Validation of a new level set approach in the counter flow premixed flame

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Abstract

The flamelet model based on the concept of local flame speed \( S^* \) is newly developed to describe a premixed flame with a finite thickness when defining \( G \) as the non-dimensional temperature. In the previous work the new flamelet model was validated by 1-D steady premixed flame successfully. In this paper the model of 3-D counter flow premixed methane-air is investigated. The local flame speed can be proposed as

\[
S^* = S_u + 2S_u(G - G_0)
\]

where the scalar \( G = G_0 \) represents the flame surface in the flamelet model. Considering the stretch effect the expression for the modified burning velocity is

\[
S_u = S_u^0 - S_u^0 \kappa L
\]

where \( S_u \) is smaller than the burning velocity of the unstretched flame \( S_u^0 \). The new flamelet model results are compared with the original \( G \)-model results in the velocity and the temperature profiles. The results are also validated by the detailed chemical reaction solution of GRI-Mech3.0 by CHEMKIN.

Key words: Flamelet model, Counter premixed flame, Stretch rate, Laminar flame speed

1. Introduction

Level set approach has been applied for the premixed flame. Scalar \( G \) can be described the flame surface (Williams,1985)

\[
\rho \frac{\partial G}{\partial t} + \rho \mathbf{u} \cdot \nabla G = \rho_\kappa S_u [\nabla G]
\]  

(1)

It is known as the conventional \( G \)-equation in the combustion literatures. Equation (1) seems simple, but it has the following critical weak points regarding the numerical solution:

1) A pure convection is generally unstable, so the calculation may have increased possibility when solved, or, if a stabilized scheme such as an upwind difference scheme is used, the effect of numerical viscosity must be considered.

2) In a one-dimensional flame, an initial profile of \( G \) is conserved in time evolution. This means that initial inappropriate profiles are conserved in the results, and any errors generated in the numerical procedures strongly affect the final solution.

For these reasons, we (2011) introduced the new concept of local flame speed and added the diffusion term, then

\[
S^* = S_u + \frac{dS^*}{dG} \bigg|_{G=G_0} (G - G_0)
\]  

(2)
\[ \rho \frac{\partial G}{\partial t} + \rho a_j \frac{\partial G}{\partial x_j} = \rho_u S^* |V| G + \rho_0 \Gamma_0 V^2 G \]  

(3)

Up to now, only freely propagating one-dimensional premixed flame has been considered.

\[ \frac{dS^*}{dG} \bigg|_{G=0.5} = S^* = \frac{8\rho_0 \Gamma_0}{\rho_a \delta} \]  

(4)

When the Lewis number, which expresses the ratio of the thermal diffusivity to the mass diffusivity, 
\[ Le = \frac{\lambda}{c_p} \text{ or } \frac{\lambda}{c_p} \]  
is assumed to be unity, then:

\[ (\lambda / c_p)_0 = \rho_0 \Gamma_0 \]  

(5)

We use the simplified transport coefficient model to get the diffusion coefficient \( \rho_0 \Gamma_0 \) as following:

\[ (\lambda / c_p)_0 = A \left( \frac{T}{T_f} \right)^{\gamma} \]  

(6)

\[ A = 2.58 \times 10^{-5} \text{ kg} / \text{m} \cdot \text{sec} \]  

At: \( T_f = 298 \text{ K} \)

For eq.(3) based on the local flame speed \( S^* \), the level-set function \( G \) not only indicates the flame front position by the iso-surface of \( G=0.5 \), but also has a physical profile in the flame thickness, which can be defined as a non-dimensional temperature \( G = \frac{(T - T_u)}{(T_b - T_u)} \). On the “conventional G-equation model” by eq.(1), this definition may give the correct value just at the flame front defined by a specified temperature \( T_0 \) (not necessary to correspond to \( G=0.5 \)), but the profile around it has no physical meaning without the additional procedures such as a re-initialization of thickness profile (Russo and Smereka, 2000) and a temperature profile model fitting it.

