# Application of the Flame Hole Dynamics to a Diffusion Flame in Channel Flow

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The method of flame hole dynamics is demonstrated as a mean to simulate turbulent flame extinction. The core of the flame hole dynamics involves derivation of a random walk mapping for the flame holes, created by local quenching, between burning and quenched states provided that the dynamic characteristics of flame edges is known. Then, the random walk mapping is projected to a background turbulent field. The numerical simulations are carried out with further simplifications of flame string and unconditioned scalar dissipation rate. The simulation results show how the chance of partial quenching is influenced by the crossover scalar dissipation rate. Finally, a list of improvements, necessary to achieve more realistic turbulent flame quenching simulation, are discussed.

**Key Words :** Turbulent Flame Extinction, Flame Edge, Flame Hole Dynamics, Random Walk, Partial Quenching

## 1. Introduction

Extinction of flame is one of the most nonlinear physical processes in the nature. For ordinary flames with overall activation energy much greater than thermal energy contained in flames, their extinction conditions can be described by the bifurcation condition corresponding to the turning point of the quasi-steady flame response curve. The conditions at the turning points enable us to calculate the fluid dynamic conditions at extinction. Since the extinction condition corresponds to a subcritical bifurcation condition, the accessible solution branches at extinction are not continuous and extinction occurs in an abrupt manner (Williams, 1985). However, this perspective is valid only to laminar flames, but not necessarily true for turbulent flames.

Turbulent flames are widely viewed as an ensemble of laminar flamelets, so that local extinction behavior in turbulent flames is almost similar to that of laminar flames. However, their collective behavior, that can be recognized by global extinction of turbulent flame, could be quite different from extinction of each local laminar flamelet. Turbulent flame is in general subject to random fluctuations of the characteristic flow time with a rather wide dynamic range. Since each flamelet undergoes a distinct random walk process between the extinction and burning states, it is natural to anticipate that extinction of tur-

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bulent flame occurs in a much more gradual manner. Consequently, the average flow dynamic condition at global extinction differs from that of the laminar flame extinction and identification of the turbulent extinction condition is not a simple task either.

The core element to the statistical description of turbulent flame extinction is the random walk process between the reacting and nonreacting states and one of such random walk models is the flame hole dynamics, proposed by Dold and Hartley (1991)[1]. The flame hole dynamics is based on the theory of flame edge, a structure existing at the boundary between the reacting and nonreacting states. Flame edges are capable of propagating to either burnt or fresh mixture side depending on the flow condition imposed on the edge. Consequently, the flame edge plays a role of controlling the expansion or contraction of flame holes created by local quenching of laminar flamelets. If the random walk process derived from the flame edge dynamics is simulated for a given background turbulent flow condition, the gradual transition of turbulent flame from a burning state to the quenched state can be obtained.

The flame edge has been one of the hottest recent research topics in the combustion community (Buckmaster, 2002 ; Nayagam and Williams, 2002). However, its full potential to describe turbulent flame extinction is not appreciated even though turbulent extinction is where the flame edge theory should be eventually applied. It is thus the aim of the present paper to demonstrate how the flame hole dynamics model is applied to the simulation of turbulent flame extinction, which has not been fully understood by the general combustion community. Since this paper is only the beginning of the following developments in the simulation technique to describe turbulent flame extinction, a model, that is rather oversimplified to be realistic, is employed while the essence of the physical and mathematical process leading to turbulent flame extinction is preserved. In the next section, the basic concept of the flame hole dynamics is introduced. Then, the turbulent flow, that serves as a background to the turbulent flame dynamics, is presented. Finally, the flame hole dynamics is applied to the turbulent flow field, obtained by DNS, to demonstrate the description of partial quenching behavior in turbulent combustion, and the future improvements of the flame hole dynamics to achieve more realistic simulation will be discussed.

## 2. Basic Concept of the Flame Hole Dynamics

In this section, the basic concept of the flame hole dynamics is introduced. The flame hole dynamics consists of two elements, namely the flame edge dynamics and random walk mapping of flame edge.

As mentioned in the introduction, flame edge is the structure that exists at the boundary of reacting and frozen surfaces. Since the iso-scalar surface, that flame is supposed to be located, is a two dimensional structure and flame edge is the boundary to its quenched part, the flame edge is the one-dimensional structure existing at the boundary of flame holes. Since the flame edge is the dynamic structure controlling random variation of flame holes, the dynamic behavior of flame edge is first introduced.

