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Analysis of Turbulent Flames of Wildfire using Direct Numerical Simulation – Implication for
Development of Predictive Capability of Wildfire Behavior

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Abstract

Wildland fire has been studied for extreme or intense fire behavior. Researchers have tried to advance the capability to predict such a behavior through physically based models. Gaseous products released during high temperature pyrolysis of wood, is the main source of fuel to the largely gaseous flames in an intense wildfire. A fully compressible database of turbulent nonpremixed (diffusion) flames of wood pyrolysis gas is developed using direct numerical simulation (DNS). A previously developed reduced 4-step mechanism is used to model the combustion of pyrolysis mixture gas and air. The resulting field variables under the influence of turbulent eddy flow is analyzed. The roles of flame displacement speed and its contributions are examined. The normal component of the displacement speed is nearly constant with respect to curvature, while the curvature related component tries to restore the flame front to a planar shape. Effects of strain and curvature are analyzed by considering their correlations with reaction rates. Reaction rates are enhanced with increased positive strain rates due to an increase in flame surface area, and with a reduced curvature. The analyzed results aid in the development of turbulent combustion models.

1. INTRODUCTION

Wildfires are a commonly occurring threat to mankind in many nations of the world. Researchers have tried to advance the capability to predict such a behavior through physically based models [1-4]. Because of the strong coupling that exists between the chemical heat release and the fine scale turbulent motion, wildland fires are intrinsically difficult to model. In some situation when a fire is intense, rapid transition events can occur. An example of rapid transition event is transition from ground to crown fire [5-7]. For such transition events, the detail of the gas—phase combustion through which a large amount of energy is released, needs to be included in developing a physically sound fire model.

In this paper, the resulting database is introduced with descriptions of its fundamental features. Flame displacement speed and the role of curvature on the dynamics of the FSD are physically interpreted and investigated. The relative importance of curvature and strain rate is a subject of discussion. Some preliminary findings with regard to the effects of curvature and strain rate on the structure of turbulent flame.

2. NUMERICAL PROCEDURE AND FLAME PARAMETER

In the present study, we use a two-dimensional DNS of turbulent nonpremixed flames of wood pyrolysis mixture gas, which is a gaseous fuel mixture released from high temperature pyrolysis of ground fuel. This fuel is a complex mixture, including four main gases (CO, H₂, CH₄ and CO₂) [7]. The combustion of pyrolysis gas mixtures occurs through several hundred elementary reactions. Although a detailed reaction mechanism to accurately describe the complex chemistry is possible, the computational cost is high. Therefore a recently derived reduced 4-step chemical kinetic scheme to model the combustion of wood pyrolysis gas is employed [8].

The governing equations solved, include the mass, momentum, energy and species conservation equations which describe pyrolysis gas combustion [9]. A two dimensional 1.0 cm x 1.0 cm domain with a uniform finite-difference grid resolution of 256 x 256, sufficient to resolve the smallest reaction zones, is utilized. An initially strained, one-dimensional laminar diffusion flame, between pyrolysis gas mixture and air, computed using OPPDIF [10] is used. The strain is as the flame becomes unstrained for the reaction zone initialization. Initial profiles of reactant mass fractions and temperature are given in Figure 1. A homogeneous turbulence field is initialized in the computational domain after the initial disturbance acoustic waves exit the domain. The fluctuating velocity field is generated according to the turbulent kinetic energy Passot-Pouquet spectrum [11]. The initial turbulence Reynolds number based on the integral length scale is 118.

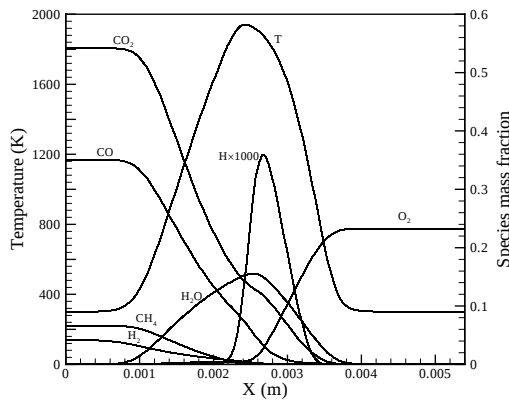


Figure 1. Initial profiles of mass fractions and temperature of opposed-flow diffusion flames for wood pyrolysis gas.

