-adiabatic flames as shown in Figs.5-6. However, a slightly upstream movement is observed. This indicates a higher burning velocity.

For $Le=0.5$ flames, Figs.7-10 show the cellular flame front at $E=14$ and 35 for adiabatic and non-adiabatic flames. When the cellular flame front forms, the flame moves upstream. This result indicates that increase in the burning velocity at $Le<1.0$ is larger compared to that of the $Le=1.0$ flames. In addition, the moving rate, namely the increase in the burning velocity, increase as the heat loss increases. In the case of $E=35$, the lateral movement of cellular flame is found for both adiabatic and non-adiabatic flames. Thus, the increase of heat loss promotes the unstable behavior of the cellular flame fronts at $Le<1.0$. Even with the small activation energy, the movement of

cellular flames of non-adiabatic flame moves upstream. This is caused by the increase in the instability intensity owing to the hydrodynamic effects.

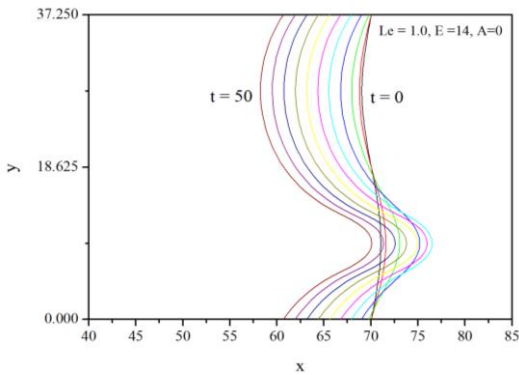


Fig.5. Cellular flame front at $Le=1.0, E=14$ for $A=0$.

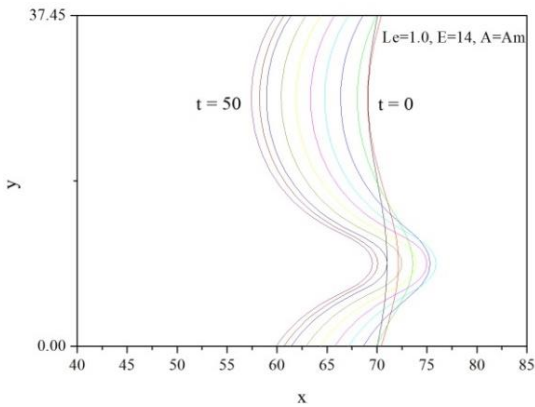


Fig.6. Cellular flame front at $Le=1.0, E=14$ for $A=Am$.

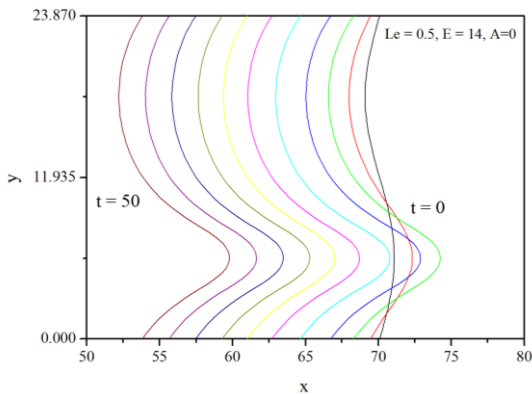


Fig.7. Cellular flame front at $Le=0.5, E=14$ for $A=0$.

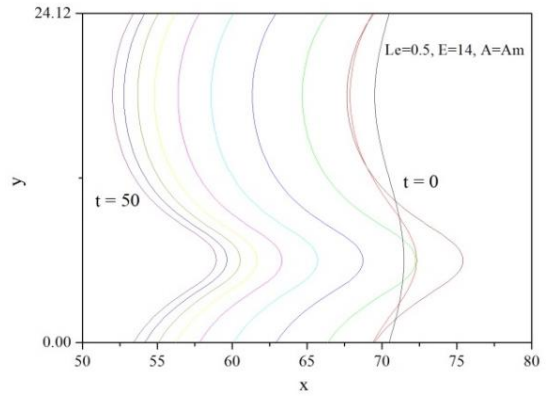


Fig.8. Cellular flame front at $Le=0.5, E=14$ for $A=Am$.

