Iso-Surface Analysis of a Turbulent Diffusion Flame

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Summary. We analyze the evolution of a diffusion flame in a turbulent mixing
layer. The location of the flame-center is defined by the "stoichiometric" interface.
Geometrical properties such as its surface-area, wrinkling and curvature are char-
acterized using an accurate numerical level-set quadrature method. This allows to
quantify flame-properties as well as turbulence modulation effects due to coupling
between combustion and turbulent transport. We determine the active flame-region
which is responsible for the main part of the chemical processing in the flame.

Key words: Turbulence, combustion, iso-surface analysis, flame properties.

1 Introduction

In various combustion processes turbulent diffusion flames arise. These are
characterized by a thin, distorted and lively evolving region where the con-
ditions for combustion, such as presence of chemical species at appropriate
concentration and temperature, are fulfilled. We will consider combustion in
a turbulent mixing layer with stylized chemical reaction process. This model
can be treated in full detail and provides an impression of the dominant tur-
bulence modulation that arises from the coupling between the fluid-flow and
the chemical reaction equations. Important global flame-properties will be
quantified in detail by applying a new iso-surface quadrature method.

The central region of a diffusion flame may be visualized by monitoring the
so-called "stoichiometric" interface. In a turbulent flow this interface develops
into a complex, highly wrinkled surface. Fundamental properties such as the
flame's surface-area and its wrinkling can be appreciated roughly by visual
inspection. However, in order to become meaningful, a quantitative method of
analysis is required. In this paper we will apply a new method for numerical
integration over complex level-sets and show that an accurate impression of
these properties and trends associated with variations in physical parameters

can be obtained. Access to these fundamental aspects can be used as under-pinning of theoretical and modeling studies aimed at better understanding of the combustion process or to allow more complex flames to be simulated.

The organization of this paper is as follows. In Section 2 we will introduce the model used to describe a diffusion flame in a temporal mixing layer. Section 3 is devoted to a description and application of the method of iso-surface analysis of the flame-center and the determination of the active flame region is discussed together with some concluding remarks.

2 Diffusion flame in a mixing layer

In this section we will introduce the mathematical model describing the flame problem studied in this paper. Subsequently, we will introduce the temporal mixing layer [3] and visualize the evolution of the flame.

The computational model is composed of the compressible flow equations for ideal gases, coupled to a system of advection-diffusion-reaction equations. The dimensionless equations can be expressed as

$$\partial_t \rho + \partial_j(\rho u_j) = 0 \tag{1}$$

$$\partial_t(\rho u_i) + \partial_j(\rho u_i u_j) + \partial_i p - \partial_j \sigma_{ij} = 0 \quad ; \quad i = 1, \ldots, 3 \tag{2}$$

$$\partial_t e + \partial_j((e+p)u_j) - \partial_j(\sigma_{ij} u_i) + \partial_j q_j - h_k \omega_k = 0 \tag{3}$$

$$\partial_t(\rho c_k) + \partial_j(\rho c_k u_j) - \partial_j(\pi_{kj}) - \omega_k = 0 \quad ; \quad k = 1, \ldots, N_s \tag{4}$$

where ρ denotes the fluid mass-density, u_i the velocity in the x_i direction, e the total energy density, c_k the k-th chemical species concentration and N_s the number of species respectively. In order to close this system of equations, additional constitutive equations need to be provided. The viscous fluxes are specified by $\sigma_{ij} = S_{ij}/Re$ and $\pi_{kj} = \partial_j c_k/(ReSc)$ with rate of strain tensor given by $S_{ij} = \partial_i u_j + \partial_j u_i - (2/3)\delta_{ij}\partial_k u_k$. The Reynolds ($Re$) and Schmidt ($Sc$) numbers characterize the strength of the viscous fluxes relative to the nonlinear convective contributions. The equation of state specifies the pressure p through $e = p/(\gamma-1) + \rho u_i u_i/2$ where $\gamma \approx 7/5$. Finally, the heat flux vector $q_j = -\partial_j T/\{(\gamma-1)RePrM^2\}$ where Pr is the Prandtl number, M the Mach number and the temperature T follows from the ideal gas law $\rho T = \gamma M^2 p$. We will use $Re = 50$, $M = 0.2$, $Pr = 1$ and consider different values for Sc in the sequel.