A compressible DNS code originally developed for combustion of perfect gases with constant specific heat [12] was modified to accurately treat mixture gases having variable thermodynamic properties with complex chemistry. Simple Fickian diffusion with the Lewis number approximation recommended by

Smooke and Giovangigli [13] is employed as a transport model for the individual species. Spatial derivatives are discretized using a sixth-order accurate compact finite difference scheme [14]. A third-order Runge-Kutta scheme is used to integrate the equations in time. The modified Navier Stokes Characteristic Boundary Conditions (NSCBC) are used to handle boundary conditions [9]. Non-reflecting boundary conditions are prescribed in the y-direction. The x-direction boundaries are periodic.

3 FLAME SURFACE DENSITY AND MIXTURE FRACTION

In the case when chemistry is sufficiently fast, the chemical time scale is short compared to the convection and diffusion time scales. Consequently, combustion takes place within asymptotically thin elements embedded in the flame. These elements are called flamelets [15]. In the flamelet regime, burning rate of combustion can be estimated through the flame surface density (FSD), which is defined as the flame surface area per unit volume. Under the flamelet assumption, the diffusion flame is located near the stoichiometric iso-level $Z(\mathbf{x}, t) = Z_{st}$, where $\mathbf{x}$ is a spatial coordinate vector, t is time, and Z is the mixture fraction, which has a value of one in the oxidizer stream and zero in the fuel stream. In this work, Z is defined for the pyrolysis gas mixture [8].

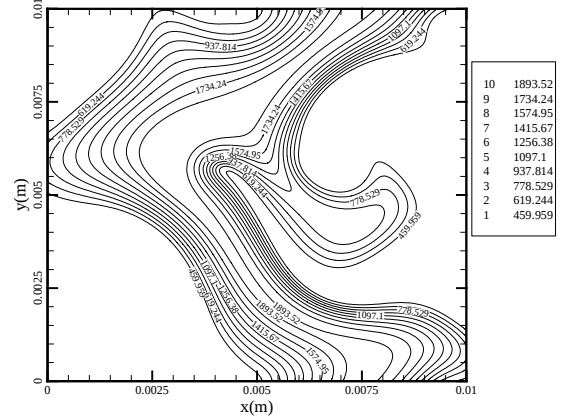


Figure 2. Equispaced temperature contour at 1.0 eddy turnover time.

4 FLAME DISPLACEMENT SPEED

The displacement speed measures the iso-scalar propagation speed relative to the flow field. An iso-surface of mixture fraction Z is considered. If this iso- Z surface propagates in the normal direction in the flow field $\mathbf{u}$, similar to the premixed combustion case [16], absolute propagation speed $\mathbf{v}$ of the iso- Z surface is given by

$$\mathbf{v} = \mathbf{u} + w\mathbf{n}, \quad (1)$$

where the unit normal vector $\mathbf{n}$ of the iso- Z surface is defined pointing toward oxidizer side:

$$\mathbf{n} = -\frac{\nabla Z}{|\nabla Z|}. \quad (2)$$

The displacement speed w is defined as

$$\begin{aligned} w &= \frac{1}{\rho|\nabla Z|} \nabla \cdot (\rho D \nabla Z) \\ &= -\underbrace{\frac{1}{\rho|\nabla Z|} \frac{\partial}{\partial n} (\rho D |\nabla Z|)}_{w_n} - \underbrace{\frac{D \nabla \cdot \mathbf{n}}{w_c}}_{w_c} \end{aligned} \quad (3)$$

where $\partial/\partial n$ denotes derivative along the flame normal vector $\mathbf{n}$ and D is the diffusion coefficient. The curvature $K = \nabla \cdot \mathbf{n}$, is

defined positive when the flame is convex towards the oxidizer. The first contribution w_n represents the displacement speed due to diffusive processes normal to the flame front at the stoichiometric mixture fraction. The second contribution w_c is related to the curvature of the iso- Z surface.