For flames with Lewis number sufficiently close to unity, their edges typically behave as what is outlined in Fig. 1, showing variation of the flame temperature as a function of the Damkohler number (or the inverse of the scalar dissipation rate, $\chi^{-1}$). The scalar dissipation rate, denoted by $\chi$, will be used as the primary variable to define the characteristic diffusion time hereafter. The quasi-steady response of the flame temperature with respect to the characteristic diffusion time, proportional to $\chi^{-1}$, shows its typical S-shaped response curve. The turning point at the intersection of the upper and middle branches is the quasi-steady extinction condition whereas

1) Dold and Hartley have never published any paper describing the flame hole dynamics except the PhD thesis of Hartley. However, an introductory paper on the flame hole dynamics is published in the journal of Korean Combustion Society in Korean (Kim, 2001).

the turning point at the intersection of the lower and middle branches is the quasi-steady ignition condition. Initial flame holes can be formed where the local scalar dissipation rate exceeds the extinction scalar dissipation rate, denoted by $\chi_E$, perhaps for a period longer than the characteristic diffusion time. Once a flame hole is formed, its edge begins to control the fate of the flame hole.

The flame edge is usually weaker than the ordinary flames at the same scalar dissipation rate because the flame suffers an extra heat loss from the edge. Consequently, near extinction condition, the flame hole will expand to create even a greater quenching hole by retreating the edge toward the reacting surface. As the scalar dissipation rate decreases, the flame edge becomes strengthened to withstand the heat loss and to decrease its retreating speed. Eventually, at a critical scalar dissipation rate, called the crossover scalar dissipation rate denoted by $\chi_C$, the flame edge changes its direction of propagation to the quenched side so as to contract the flame hole. If the scalar dissipation rate is further decreased, the advancing speed continuously increases till it reaches an asymptotic value. It is conjectured that the asymptotic value for the propagation speed of edge's ignition front corresponds to the laminar flame speed times the square root of the ratio of the unburnt mixture density to the burnt gas density (Reutsch et al., 1995) even though it is not theoretically proved yet.

It must be noted in Fig. 1 that there exists a metastable region between the extinction scalar dissipation rate and the crossover scalar dissipation rate. In the metastable region, a section of flame surface is either in a burning state or in a quenched state depending on the combustion state in the neighboring flame surface segment. Because of this duality of the combustion state in the metastable region, we need to clearly define the response mapping of flame edges to the scalar dissipation rate fluctuation, and the response mapping is the second core element of the flame hole dynamics.

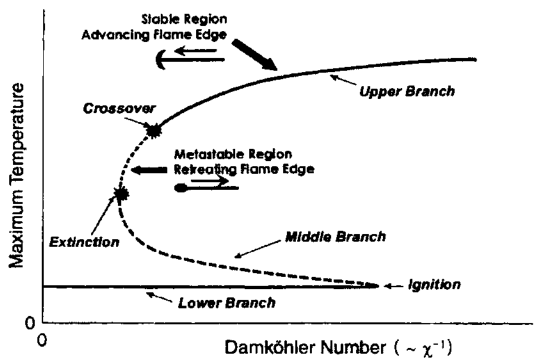
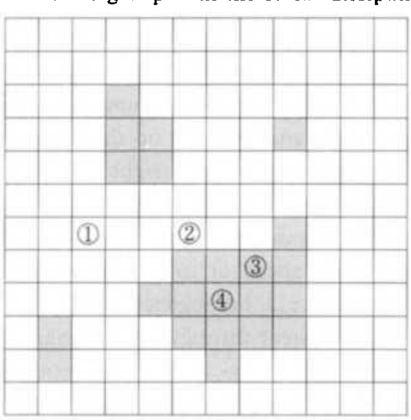



**Fig. 1** Schematic diagram for the response characteristics of flame and its edge with respect to the scalar dissipation rate

**Table 1** The classification of the flame groups where the shaded grids correspond to the quenched sectors and the white grids correspond to the reacting sectors, and the flame hole random walk mapping for each flame group with the scalar dissipation rate




| Flame Group | Scalar Dissipation Rate | Burning State |
|---|---|---|
| ① | $\chi > \chi_E$ | Quenching |
| | $\chi < \chi_E$ | Burning |
| ② | $\chi > \chi_C$ | Quenching |
| | $\chi < \chi_C$ | Burning |
| ③ | $\chi > \chi_C$ | Quenching |
| | $\chi < \chi_C$ | Burning |
| ④ | $\chi > \chi_I$ | Quenching |
| | $\chi < \chi_I$ | Re-Ignition |