The source terms in the species and energy equation represent the chemical processes that take place. The chemical reactions are characterized by reaction rates ω_k and the heat released in these reactions is given by $h_k \omega_k$ in which h_k is the specific enthalpy associated with species k. The chemical reaction rate ω_k is assumed to be determined by an Arrhenius law. We will consider a single reaction in which fuel F reacts with oxidizer O to yield product P: $F + O \rightarrow P$. For this particular reaction we may express the reaction-rates as [1]

$$\omega_1 = -(\rho c_F)(\rho c_O)Da_O \exp(-\frac{Ze}{T}) \;\; ; \;\; \omega_2 = \alpha\omega_1 \;\; ; \;\; \omega_3 = -\omega_1(1+\alpha) \quad (5)$$

where we introduced the Zeldovich number Ze, put $Da_O = Da/W_O$ with Da the Damköhler number and W_i the molecular weight of species i. In addition, $\alpha = W_O/W_F$ and use was made of $W_P = W_F + W_O$. The source term for the energy equation may be written as

$$h_j\omega_j = h_1\omega_1 + \alpha h_2\omega_1 - (1+\alpha)h_3\omega_1 = \omega_1(h_1 + \alpha h_2 - (1+\alpha)h_3) = Q\omega_1 \quad (6)$$

where Q will be referred to as the effective standard enthalpy of formation. In total this model requires four additional parameters: Da_O, Ze, Q and α. We will assume $\alpha = 1$, $Ze = 1$, $Da_O = 1$ and study variations in Q.
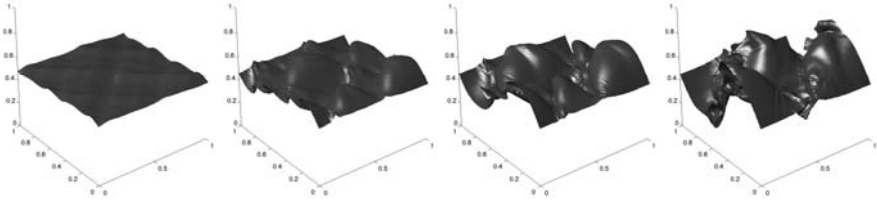
Fig. 1. Evolving stoichiometric surface $c_F - c_O = 0$ in a turbulent mixing layer. The snapshots are taken at $t = 15, 35, 55, 75$ (from left to right).

The consequences of combustion on turbulence may be illustrated with the canonical flow in a temporal mixing layer. In this flow two parallel fluid streams with different velocities merge and rapidly mix [3]. Initially, we consider the upper stream to contain fuel ($c_F = 1, c_O = 0$) and the lower stream to contain oxidizer ($c_O = 1, c_F = 0$). We adopt explicit Runge-Kutta time-stepping and finite volume discretization. The 'center' of the flame is defined through the "stoichiometric surface" $c_F - c_0 = 0$ as shown in Fig. 1.

3 Iso-surface analysis of turbulent flame properties

To quantify basic properties of an evolving diffusion flame we concentrate on "global" variables, such as the flame-area or wrinkling. The global variable corresponding to a density function f and a level-set $S(a,t)$ is defined as

$$I_f(a,t) = \int_{S(a,t)} dA \; f(\mathbf{x},t) = \int_V d\mathbf{x} \; \delta(F(\mathbf{x},t) - a)|\nabla F(\mathbf{x},t)|f(\mathbf{x},t) \quad (7)$$

where V is a fixed and arbitrary volume which encloses the level-set $S(a,t)$ defined as the set where $F(\mathbf{x},t) = a$ for a "level-function" F. The formulation in (7) was used as the basis of the numerical quadrature method in [2].

(a)   (b)
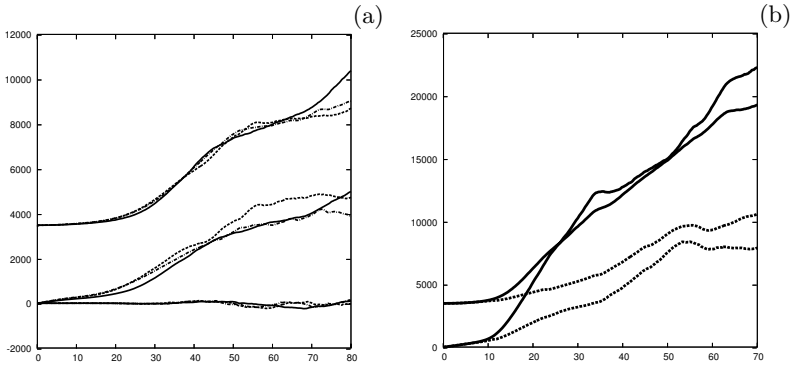
Fig. 2. Evolution of A (top), W (middle) and C (bottom) for the flame in Fig. 1 at 32^3 (solid), 64^3 (dashed) and 96^3 (dash-dot) with $Sc = 10$ and $Q = -1$ (a). Heat-release variations (b): solid: $Q = 0$, dashed: $Q = -100$ at $Sc = 50$.

