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Strain rates normal to approaching iso-scalar surfaces in a turbulent premixed flame

Cesar Dopazo [a], Luis Cifuentes [a,*], Jesus Martin [a], Carmen Jimenez [b]

[a] LIFTEC, CSIC-University of Zaragoza, Spain
[b] Department of Energy, CIEMAT, Spain

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ABSTRACT

A Direct Numerical Simulation (DNS) dataset of a turbulent premixed propagating flame with an Arrhenius one-step chemistry in an input–output configuration is examined. Combustion takes place in the 'corrugated flamelets' regime. Heat release causes the flow volumetric dilatation rate to be positive over most of the computational domain, with associated positive strain rates normal to iso-scalar surfaces and both positive or negative strain rates tangent to them. The normal propagation of convex and concave iso-surface infinitesimal area elements produces stretching and reduction, respectively, superposed to tangential flow strain rate effects. The normal propagation speed of iso-surfaces increases monotonically from 'fresh gases' to 'hot products', which draws two adjacent ones closer; this contribution, due to both chemistry and molecular diffusive transport, is much greater than that of the normal flow strain, and enhances mixing and chemical conversion. Many aspects of turbulent premixed flames traditionally explained in terms of tangential strain rates can likely be well understood using the normal ones.

1. Introduction

The importance of the tangential strain rate on the propagation speed and stability of laminar, premixed flames has been investigated for some time (Matalon [1], and references therein). Interpretations of turbulent mixing in terms of the iso-scalar surface evolution have also been proposed [2,3].

Transport equations for flame area and surface density function have been derived with an explicit dependence on tangential stretching [4,5].

Flows with important density changes, due, for example, to chemical heat generation, will presumably undergo large volumetric dilatation rates. Intuitively, this situation may lead to mostly positive values for both tangential and normal strain rates [6]; the former will imply iso-scalar surface stretching, whereas the latter will, in principle, yield a reduction of the scalar-gradient modulus, as iso-surfaces separate. This fact seems at first glance to hamper scalar molecular fluxes and dissipation of composition inhomogeneities. Chakraborty [7] has documented, via DNS, the occurrence of positive normal strain rates in a 'corrugated flamelets' regime. and negative ones in a 'thin reaction zone regime'; while in the first case the scalar gradient aligns preferentially with the strain rate tensor eigenvector corresponding to its most extensive eigenvalue, in the second instance the scalar gradient is mainly parallel to the most compressive eigenvector. This latter feature coincides with that described for turbulent scalar mixing in constant density flows [8,9]. Chakraborty et al. [10] have scrutinized via DNS the Lewis number effect on the scalar gradient alignment in turbulent premixed flames; they have documented mainly positive normal strain rates and concluded that 'the most extensive principal strain rate' is preferentially perpendicular to iso-scalar surfaces and 'destroys the scalar gradient' with a 'magnitude' that 'increases with decreasing Lewis number for given turbulent Reynolds and Damköhler numbers'.

This works aims at explaining why scalar-gradients can grow and mixing is not hampered under mostly positive flow strain rates normal to iso-surfaces. DNS results for a propagating turbulent premixed flame with one-step Arrhenius chemistry in an input–output configuration are examined. Normal strain rates caused by changes in iso-scalar surface propagation speed in the normal direction, due to both molecular transport and chemistry, are negative and lead to 'effective' strain rates that bring iso-surfaces closer together and enhance scalar-gradients.

Section 2 describes the kinematics of non-material iso-scalar surfaces and summarizes the assumptions underlying the direct numerical simulations. The practical execution of the latter is presented briefly in Section 3. Numerical results are discussed in Section 4 and some conclusions are drawn in Section 5.

* Corresponding author.
E-mail address: lcifuentes@unizar.es (L. Cifuentes).

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2. Formulation

2.1. Kinematics of iso-scalar surfaces

Scalar mixing can be viewed as a combination of iso-scalar surface stretching and scalar-gradient growth induced by the flow field. Figure 1 depicts an infinitesimal surface, S, on the non-material iso-surface $Y(\mathbf{x},t) = \Gamma$, with a normal unit vector $\mathbf{n}(\mathbf{x},t) = \nabla Y/|\nabla Y|$.