The flame edge response mapping is shown in Table 1. The virtual flame surface, the surface corresponding to the iso-scalar surface of the stoichiometric mixture fraction, can be divided by a grid system to give an identification to each virtual flame surface sector. Each virtual flame sector can be first classified into the flame sector or quenched sector depending on whether reaction takes place or not. However, when their boundary conditions are taken into account, the virtual flame sectors can be further classified by four groups, namely the group 1 through group 4. The group 1 is the flame surface group, in which the periphery of a flame sector is completely surrounded by the reacting flame sectors, while the group 2 is the group of flame sectors bordering with at least one quenched sector. On the other hand, the group 3 is made of the quenched sectors bordering with at least one flame sector, while the group 4 is the group of quenched sectors completely surrounded by the quenched sectors.

For the flame sectors in the group 1, the random walks between the flame and quenching sectors are controlled by local extinction of the flame sector, so that the flame sector remains as a flame sector if the local scalar dissipation rate is smaller than the extinction scalar dissipation rate. Otherwise, the flame sector will be quenched. On the other hand, in the quenched sectors in the group 4, the random walks are controlled by local ignition and the critical value controlling on-or-off of the quenched sectors is the ignition scalar dissipation rate. For the sectors in group 2 and 3, the random walks are controlled by the crossover scalar dissipation rate. If the scalar dissipation rate is greater than the crossover value, the burning sectors adjacent to the flame hole boundary will be quenched by the retreating flame edge, whereas the quenched sectors adjacent to the hole boundary can return to the burning state if the scalar dissipation rate is smaller than the crossover value.

As outlined in the flame hole dynamics mapping in Table 1, the chance of being in a reacting state for laminar flamelets in turbulent flame is influenced not only by the extinction condition, but also by the crossover condition determining the direction of flame edge propagation.

## 3. DNS of Fuel-Oxidizer Channel Flow

In order to apply the flame hole dynamics to the turbulent flame quenching phenomenon, it is necessary to prepare the background turbulent flow and mixing fields to provide a random sequence of the scalar dissipation rate to each flame sector. For the present investigation, the flow field and mixture fraction field are obtained by a direct numerical simulation technique. The governing equations are integrated in time using a semi-implicit scheme. A low-storage three-sub-step, third order Runge-Kutta scheme (Spalart et al., 1991) is used for treating convective terms explicitly and a second order Crank-Nicolson scheme is used for treating the viscous terms implicitly. All spatial derivatives are approximated with the second order central difference scheme. At the downstream exit, the convective boundary condition is used to allow the vortical structures to leave the domain smoothly. Detailed numerical algorithms are described in Na and Moin (1998) and Na (2001, 2003).

The mixing channel is configured in terms of the half channel width $h$. In the streamwise direction, denoted by the $x$-direction, the calculation domain is set to be $0<x/h<10$. The vertical $y$-direction extends from $y/h=0$ to $y/h=2$, where the wall boundary condition is imposed at the lower and upper walls located at $y/h=0$ and 2. At the center of the y-direction, i.e. $y/h=1$, is the splitter plate, extending up to $x/h=0$, that separates the fuel and oxidizer stream. On the other hand, the transverse depth is assigned for $0<z/h<5$ with the periodic boundary condition. The Reynolds number based on the inlet friction velocity and a half channel height is 135 and the calculation domain is discretized by a $64\times64\times64$ grid system. A snapshot of the simulated turbulent flow field, sliced at $z/h=2.5$, is shown in Fig. 2(a), where a homogeneous turbulence is seen to be persistent throughout the channel.

If the Lewis numbers of fuel and oxidizer are assumed to be unity, the mixing of fuel with

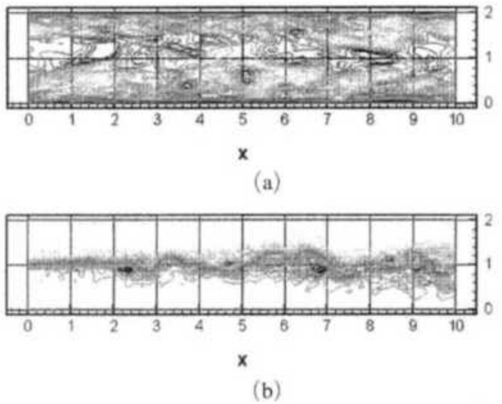



**Fig. 2** Snapshots for the DNS results ; (a) turbulent flow field represented by the contours of the streamwise velocity and (b) turbulent mixing field in terms of the mixture fraction