For a diffusion flame the level-set function $F = c_F - c_O$. To determine the surface-area A of the flame we adopt $f_A = 1$. A measure for the global "curvature" C is obtained using as density

$$f_C(\mathbf{x}, t) = \nabla \cdot \mathbf{n} \quad ; \quad \mathbf{n}(\mathbf{x}, t) = \frac{\nabla F(\mathbf{x}, t)}{|\nabla F(\mathbf{x}, t)|} \tag{8}$$

where $\mathbf{n}$ denotes the unit normal on the flame surface. The 'wrinkling' W is obtained using $f_W(\mathbf{x}, t) = |\nabla \cdot \mathbf{n}|$. In Fig. 2(a) we show estimates for A, C and W obtained at different resolutions. Already at a resolution of 96^3 an acceptable accuracy is obtained which was further confirmed by results on finer grids. In Fig. 2(b) we varied the heat release parameter Q and Schmidt number Sc. Evidently, a strong heat release induces a significant reduction in the area and wrinkling of the flame.

Motivated by the interpretation of the stoichiometric surface, we may introduce a "thick" active flame region around this surface, defined by $S(a) = \{\mathbf{x} \in R^3 | \ |c_F - c_O| \leq a\}$ in which the parameter a is referred to as the stoichiometric interval width. The fuel processing-rate Γ_F associated with $S(a)$ is

$$\Gamma_F(a, t) = \int_{-a}^{a} ds \int_{c_F - c_O = s} dA \ \omega_F(\mathbf{x}, t) \tag{9}$$

The processing rate Γ_F arises mainly from nearby iso-surfaces $c_F - c_O = s$ where s runs from $-a$ to a. When a increases Γ_F increases as well with a maximum at $a = 1$. This allows to define the ε-flame-region by $\Gamma_F(a, t)/\Gamma_F(1, t) = \varepsilon$ from which $a(\varepsilon, t)$ may be solved.

In Fig. 3 we collected the evolution of the stoichiometric interval width a. After the transitional stages a fairly constant value of a defines the active flame region. The corresponding physical space region increases with time, as shown in Fig. 4.
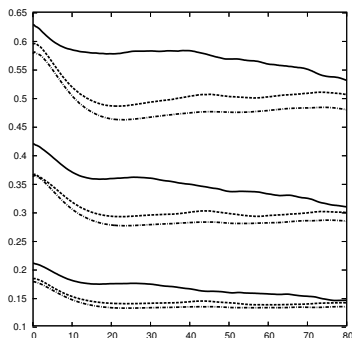
Fig. 3. Effective flame region corresponding to 75 % (top), 50 % (middle) and 25 % (bottom) of the total processing rate on 32^3 (solid), 64^3 (dashed) and 96^3 (dash-dot).
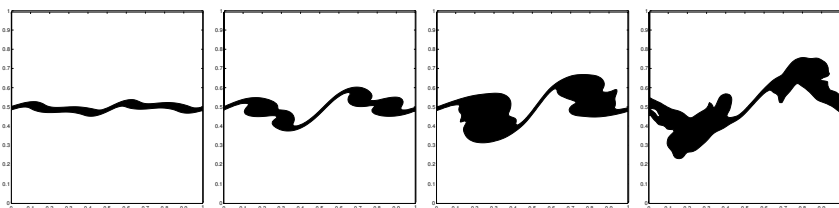
Fig. 4. Active flame region corresponding to 50% of the total combustion. A characteristic slice is shown at $t = 15, 35, 55, 75$ (from left to right).

In summary, we introduced a simple combustion model and studied a turbulent diffusion flame in a temporal mixing layer. The coupling between the combustion and the turbulent transport induces a significant modulation of the turbulent flow properties, e.g., characterized by a strongly reduced spreading rate of the mixing layer. Using a new method for integration over geometrically complex evolving level-sets, basic properties such as flame-area, wrinkling, curvature and active flame region were quantified.

References

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