First the effects of the stretch need to be considered when applying 3-D counter flow case. If the strain is sufficiently small, a linear analysis (Candel and Poinsot, 1990) shows that the flame speed is reduced to \( S_u^0 \):

\[ S_u = S_u^0 - S_u^0 L \delta \]  

(5)

where \( S_u \) is the rate of propagation of the flame relative to the unburned gas, \( S_u^0 \) is the value of \( S_u \) for an unstretched (plane) flame \( (k = 0) \), \( k \) is the stretch rate. The coefficient \( L \) is a measure of the response of the flame to stretch, called the Markstein length. Naturally, it is an important issue to gain an understanding of the factors that can influence the value of the Markstein length. Kwon, et al.(1992) makes an assumption that the Markstein length is proportional to the local characteristic flame thickness, because both are representative of the scale of distance over which the diffusion of mass and heat occurs in flames. Thus, a dimensionless Markstein number is defined as following:

\[ Ma = L \delta \]  

(6)

\( \delta \) is unstretched flame thickness. The Markstein number is a physicochemical parameter that expresses the response of a flame to stretching. Neither its theoretical nor its experimental evaluation is easy, although Searby and Quinard(1990) have recently presented some experimental values. The value depends in a detailed way upon chemical kinetics and the transport properties. For a two reactant mixture with a single step reaction rate the asymptotic analysis of Clavin(1985) yields
\[ Ma = \frac{1}{\gamma} \ln\left( \frac{1}{1-\gamma} \right) + \frac{1}{2} \beta (Le-1) \int_{0}^{\frac{x}{\gamma}} \ln(1+x) dx \]  

(7)

where \( \gamma = (T_b - T_0) / T_b \), \( \beta \) is the reduced activation energy, Zel’dovich number

\[ \beta = \frac{E}{RT_b^2} (T_b - T_u) \]  

(8)

The flame stretch is defined by the fractional rate of change of a flame surface element \( A \) (Matalon and Matkowsky, 1982):

\[ k = \frac{1}{A} \frac{dA}{dt} \]  

(9)

A flame front propagating in a non-uniform flow is subject to strain and curvature effects which lead to changes in the flame area. These changes are measured by stretch. The curvature is 0 in the counter flow premixed flame and the stretch rate is only considered. In counter flow, the stretch rate can be calculated by

\[ k = -\frac{du}{dx} \]  

(10)

When considering the stretch effect, the laminar flame speed changed with the different \( Ma \) number. Table 1 shows the different Makerstein number in different experimental set up when the equivalence ratio equal to 0.6. When assuming \( Le \approx 1 \), by Eq.(7) the \( Ma = 2.04 \) can be obtained. In the table 1, there are different values about \( Ma \) number when equivalence ratio equal to 0.6. These values are categorized two groups, one represents large values more than 2 and the other represents small values nearly to 0. In this research the values of \( Ma = 2.04 \) and \( Ma = 0 \) are chosen as the representations of two groups. Excluded the experiment difficulties the difference by previous researchers may depend on the position of the flame front measuring the flame speed, which varies in the non-uniform convection velocity field. Our new model has a good merit that local flame speed is introduced to describe the whole region profile in the flame thickness, which can globally match to the profile of velocity. The results show that the new G-equation predicts a good enough matching profile when \( Ma = 0 \) rather than \( Ma = 2.04 \).