oxidizer can be formulated in terms of the mixture fraction defined as

$$Z=\frac{Y_F-Y_O+Y_{O0}}{Y_{F1}+F_{O0}} \tag{1}$$

where $Y_{F1}$ and $Y_{O0}$ are the fuel and oxidizer concentrations at their inlets, respectively. To the leading order approximation, the fuel and oxidizer are completely consumed at the reaction sheet, at which the mixture fraction takes a specific value, namely the stoichiometric mixture fraction $Z_{st}$ defined as

$$Z_{st}=\frac{Y_{O0}}{Y_{F1}+Y_{O0}} \tag{2}$$

The unsteady, convective-diffusive balance of the mixture fraction can be directly solved with the background turbulent flow field to yield the corresponding turbulent mixing field. From the definition of the mixture fraction in Eq. (1), the applicable boundary condition at the inlet, i.e. at $x/h=0$ becomes

$$Z=\begin{cases} 1 \text{ for } y/h>1 \\ 0 \text{ for } y/h<1 \end{cases} \tag{3}$$

while the gradient of the mixture fraction is imposed to be zero at the wall boundaries. A snapshot of the mixture fraction field corresponding to the flow field snapshot in Fig. 2(a) is given in Fig. 2(b). From the end of the splitter plate located at $x/h=0$ and $y/h=1$, a turbulent mixing layer begins to develop as fuel and oxidizer is mixed in the downstream direction. In addition, the large scale eddy structures first appear near $x/h=2.5$ and persist throughout the downstream direction.

## 4. Simulation of the Flame Hole Dynamics

### 4.1 Simplifications of the problem

In order to demonstrate how the flame hole dynamics works, further extreme simplifications are introduced while not sacrificing the essence of the flame hole dynamics model.

First the flame surface, anchored at the end of the splitter plate, is assumed to be extending downstream along the center surface of $y/h=1$. In general, the flame surface is located at the iso-scalar surface of the stoichiometric mixture fraction $Z_{st}$. Since the mixture fraction itself is a turbulent quantity, the flame location also fluctuates. Under such condition, it is quite difficult and expensive, even if doable, to track the flame surface in order to calculate the turbulent quantities conditioned at $Z_{st}$. Even the conditioned moment closure model uses the turbulent quantity evaluated at the average mixture fraction instead of the instantaneous stoichiometric mixture fraction (Klimenko and Bilger, 1999). In this paper, we are concerned with a case of $Z_{st}=0.5$, and the turbulent quantity, namely the scalar dissipation rate, will be evaluated at its average location, i.e. the center plane, instead of the instantaneous location.

In addition, the flame is assumed to be a string instead of a surface by replacing the $z$-direction variation for time variation. Then, each $x$-$y$ plane data set forms a separate two-dimensional realization of the background turbulence. By doing so, the expense to generate the background turbulent information is dramatically reduced. Since 64 grid points are used in the $z$-direction, we have a sequence of 64 scalar dissipation rate vectors that also has a size of 64 $x$-direction components. Once the 64 scalar dissipation rate vectors are used up, they will be used again in a periodic manner to make up a larger sequence of scalar dissipation rate vectors. In this paper, we used 1200 scalar dissipation rate vectors. Here it must be noted that the $z$-direction turbulent variation is homogeneous. Therefore, it will have some resemblance with time variation even though it is not fully turbulent but periodic with 64 random sequences. Since the initial condition is random, the subsequent flame variation is likely to remain random. Nonetheless it is not clear that the flame hole variation will eventually be attracted to a limit cycle. Under this flame-string simplification, the flame group is determined by considering only two neighboring flame grids instead of four neighboring flame grids for the case of flame surface. Apart from this difference, the flame hole random walk mapping is not altered at all.

### 4.2 Characteristics of the scalar dissipation rate

For the flame string located along the centerline of the mixing layer, the scalar dissipation rate is defined as

$$\chi=\nabla Z\cdot\nabla Z=\frac{\partial^2 Z}{\partial x^2}+\frac{\partial^2 Z}{\partial y^2} \tag{4}$$

Then we can sample 64 scalar dissipation rate vectors, whose length is also 64. Figure 3 shows the statistical behavior of the scalar dissipation rate as a function of the $x$-direction grid point. It is seen from the figure that the average of the scalar dissipation rate decreases monotonically in the downstream direction whereas its standard deviation shows a non-monotonic behavior. In particular, the standard deviation becomes saturated around $x/h=3$, near which the first large scale mixing eddy is formed, and remains rather invariant thereafter.