$Y(\mathbf{x},t)$ is, for example, the normalized reactant mas fraction ($Y = 1$ in the 'fresh gases' and $Y = 0$ in the 'hot products').

An infinitesimal vector, $\mathbf{r}(\mathbf{x},t)$, joins a point $\mathbf{x}$ at the center of S to a point $\mathbf{x}+\mathbf{r}$ on a neighboring iso-scalar surface $Y(\mathbf{x},t) = \Gamma + d\Gamma$. The two extremes of $\mathbf{r}$ move with velocities $\mathbf{v}^Y(\mathbf{x},t)$ and $\mathbf{v}^Y(\mathbf{x}+\mathbf{r},t)$, where the velocity of a point of the non-material iso-scalar surface is decomposed as

$$\mathbf{v}^Y(\mathbf{x},t) = \mathbf{v}(\mathbf{x},t) + V^Y(\mathbf{x},t)\mathbf{n}, \tag{1}$$

$\mathbf{v}$ is the fluid velocity and V^Y is the normal displacement speed of $Y(\mathbf{x},t) = \Gamma$ relative to the local fluid. The time rate of change of $\mathbf{r}$ is

$$\frac{d\mathbf{r}}{dt} = (\mathbf{r}\cdot\nabla)\mathbf{v}^Y. \tag{2}$$

The right side of (2) can be expanded as

$$\frac{d\mathbf{r}}{dt} = \mathbf{r}\cdot\mathbf{s} + \mathbf{r}\cdot\mathbf{w} + (\mathbf{r}\cdot\nabla)V^Y\mathbf{n} + V^Y(\mathbf{r}\cdot\nabla)\mathbf{n}, \tag{3}$$

where $\mathbf{s}$ and $\mathbf{w}$ are the strain and rotation rate tensors, respectively, and $\nabla\mathbf{n}$ is the curvature tensor. $\mathbf{r}\cdot\mathbf{w}$ can be recast as $1/2(\boldsymbol{\omega}\times\mathbf{r})$, in terms of $\boldsymbol{\omega} = \nabla\times\mathbf{v}$, the vorticity vector.

If $\mathbf{r} = \Delta x_N\mathbf{n}$, one can readily obtain from (3)

$$\frac{1}{\Delta x_N}\frac{d\Delta x_N}{dt} = a_N + \frac{\partial V^Y}{\partial x_N}, \tag{4}$$

$$\frac{d\mathbf{n}}{dt} = (\boldsymbol{\delta} - \mathbf{nn})\cdot\mathbf{s}\cdot\mathbf{n} + \frac{1}{2}\boldsymbol{\omega}\times\mathbf{n} + V^Y(\mathbf{n}\cdot\nabla)\mathbf{n}, \tag{5}$$

where

$$a_N = \mathbf{n}\cdot\mathbf{s}\cdot\mathbf{n}, \tag{6}$$

is the flow strain rate normal to $Y(\mathbf{x},t) = \Gamma$. $\partial V^Y/\partial x_N$ is the derivative of the propagation velocity in the normal direction to the iso-surface. $\boldsymbol{\delta}$ is the identity Kronecker delta tensor. While the vorticity has no influence on the variation of the modulus of $\mathbf{r}$, Δx_N, it obviously rotates its direction, $\mathbf{n}$.

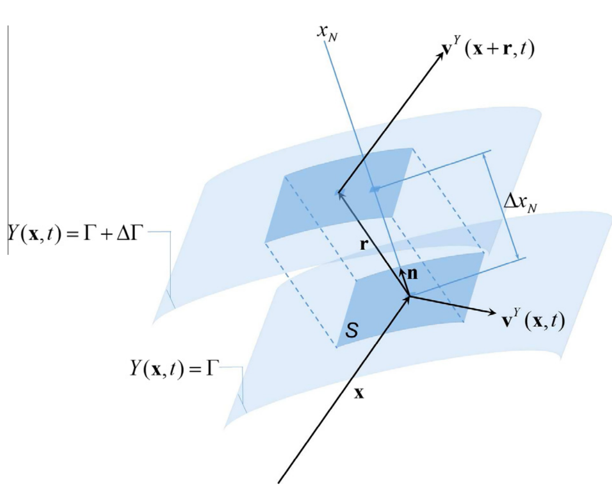

Fig. 1. Schematic representation of two elements of flame surface.