<table>
<thead>
<tr>
<th>Researchers</th>
<th>Data method</th>
<th>Ma [-]</th>
<th>Makerstein length</th>
</tr>
</thead>
<tbody>
<tr>
<td>Clavin (1985)</td>
<td>Calculation</td>
<td>2.04</td>
<td>0.00047</td>
</tr>
<tr>
<td>Davis (2002)</td>
<td>Calculation</td>
<td>2.98</td>
<td>-</td>
</tr>
<tr>
<td>Davis (2002)</td>
<td>Consumption velocity</td>
<td>0</td>
<td>-</td>
</tr>
<tr>
<td>Nakahara (2005,2011)</td>
<td>Experiment</td>
<td>0.5</td>
<td>-</td>
</tr>
<tr>
<td>Searby (1990)</td>
<td>Experiment</td>
<td>2.76</td>
<td>-</td>
</tr>
</tbody>
</table>
Nomenclature

\( G \): flame index parameter (unitless)

\( k \): stretch rate (1/sec)

\( Le \): Lewis number (unitless)

\( S_\infty \): laminar flame speed (m/s)

\( S^* \): local flame speed (m/s)

\( u \): flow velocity (m/s)

\( T \): temperature (K)

\( \beta \): the reduced activation energy

\( \delta \): flame thickness (m)

\( \lambda \): thermal conductivity (W/m·K)

\( \rho \): density (kg/m³)

\( \Gamma \): diffusion coefficient (m²/s)

\( \phi \): equivalence ratio (unitless)

\( \gamma \): \((T_b - T_0)/T_b \) (dimensionless)

\( L \): a measure of the response of the flame to stretch (unitless)

\( A \): flame surface element (unitless)

\( \xi \): the mixture fraction (unitless)

Subscripts:

\( b \): burned state

\( u \): unburned state

\( 0 \): flame surface state

2. Numerical set up

Previously Smooke, et al. (1991) investigated the structure and extinction of counter flow premixed methane-air flames in the fresh reactant-hot product configuration. Here we referred the experimental set up to reach our goal. We slightly changed the physical condition that the burned gas temperature is higher than the experimental set up. The characteristic scale lengths are drawn in the figure 1. Fig.1 shows the result of the experiment set up. The burned configuration is such that methane and air are introduced as reactant from the lower duct the exit diameter \( D \) of which is 0.02314 m. The separation distance \( L \) between the ducts is 0.01486 m. The upper duct’s diameter is also 0.02314 m. The burned gas is introduced at the entrance of upper duct. The products of combustion of this flame are used to stabilize the counter flow premixed flame in the region between the upper duct and the lower duct. The unburned gas temperature is 300 K and the burned gas temperature is 1680 K which is higher than the experimental boundary condition. The temperature 1680K is determined by the equilibrium calculation by CHEMKIN where the equivalence ratio is 0.6. Accordingly we slightly changed the boundary condition at the upper side the temperature is increased as the burned temperature in order to validate our new level set approach. The velocity of the burned gas is 2 m/s and the unburned gas is 1.14 m/s, which are referred by the experiment. The fuel lean case is applied where the equivalence ratio is 0.6. Because the boundary condition is changed, we could not compare our numerical result...
with the experimental result. Here we referred the CHEMKIN results of counter flow case by using the same boundary condition to compare our results.

![Image](image_url)

**Figure 1** The experimental set up

In this paper, the axial direction along the central line is defined as the x-direction. To conduct the present numerical simulation, the CFD code “Frontflow/red ver.3.1” is modified to allow the installation of the new level set approach. The code is based on the SMAC/SIMPLE algorithms and the Finite Volume Method with an unstructured grid system. The computational grid system in the present calculation consists of about 993555 cells. The Euler implicit scheme is applied for the time integrations of the governing equations. The time increment is set to 1.0×10⁻⁵ sec. The cell size is set to 1.0×10⁻⁶ m. A convection term in the momentum equation is discretized by a 1st order upwind convection scheme and the 2nd order central difference is also validated.

3. Flamelet data

In the flamelet approach, the temperature, density and the chemical components of the burned mixture are determined by the constant value of the mixture fraction $\xi$ in the pure premixed flame. The flamelet database for the present calculations is constructed from the results of chemical equilibrium simulations using a detailed chemical reaction system. The simulations are conducted on the commercial software CHEMKIN (Kee, 2004) with the thermodynamic data provided in Gri-Mech 3.0. For the laminar flame speed, which also depends on the chemical components of the premixed gas and thus depends on the constant value of the mixture fraction in the premixed flame, one-dimensional of a freely propagating flame in a uniform premixed gas is calculated.