The characteristics of the PDF for the scalar dissipation rate is shown in Fig. 4, where the PDFs of the scalar dissipation rates at $x/h=4$ and 8 are plotted. Comparing the both plots, we can easily notice that the PDF at the downstream has a greater chance to stay in a low scalar dissipation region. This is perhaps caused by the fact that the viscous dissipation decreases the average scalar dissipation rate in the downstream while its standard deviation remains almost constant because of the large scale eddy motion.

In this subsection, the basic statistical properties of the scalar dissipation rate is examined.

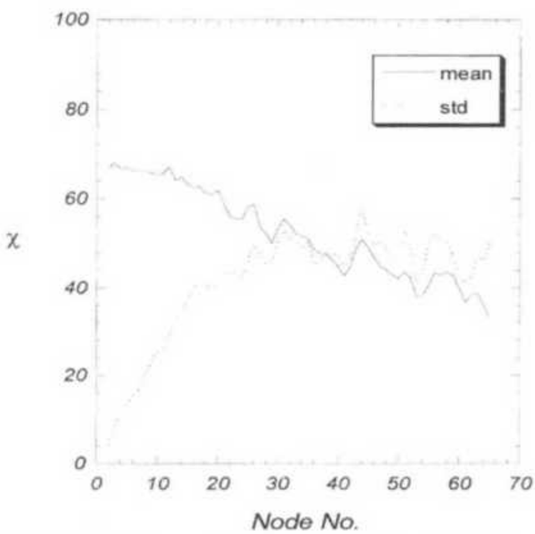



**Fig. 3** Variations of the average scalar dissipation rate and its standard deviation with the $x$-direction node number

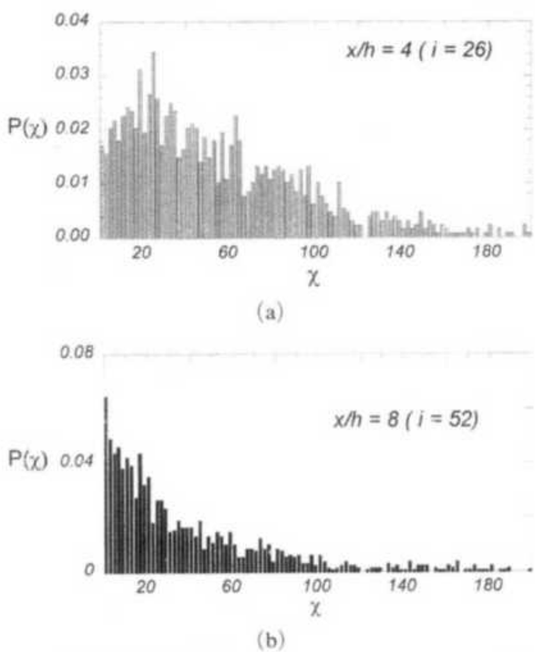



**Fig. 4** Probability density functions for the scalar dissipation rate (a) at $x/h=4$ and (b) at $x/h=8$

However, the statistical behavior is not sufficiently smooth since the number of sampling is limited. The better statistical properties can be obtained if larger turbulent flow data are available and a new DNS is currently being conducted to prepare the large turbulent flow data in a mixing layer.

### 4.3 Simulation of partial quenching in turbulent flame string

Prior to carrying out simulations of the flame hole dynamics, the critical values for the scalar dissipation rate must be specified. In this simulation, we first exclude annihilation of the flame holes by re-ignition of the flame group 4. The ignition Damkohler number is usually several orders of magnitude greater than the extinction Damkohler number, so that re-ignition is an event which seldom occurs unless there exists a special circumstance to add a significant amount of heat flux into the unburnt mixture. Therefore, we only need to specify the extinction and crossover scalar dissipation rates, and the events of turning on the reaction in quenched sectors can be realized only by advance of flame edges.

Figure 5 is a realization of the flame hole dynamic simulation, where the extinction scalar dissipation rate is assigned to be $\chi_E=90$ and the crossover scalar dissipation rate is assigned to be $\chi_C=50$. Considering the experimental results on the extinction strain rate and the crossover strain rate, measured by Shay and Ronney (1998), a factor of 2 difference in their values seems to be realistic even if only a limited amount of the experimental and theoretical results are available up to date. The horizontal coordinate is the initial 160 Lagrangian time steps among 1200 time steps taken in the numerical simulation. The vertical coordinate shows the reaction status by colors, where the red parts are the burning segments and blue parts are the quenched segments in the flame string. Therefore, we can observe random walks of the flame holes created in the flame string evolving in the time coordinate.