The infinitesimal volume $V = S\Delta x_N$, between the two iso-scalar surfaces, changes in time according to

$$\frac{1}{V}\frac{dV}{dt} = tr(\mathbf{s}) + \frac{\partial V^Y}{\partial x_N} + 2k_m V^Y, \tag{7}$$

where $tr(\mathbf{s}) = \nabla\cdot\mathbf{v}$, the trace of the strain rate tensor, yields the flow volumetric dilatation rate, and k_m is the local mean curvature, $k_m = (\nabla\cdot\mathbf{n})/2$, of the iso-scalar surface. $k_m > 0$ for iso-surfaces convex towards 'fresh gases' and $k_m < 0$ for concave ones. The time rate of change of the infinitesimal surface S can thus be obtained from

$$\frac{1}{S}\frac{dS}{dt} = \frac{1}{V}\frac{dV}{dt} - \frac{1}{\Delta x_N}\frac{d\Delta x_N}{dt}, \tag{8}$$

and using (4) and (7)

$$\frac{1}{S}\frac{dS}{dt} = a_T + 2k_m V^Y, \tag{9}$$

with

$$a_T = (\boldsymbol{\delta} - \mathbf{nn}) : \mathbf{s}, \tag{10}$$

the flow strain rate tangential to $Y(\mathbf{x},t) = \Gamma$. This expression has been derived for flame stretch by several authors (Poinsot and Veynante [11], and references therein). a_N and a_T satisfy $a_N + a_T = \nabla\cdot\mathbf{v}$.

The mass flow rate per unit volume of $Y(\mathbf{x},t)$, which determines the local mixing rate, is

$$\frac{\mathbf{f}^Y\cdot S\mathbf{n}}{V} \sim -\rho D\frac{S}{V}\frac{\Delta\Gamma}{\Delta x_N}, \tag{11}$$

where $\mathbf{f}^Y$ is the Fickian molecular flux, $\sum(\Gamma;x,t) = S/V = 1/\Delta x_N$ is the surface density function [5], and $|\nabla Y| = \partial Y/\partial x_N = \Delta\Gamma/\Delta x_N$.

For the two given iso-scalar surfaces, the local mixing rate increases with time if Δx_N diminishes. From (4) one concludes that $d\Delta x_N > 0$ if $(a_N + \partial V^Y/\partial x_N) > 0$, and $d\Delta x_N < 0$ if $(a_N + \partial V^Y/\partial x_N) < 0$.

For combusting flows with significant heat release $\nabla\cdot\mathbf{v} > 0$, and the probability of finding $a_N > 0$ in most of the flow domain might be large. Therefore, for the scalar-gradient and the mass flow rate per unit volume to increase, $\partial V^Y/\partial x_N$ should be negative and its absolute value greater than a_N.

Surface stretching $(dS > 0)$ occurs if $(a_T + 2k_m V^Y) > 0$, but seems to bear no direct influence on the local mixing rate.

On the other hand, the evolution of an iso-scalar surface obeys the equation

$$\frac{\partial Y}{\partial t} + (\mathbf{v}^Y\cdot\nabla)Y = 0, \tag{12}$$

which can be rephrased as

$$\frac{\partial Y}{\partial t} + (\mathbf{v}\cdot\nabla)Y = -V^Y|\nabla Y|. \tag{13}$$

An equation for the evolution of $|\nabla Y|$ can be readily obtained from (12),

$$\frac{\partial|\nabla Y|}{\partial t} + (\mathbf{v}^Y\cdot\nabla)|\nabla Y| = -\left(a_N + \frac{\partial V^Y}{\partial x_N}\right)|\nabla Y|, \tag{14}$$

The scalar-gradient associated to a point on a non-material iso-surface moving with velocity $\mathbf{v}^Y$ decreases or increases depending, once again, on positive or negative values, respectively, of the 'effective' normal strain rate, $(a_N + \partial V^Y/\partial x_N)$.