4. Results and discussion

To more clearly explain the results, the following table shows the differences of the figures’ labels.

<table>
<thead>
<tr>
<th>Table 2: The differences of the labels</th>
</tr>
</thead>
<tbody>
<tr>
<td>Conventional model $Ma=0$ (simplified conventional model)</td>
</tr>
<tr>
<td>Conventional model $Ma=2.04$</td>
</tr>
<tr>
<td>New model $Ma=0$ (simplified new model)</td>
</tr>
<tr>
<td>New model $Ma=2.04$</td>
</tr>
</tbody>
</table>

When $G$ is defined as the non dimensional temperature, the temperature can be estimated by calculating scalar $G$. First the profiles of the new model with the time step are shown in Fig.2. From the results, the profile rapidly
converges to the plane flame. Along the central position, the temperature is plotted with different time steps. From Fig.3, the temperature rapidly converges into the same profile as that formed in the stagnation surface.

**Time = 0.005 s**

![Image](image1.png)

**Time = 0.01 s**

![Image](image2.png)

**Time = 0.025 s**

![Image](image3.png)

**Time = 0.15 s**

![Image](image4.png)

**Figure.2** Temperature profiles for various times calculated by using the new model
Figure 3 The temperature profile along the central line

The temperature was also calculated by calculating the conventional $G$-equation when treating $G$ as non-dimensional temperature; the second central difference convection term was also applied in the convection term. The pure convection term has a non-physical profile. On removing the numerical diffusion by applying the second central difference, the profile becomes more unstable than that calculated by using the first-order upwind scheme shown in Fig.4. The conventional $G$-equation was also calculated by the first-order upwind scheme. When the upwind scheme was applied in the conventional $G$-equation, the profile diverged. The upwind scheme does not include physical diffusion and includes only the numerical diffusion. The numerical diffusion, which is not constant, depends on the flame velocity. In Fig.5, near the stagnation point the velocity is very low and, as a result, the numerical diffusion is also very low. The temperature instability appears at the stagnation point which shows a hump.

Figure 4 Temperature calculated by the conventional $G$-model with the second central difference

Figure 5 Temperature calculated by using the old $G$-model with a first-order upwind
Furthermore, we also calculated conventional $G$-equation by using a second-order upwind in the convection term, and the results were similar to those for the first-order upwind scheme shown in Fig. 7. In contrast, the new $G$-equation’s results are stable regardless of which central difference scheme or first-order upwind scheme was applied in the convection term. Figures 2 and 8 show the identification between the two different schemes.

**Figure 6** Velocity profile by using the conventional $G$-model with a first-order upwind

**Figure 7** Temperature calculated by the conventional $G$-model with the second-order upwind scheme

**Figure 8** Temperature calculated by the new $G$-model with a second-order central difference

Figure 9 shows the velocity profile calculated by means of the new $G$. In terms of the coupling with the stagnation point along the central line in Fig. 10, the results from the new model result are identical with those by CHEMKIN. The results calculate by conventional model in the center part are not identical with those by CHEMKIN. Also the conventional model’s trend does not agree with other results. Figure 11 compares the temperature profile calculated by the new $G$-equation and the CHEMKIN result based on the stagnation point; these results show the excellent agreement with one another. By watching Fig.12, the flame position defining at $G=0.5$ is predicted by all models (both new and conventional models) in the same position and agree with that by CHEMKIN. It indicates that in the flame case (equiv. ratio is 0.6), the stretching velocity gives little effect ($Ma~0$) to the “flame speed defined at the center of flame thickness ($G=0.5$)”, where the all model give the same “flame speed” in the model formulation by eq.(1) and (3). Figure 12 compares the temperature distributions calculated by the various models. Only the new model produces a high degree of similarity with the CHEMKIN results.
Figure 9 The velocity profile calculated by means of the new $G$-equation

