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# MODELING OF FLAME-GENERATED TURBULENCE BASED ON DIRECT NUMERICAL SIMULATION DATABASES

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Turbulent premixed flames propagating in homogeneous isotropic turbulent flows were simulated directly with a single-step irreversible reaction. Two cases were calculated, case H, with a high-density ratio of flame $\rho_u/\rho_b = 7.53$, and case L, low-density ratio of flame $\rho_u/\rho_b = 2.50$, while $u'/u_L$ was nearly equal to unity. We obtained databases of fully developed stationary turbulent flames. These databases were investigated by analyzing the transport equation for turbulent kinetic energy to study flame-generated turbulence and its models. We found that turbulent fluctuations of all components, especially the streamwise component, were amplified in the flame brush and that flame-generated turbulence increased for a larger density ratio of the flame. Analysis based on the Favre-averaged transport equation for turbulent kinetic energy showed that pressure-related terms produced kinetic energy in the flame brush, the mean pressure gradient term was most important in case H and the pressure work term was most important in case L. On the other hand, the diffusion and dissipation term and velocity gradient term decreased kinetic energy. Next, modeling of the important terms in the balance equations were discussed. The mean pressure gradient term, pressure dilatation term, and additional dissipation components were modeled and compared with the direct numerical simulation (DNS) results. The mean pressure gradient term was modeled with assumption on the density, and the model was in good agreement with DNS. The other two terms were also modeled by scaling, and these models mimicked DNS well.

## Introduction

Flame-generated turbulence, which is characteristic physics in the premixed turbulent combustion and must be included in the turbulent combustion model, was first proposed by Karlovitz et al. in 1953 [1]. Non-gradient diffusion in turbulent premixed combustion was observed experimentally in 1980 by Moss [2] and considered theoretically, in 1981, by Libby and Bray [3]. However, since these early efforts, progress toward understanding the importance of these phenomena, their physical explanation and practical models has been limited. Following the approach initiated by Rutland and Trouvé [4] that uses direct numerical simulations (DNS), this paper presents new results for a statistically steady and planar propagating turbulent premixed flame. These results enabled us to explain how the turbulent kinetic energy is influenced by the expansion of gases in the so-called flamelet regime. The modeling of the important terms in the balance equations for these quantities is also discussed.

After a synthetic presentation of the present knowledge and open questions about these related phenomena, the paper describes the DNS. Then, using the new data, flame-generated turbulence and its modeling are separately discussed, as thoroughly as possible.

This study was done by the following background. Flame-generated turbulence was a simple hypothesis proposed by Karlovitz et al. [1]. More precisely, Bray and Libby, in 1976 [5], first related this phenomenon to the mean velocity gradient that expansion of gases is able to produce in a flow confined within a duct. The experiment of Moreau and Boutier [6] confirmed this effect. However, they understood very soon that another mechanism was involved. It was more unusual and related to the mean pressure gradient that preferentially accelerates burned, light, fluid particles compared to unburned and heavy particles [7]. This phenomenon was experimentally exposed and modeled by the careful work of Borghi and Escudie [8] and later by Chomiak and Nisbet [9]. The modeling of this effect must consider the turbulent mass diffusion flux, with possible countergradient behavior.

The influence of fluctuating pressure gradient in the flame has been considered important since the papers of Kuznetsov, in 1979 [10], and Stralhe, in 1982 [11], but was confirmed only recently (1994) through DNS by Rutland and Cant at Stanford University [12]. Until very recently, the most advanced version of the Bray-Libby-Moss-Champion model (the last version of the model called Bray-Moss-Libby model) of turbulent premixed combustion in the flamelet (c.f. [13]) simply neglected this effect, without producing any clear disagreement with experimental results. An important step in modeling was accomplished recently, and now Bray et al. [14] have included this effect in a new model that seems to agree well with experiments for a flame stabilized in a stagnating flow.

It has often been claimed that the increase in turbulence that can be measured on the bases of statistical mean values may be simply the signature of some flapping of the flame, especially for the flamelet regime. This is only partially true, as confirmed with conditional measurements (in unburned or burned gases), in physical experiments or with DNS. Even conditional values show that the turbulent kinetic energy is increased in burned gases (see Ref. [15], although turbulence is defined without conditioning in our new models and needs to be predicted.

Combustion is expected also to contribute the decrease of turbulence. First, the increase in temperature and molecular viscosity can be invoked, but this will play a role only at small Reynolds numbers. A second effect is directly related to the expansion of gases, because it is readily seen that there is a negative mean dilatation term in the balance equation for the turbulence kinetic energy. A third factor is expected because additional components do appear in the viscous dissipation term when density is not constant. Although these terms have been discussed already [12], they have not been modeled explicitly [13,14].

Important steps have been made since flame-generated turbulence and countergradient diffusion were discovered, in particular very recently by Bray and coworkers [14,16]. However, it is of particular interest to verify the previous findings for the case of truly statistically steady flames and address the questions of

- The role of fluctuating pressure in the turbulent kinetic energy balance
- The role of viscous terms, modified by the flamelets, in dissipation of turbulent kinetic energy

For each of these questions, a discussion concerning modeling is in order.

It seems clear that the role of fluctuations in the pressure gradient, either for flame-generated turbulence or for countergradient diffusion, is related to the well-known Landau-Darrieus instabilities of flamelets. These instabilities occur very often in laminar flames (except in certain cases, for instance, when they can be stabilized by gravity forces), and it is expected that they occur also for flamelets when these are maintained within the flame brush. The role of these instabilities for the mean properties of the flame brush is important when the incoming turbulence is weak, but can be expected to be shrink as the ratio $u'/u_L$ increases. These instabilities saturate at a certain level due to flamelet interactions, and the interactions occur most easily in turbulent flames, all of which results in strongly nonlinear behavior. It is very difficult to describe theoretically this nonlinear behavior, and the proposed models are expected to avoid this difficulty.

## Numerical Method and Flow Conditions

We calculated steady and planar propagating turbulent premixed flames in three dimensions by the compressible Navier-Stokes equations with the following assumptions [15,17]. (1) The chemical reaction is a single-step irreversible one with heat release. (2) The bulk viscosity, the Soret and the Dufour effects, and the pressure gradient diffusion can be neglected. (3) The specific heat at constant pressure and the specific heat ratio are constant. (4) The equation of state for the burned and unburned gases is ideal. (5) The transport coefficients are temperature dependent, as follows: $\mu = \mu_0(T/T_0)^{0.7}$, $Le = (\lambda/\rho DC_p) = 1.0$, and $Pr = (\mu C_p/\lambda) = 0.75$.

The simulation domain was a box $8 \times 4 \times 4$ mm containing a grid with $512 \times 128 \times 128$ points. The long dimension of 8 mm was taken in the streamwise direction and the other dimensions were transverse. Boundary conditions in the transverse directions were periodic, and the Navier-Stokes characteristic boundary conditions [18,19] was applied to the streamwise direction. At the inflow boundary, precalculated homogeneous isotropic turbulence entered the domain with a mean inflow velocity; the velocity was assigned by assuming Taylor's hypothesis and a phase shift. The sixth-order central finite difference method was used for the streamwise direction to treat non-periodic boundary conditions and the Fourier spectral collocation method was used for the transverse directions. The third-order Runge-Kutta method was used for time integration.

A premixed gas was presumed to have a pressure, $p_0$, of 0.1 MPa, initial temperature, $T_0$, of 300 K,