4 RESULTS AND DISCUSSION

4.1 Resulting Field and Flame Displacement Speed

The resulting computational fields are extracted and investigated. Temperature contour at one instance is plotted in Figure 2. The area of very high temperature indicates the location of the flame, where major chemical reactions take place.

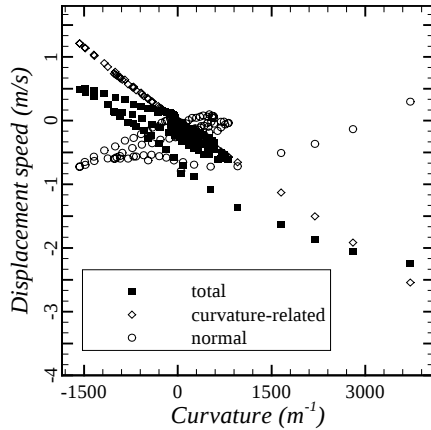


Figure 4. Scatter plots of displacement speeds as a function of curvature. Total displacement speed and its normal and curvature-related contributions are shown.

Figure 3 displays contours of instantaneous vorticity and FSD at different turbulence interaction times, based on the initial eddy turnover time $t_e = l_t/u_t$, where l_t is the initial integral length and u_t is the initial turbulent velocity. The initially planar laminar flame is stretched and distorted by the turbulence. However, vorticity near the flame zone is weakened both due to an increase in kinematic viscosity with temperature and volumetric expansion. As the

turbulence distorts the flame, peak values of FSD appear near the curved regions of the flame front.

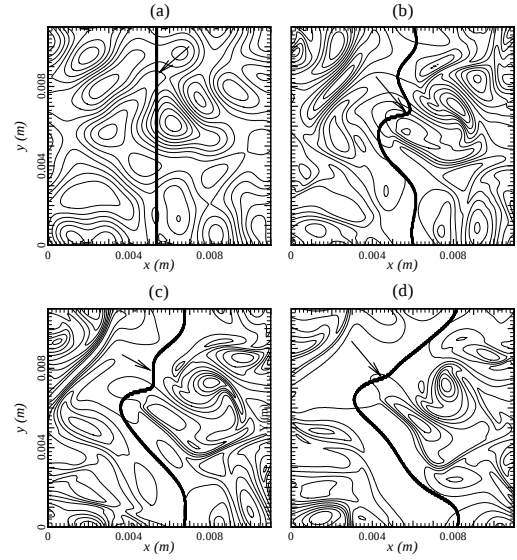


Figure 3. Equispaced vorticity contours overlaid by equispaced flame surface density contours (indicated by arrows) with 10 levels.

As given in Eq. 3, the displacement speed has two contributions. Figure 4 shows variation with curvature of displacement speeds and its contributions along the stoichiometric line. As expected, the curvature-related displacement speed w_c , which is inversely proportional to curvature, is positive (negative) at negative (positive) curvature and becomes zero at zero curvature. As a result, the flame surface is displaced towards the fuel (oxidizer) stream at positive (negative) curvature. In other words it moves in the direction to pull back the flame surface to its planar shape. The normal displacement speed w_n , appears to be weakly curvature dependent. It has mostly negative values with smaller magnitudes. Due to this fact, the curvature-related displacement speed contributes more significantly to the total displacement speed.