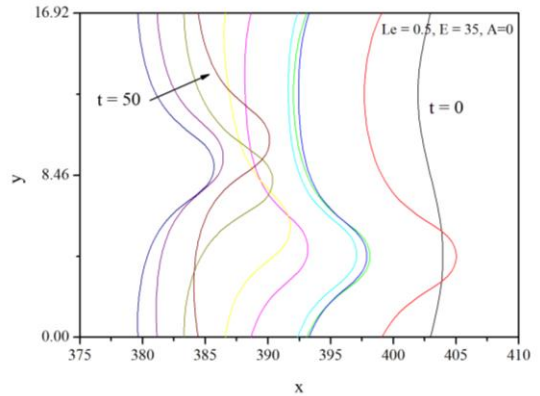


Fig.9. Cellular flame front at $Le=0.5, E=35$ for $A=0$.

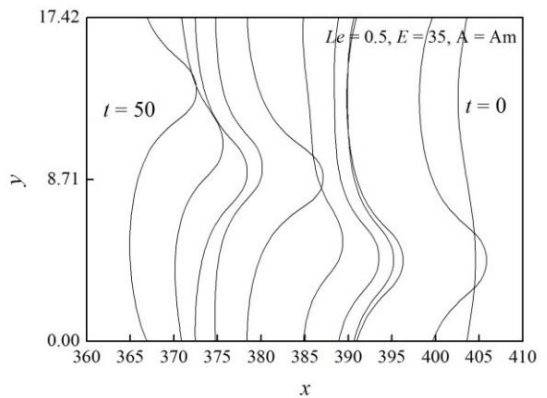


Fig.10. Cellular flame front at $Le=0.5, E=14$ for $A=Am$.

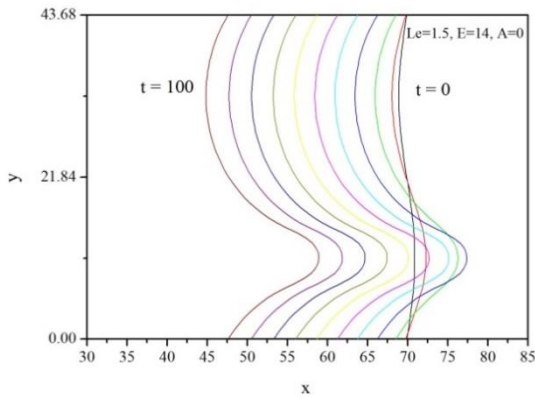


Fig.11. Cellular flame front at $Le=1.5, E=14$ for $A=0$.

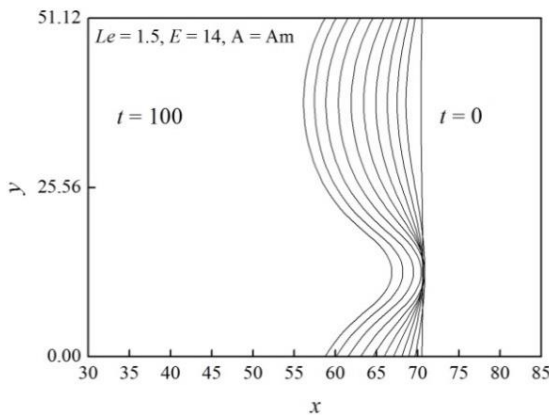


Fig.12. Cellular flame front at $Le=1.5, E=14$ for $A=Am$.

For $Le=1.5$ flames, Figs.11-12 show the cellular flame front at $E=14$ for adiabatic and non-adiabatic flames. This result shows that the decrease in the burning velocity at $Le < 1.5$ is slightly smaller compared that at $Le=1.0$. In addition, the moving rate, namely the decrease in the burning velocity increases as the heat loss increases. Even with the small activation energy, the movement of cellular flames of non-adiabatic flame moves upstream owing to thermal expansion effects.

5.3 Burning velocity

The burning velocity of a cellular flame S_{cf} , is larger than that of planar flame, which is obtained by the integrating the reaction rate throughout the computational domain then normalizing the burning

velocity of a planar flame to obtain the normalized the burning velocity S_{cf}/S_h .

Following the calculation, the relations of the Lewis number and the normalized burning velocity of cellular flames at $E=14$ and 35 for $A=0$ and $A=Am$ are obtained. The results are shown in Fig.13. The results shows the values for S_{cf}/S_h are almost the same at $Le=1.0$ for adiabatic and non-adiabatic flames. When $Le < 1.0$, S_{cf}/S_h increases for non-adiabatic flames due to the enhancement of the intrinsic instability. On the other hands, at $Le=1.5$, S_{cf}/S_h slightly decreases for non-adiabatic flames. This is because of the heat loss which has a stabilizing influence due to the intrinsic instability for $Le > 1.0$ flames.