In the simulation, the initial flame holes are created by local quenching. Then, the holes randomly repeat on-or-off status by turbulent fluctuations of the scalar dissipation rate. It is apparent from Fig. 5 that the chance of partial quenching is much greater near the splitter plate than in the downstream region. In addition, the size of flame hole is greater near the splitter plate. The typical passage time, which measures the time scale to return to the burning state from excursion to the quenched state, appears to be about 10 Lagrangian time steps.

Figure 6 shows the variations of the burning fraction with the crossover scalar dissipation rate while the extinction scalar dissipation rate is fixed. Particularly near the splitter plate, the burning fraction is very sensitive to the crossover scalar

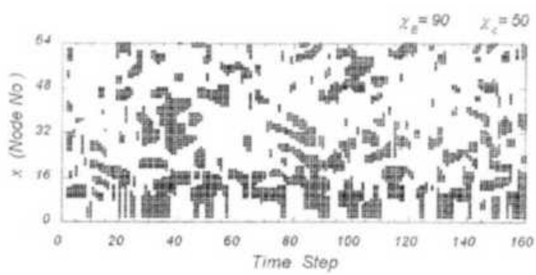



**Fig. 5** Lagrangian evolution of the holes in the flame string for $\chi_E=90$ and $\chi_C=50$. The shaded grids are the quenched flame sectors

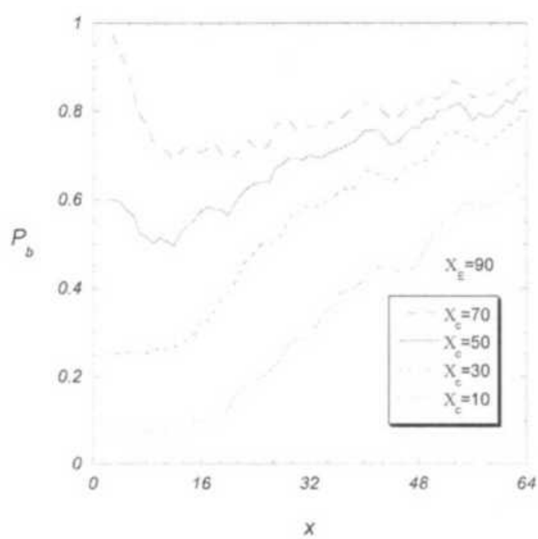



**Fig. 6** Variations of the partial burning ratio as a function of $x$ for various values of the crossover scalar dissipation rate

dissipation rate. Such dependence is perhaps caused by the fact that the crossover scalar dissipation rate controls the expansion of the flame holes while the extinction scalar dissipation rate is more responsible to the initial creation of the holes.

## 5. Concluding Remarks

The method of flame hole dynamics is demonstrated as a mean to simulate turbulent flame extinction, which controls many practical combustion phenomena such as flame lift off or blow off. The core of the flame hole dynamics is the random walk mapping for the flame holes hopping between the burning and quenched states for a specified dynamic characteristics of flame edges. Then, the random walk mapping is projected to a background turbulent field, obtained by the direct numerical simulation for a channel mixing layer. The numerical simulations are carried out with further simplification of flame string and unconditioned scalar dissipation rate. The simulation results show how the chance of partial quenching is influenced by the crossover scalar dissipation rate as well as by other statistics of the turbulent flow.

Even though the present paper is concerned with demonstration of how the flame hole dynamics works in turbulent combustion, it is apparent that the current simulation technique needs significant improvements to achieve more realistic simulations of turbulent flame quenching. The main improvements that the authors plan to develop in the future research are listed below according to their technical difficulties.

(1) More realistic background turbulent flow field is needed and a larger DNS is currently being carried out.

(2) The flame string assumption should be released to carry out the flame hole dynamics for the flame surface.

(3) The flame hole dynamics should be imposed on the instantaneous reacting surface instead of the surface located on the unconditioned average stoichiometric mixture fraction.

(4) The finiteness of the flame edge propagation speed needs be included to replace the assumption of infinitely fast flame edge response.

(5) Influences of the density variation by combustion heat release need be included to take into account the turbulence property modification by temperature increase.

Including all the above effects will take a rather extensive research efforts as well as long research period. However, it will be a worthwhile effort to make a realistic physical modelling to the phenomenon of turbulent flame extinction.

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