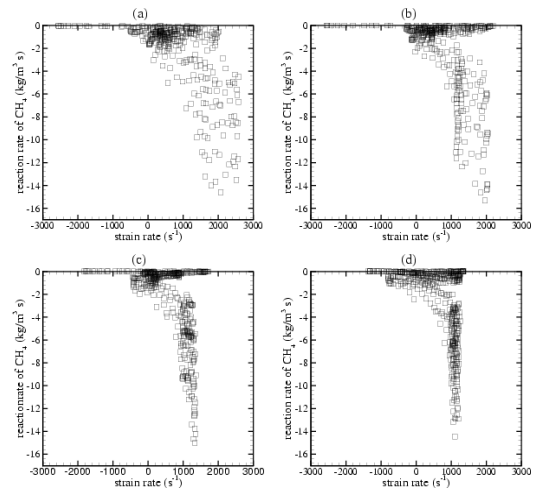


Figure 5. Scatter plots of CH_4 reaction rate as a function of strain rate at (a) 0.25 (b) 0.5 (c) 0.75 and (b) 1.0 of the initial eddy turnover time.

4.2 Turbulence Effects: Strain Rate and Curvature

To better understand turbulence combustion interaction, correlations of reaction rate with strain rate and curvature are analyzed. Strain rate is associated with the rate of tangential strain acting on the flame surface [16,17] and is given by

$$a_T = \nabla \cdot \mathbf{u} - \mathbf{nn} : \nabla \mathbf{u}.$$

Once again the curvature K is defined positive when the flame is convex towards the oxidizer [17]. Figure 5 is a scatter plot of CH_4 reaction rate and strain rate at several times. It can be concluded from these statistics that the magnitudes of the CH_4 reaction rate are very close to zero in regions of negative strain rate and increase with increased positive strain rates. This is caused by an increase in the flame surface area due to straining. As time increases, most data points are clustered together at the value of strain rate close to 1200 s^{-1} . A scatter plot of CH_4 reaction rate with K is shown in Figure 6. Magnitudes of the reaction rate increase as magnitudes of curvature decrease and reach a maximum value near zero curvature. With time, a large number of data points move closer to the location of zero curvature. Notice from Figures. 5 and 6, that the degree of scatter becomes smaller at later times due to weakened turbulence. The other marked statistical trend is that most of the data points correspond to positive strain rates resulting in its statistical average being positive, while averaged curvature is close to zero. This result is consistent with previous works observed in premixed flame combustion [18,19].

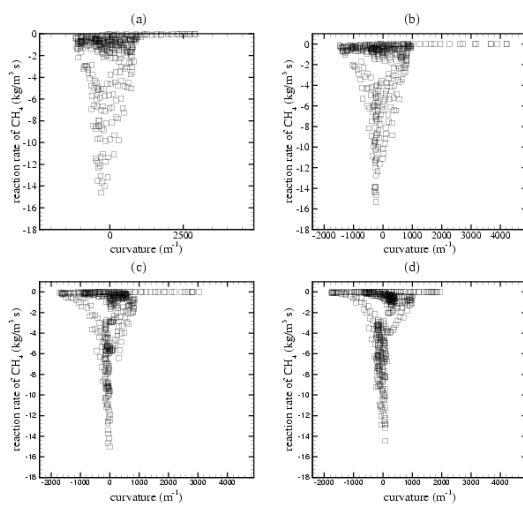


Figure 6. Scatter plots of CH_4 reaction rate as a function of curvature at (a) 0.25 (b) 0.5 (c) 0.75 and (b) 1.0 of the initial eddy turnover time.

5 CONCLUSIONS

The direct numerical simulation of turbulent nonpremixed flames of wood pyrolysis gas, coupled with a realistic chemistry, was performed. The physical problem consists of the interaction between an initially unstrained laminar diffusion flame and a homogeneous field of decaying turbulence. The effects of turbulence on the flame structure were captured as the flame was stretched and distorted. The database obtained provides a better understanding of turbulence flame structure and interaction between turbulence and chemistry. The normal component of the flame displacement speed is found nearly constant, while the curvature related component behaves in such a way to bring the curved back to flat flame.

The effects of instantaneous flame curvature and strain rate on reaction rates were investigated via statistical correlations. Reaction rates are correlated with strain rate and curvature. Reaction rates increase with increased positive strain rates. This is due to an increase in the flame surface area by Straining. As magnitudes of curvature decrease the reaction rates increase and reach a maximum value near zero curvature.

6. ACKNOWLEDGEMENTS

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