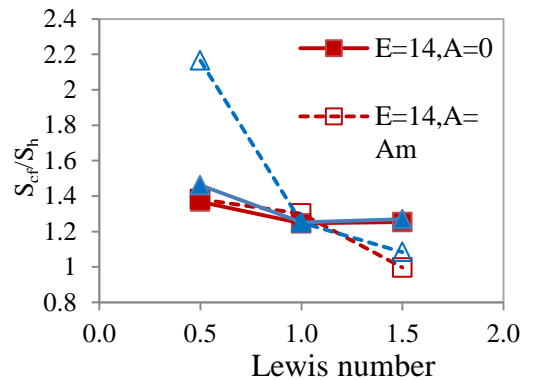


Fig.13. Relations of Lewis number and Normalized Burning velocity of Cellular flames at $E=14$ and 35 for $A=0$ and $A=Am$.

6. Conclusion

The effects of low activation energy on intrinsic instability of adiabatic and non-adiabatic cellular premixed flames studied using two-dimensional unsteady calculations of reactive flows based on the compressible Navier-Stokes equation. For the Lewis number was lower than unity ($Le=0.5$), the growth rate and the normalized burning velocity (S_{cf}/S_h) increased when the activation energy was lower for adiabatic premixed flames due to the decrease in the Zeldovich number. When the heat loss increased, the growth rate was lower and the

normalized burning velocity was higher. However, the ratio of the cell size to the critical wavelength ($D_{\text{cell}}/\lambda_c$) was smaller compared to adiabatic premixed flames. For the Lewis number equal to unity ($Le=1.0$), the growth rate and the normalized burning velocity were almost the same and slightly decreased even at sufficiently low activation energy. Moreover, the Lewis number of value higher than unity ($Le=1.5$), the growth rate and the normalized burning velocity were lower and even at sufficiently low activation energy for adiabatic premixed flames and slightly lower growth rate and lower normalized burning velocity were obtained. The results show that a lower growth rate was obtained at sufficiently low activation energy due to a decrease in the Zeldovich number. Even at low activation energy, the effects of hydrodynamic instability became higher destabilizing (stabilizing) effects for $Le<1.0$ ($Le>1.0$) when the heat loss increased due to the hydrodynamic effects.

7. Acknowledgements

The author would like to thank KMUTT for financial support, Professor KADOWAKI Satoshi from Nagaoka University of Technology for academic advisory. The author acknowledge Mr.Anupong Banchongkarn, HPC staff and National e-Science Infrastructure Consortium for providing computing resources that have contributed to the results reported within this paper.

8. References

- [1] Qin, X., Kobayashi, H., and Niioka, T., *Experimental Thermal and Fluid Science*, Vol.21 (2000), pp.58-63.
- [2] Smallbone A., Tsuneyoshi K., and Kitagawa T., *Journal of Thermal Science Technology*, Vol.1 (2006), pp.31-41
- [3] Williams F.A., *Combustion Theory*, 2nd Ed., Addison-Wesley Publishing Company, Redwood, CA, (1985), pp.349-365.
- [4] Clavin P., *Progress in Energy and Combustion Science*, Vol.11 (1985), pp.1-59.
- [5] Sivashinsky G.I., *Philosophical Transaction of the Royal Society London*, Series A., Vol.332 (1990), pp. 135-148.
- [6] Kadowaki S., and Hasegawa T., *Progress in Energy and Combustion Science*, Vol.31 (2005), pp193-241.
- [7] Kagan L., Ronney P.D., and Sivashinsky G.I., *Combustion Theory and Modelling*, Vol.6 (2002), pp.155-172.
- [8] Kaewpradap A. and Kadowaki S., *Journal of Thermal Science Technology*, Vol.2 (2007) pp.79-89.
- [9] Kaewpradap A. and Kadowaki S., *Transaction of JSASS Aerospace Technology*, Vol.8 (2010) pp.15-21.
- [10] Kaewpradap A., Maruta K., Kadowaki S., *Japan Society of Mechanical Engineers*, Vol.75/753, 2010, pp.286-291.
- [11] Thwe Thwe Aung and Satoshi KADOWAKI, *Journal of Thermal Science Technology*, Vol.8 (2013) pp.323-335.
- [12] Kadowaki S., *Combustion Flame*, Vol.143 (2005), p.174-182.
- [13] Kaewpradap A. and Kadowaki S., *Journal of FluidScience Technology*, Vol.3 (2008) pp.219-230.