Figure 10 Comparison of velocities calculated by the new model with the results by detailed reaction

Figure 11 Comparison of temperatures calculated by the new model with the results from CHEMKIN

Previous results are based on the unstretched flame speed which means $Ma = 0$. When considering the flame-stretch effect, we compared two results, one for a Makerstein number of 2.04 and the other for a Makerstein number of 0; the latter value is same as that for the unstretched flame speed. We also compared the results of applying the new model and the conventional model. Figure 13 shows the temperature distribution for $Ma = 2.04$ calculated by using the conventional model. Because of the effect of the $Ma$ number, the flame speed is lower than that at $Ma = 0$, the diffusion effect is accordingly low, and the distribution still shows an instability. The new model shows stability however (Fig. 14). Figures 15 and 16 show the velocity and temperature profiles, respectively, along the central line. When the temperature is calculated by the new model, coupling with the stagnation point, it is obvious that in the case of $Ma = 0$ the result shows better agreement with the CHEMKIN results than in the case of
Ma = 2.04. Furthermore, Figures 17 and 18 also show the similar conditions to those calculated by the conventional model.

![Temperature comparison for various models](image)

**Figure.12** Temperature comparison for various models

In counter flow the flame speed is defined as the minimum velocity point in the velocity distribution, so the flame speed can be obtained at that point in our simulations listed in the table 3. From the result the new G without stretch is very near the detailed reaction which means the new G includes the effect of stretch directly.

Table 3 Flame speed by different models.

<table>
<thead>
<tr>
<th>Flame speed (1-D plane flame)</th>
<th>0.11m/sec</th>
</tr>
</thead>
<tbody>
<tr>
<td>Flame speed (detailed reaction)</td>
<td>0.27m/sec</td>
</tr>
<tr>
<td>Flame speed (conventional model Ma = 0)</td>
<td>0.18m/sec</td>
</tr>
<tr>
<td>Flame speed (conventional model Ma = 2.04)</td>
<td>0.11m/sec</td>
</tr>
<tr>
<td>Flame speed (New model Ma = 0)</td>
<td>0.25m/sec</td>
</tr>
<tr>
<td>Flame speed (New model Ma = 2.04)</td>
<td>0.21m/sec</td>
</tr>
</tbody>
</table>

![The temperature distribution for Ma = 2.04](image)

**Figure.13** The temperature distribution for Ma = 2.04 calculated by using the conventional model
Figure 14 The temperature distribution for $Ma = 2.04$ calculated by using the new model

Figure 15 The velocity profiles for various values of $Ma$ calculated by using the new model

Figure 16 The temperature profiles for various values of $Ma$ calculated by using new models
Figure 17 Velocity profiles for various values of $Ma$ calculated by using the conventional model

Figure 18 Temperature profiles for various values of $Ma$ calculated by using the conventional model

5. Conclusions

In this paper, the stretch effect is considered and the strained premixed methane–air flames is studied in the fresh reactant–hot products configuration. Using CHEMKIN results as a basis, the various models for the lean-fuel case is compared and the following results are obtained:

1) The conventional $G$-equation was once more shown to demonstrate instability, regardless of which central-difference or upwind scheme is applied in the convection term.
2) The new level-set approach shows stability and gave results in excellent agreement with those from CHEMKIN.
3) The good prediction of the temperature profile in the flame that we obtained shows not only the flame surface, but also the entire flame distribution.
4) When considering the flame stretch effect, the speed of a stretched flame is lower in the case of $Ma = 2.04$ than the case of $Ma = 0$. Accordingly, the case of $Ma = 0$ shows better agreement with the one of the detailed reactions calculated by means of CHEMKIN.
Acknowledgements

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References


