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Assessment of a presumed joint pdf for the simulation of turbulence–radiation interaction in turbulent reactive flows

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ABSTRACT

Turbulent reactive flows are an important problem in engineering, with a major impact on combustion efficiency, pollutant emissions and climate change. The numerical simulation of these flows is difficult, not only due to the need to address different physical phenomena, but also due to the interaction between them. The interaction between turbulence and radiation, due to the strong non-linearity between temperature and radiative emission, is the subject of the present work. To account for this interaction, the time-averaged form of the radiative transfer equation may be solved. The correlation between the absorption coefficient of the medium and the radiation intensity is often neglected in simulations, because the radiation intensity depends on the temperature and chemical composition along an optical path, and therefore it may be argued that it is relatively independent of local turbulent fluctuations. However, this approximation may introduce errors that are not negligible. A model has recently been proposed to determine that correlation, which relies on the assumption that the joint probability density function of mixture fraction and radiation intensity is a two-dimensional clipped Gaussian. This assumption is investigated here using experimental data for the mean and variance of mixture fraction for a turbulent free jet flame. It is shown that the presumed joint pdf accurately allows the evaluation of the mean radiation emission and absorption, but the prediction of the correlation between fluctuations of the absorption coefficient and fluctuations of the radiation intensity is not so good near the end of radial optical paths.

1. Introduction

Turbulent reactive flows are of major importance in many practical applications, such as utility boilers, furnaces, incinerators, gas turbine combustors, rockets, internal combustion engines and fires. Mathematical modelling of these flows has been the subject of extensive research for several decades. One of the main problems in the numerical simulations lies in the interaction between different physical phenomena, particularly turbulence, combustion and radiation [1]. Turbulent fluctuations of the temperature field affect combustion, since the reaction rates are a strongly non-linear function of temperature. Similarly, radiation is affected by temperature fluctuations, because the emission of radiation is proportional to the fourth power of temperature, and the mean value of the fourth power of temperature may be quite different from the fourth power of the mean temperature. Conversely, the temperature field is strongly influenced by combustion and radiation. Furthermore, the density is closed related to the temperature and the chemical composition via the ideal gas law. Therefore, turbulent fluctuations of temperature affect the density field, which then influences the velocity field and turbulence. This implies a close coupling and interaction between these non-linear physical processes.

In the present work, we are concerned with the interaction between turbulence and radiation [2]. It has been shown that this interaction may contribute to increase the mean radiation intensities in turbulent diffusion flames by a factor of two or more [3,4]. The flames become cooler due to radiation, and numerical calculations show that turbulence–radiation interaction further contributes to decrease the flame temperature, accounting for about 1/3 of the total drop in the maximum temperature in a free, turbulent diffusion methane/air flame [5]. This has an important impact on pollutant emissions.

Turbulent flows are often modelled by solving the time-averaged form of the governing equations for mass and momentum, and using a turbulence model to deal with the unclosed terms arising from the time-averaging procedure [6]. Similarly, turbulence may be taken into account in radiative transfer calculations by solving the time-averaged form of the

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radiative transfer equation (RTE), and using a model for the unclosed terms. The mean radiative emission term may be evaluated in the framework of conserved scalar/prescribed probability density function (pdf) models [7], often employed in combustion modelling, without any further assumptions, as described in [8]. The mean radiative absorption term, given by the mean value of the product of the absorption coefficient of the medium by the radiation intensity, is much more difficult to model. In fact, the radiation intensity depends on the properties of the medium (temperature and chemical composition) along the optical path, rather than just at the point under consideration.

To simplify the evaluation of the mean radiative absorption term, it is common practice to neglect the correlation between the absorption coefficient of the medium and the radiation intensity. This is the so-called optically thin fluctuation approximation (OTFA) [9], which has been employed, e.g., in [5,8,10–12]. It is justified by the fact that the local radiation intensity should not depend significantly on local fluctuations of the absorption coefficient of the medium, since these depend only on local properties. However, this approximation is questionable in the case of optically thick media, and recent direct numerical simulations of a premixed combustion system reveal that the absorption coefficient – radiation intensity correlation is not negligible, even in the case of optically thin media, and is significant at intermediate values of the optical thickness [13]. Additional direct numerical simulations of a statistically one-dimensional nonpremixed system confirm that the contribution from that correlation is significant at intermediate to large values of the optical thickness [14].

A model based on the diffusion approximation was proposed in [15] to evaluate the absorption coefficient – incident radiation correlation, but it is restricted to optically thick media. A more general model is reported in [16]. It relies on the assumption that the shape of the joint pdf of mixture fraction and radiation intensity is a clipped Gaussian. The purpose of the present paper is to investigate the accuracy of this assumption, i.e., of the potential of a presumed joint mixture fraction–radiation intensity pdf model to simulate turbulence–radiation interaction.

2. Theory

The RTE in an emitting–absorbing medium may be written as

$$\frac{\mathrm{d}I_\nu}{\mathrm{d}s} = -\kappa_\nu I_\nu + \kappa_\nu I_{b\nu} \quad (1)$$

where I_ν is the radiation intensity, κ_ν the absorption coefficient, $I_{b\nu}$ the Planck function, and s the direction of propagation of radiation. Subscript ν stands for the wavenumber. In turbulent flows, the time-averaged form of Eq. (1) is written as

$$\frac{\mathrm{d}\bar{I}_\nu}{\mathrm{d}s} = -\overline{\kappa_\nu I_\nu} + \overline{\kappa_\nu I_{b\nu}} = -\bar{\kappa}_\nu \bar{I}_\nu - \overline{\kappa'_\nu I'_\nu} + \overline{\kappa_\nu I_{b\nu}} \quad (2)$$

where the overbar denotes time-averaged values. The absorption coefficient of the medium is a function of the temperature, pressure and molar fraction of the absorbing species, while the Planck function depends on the temperature.

Combustion models employed in the numerical simulation of turbulent reactive flows are often based on the assumption of the shape of the pdf of mixture fraction or on the solution of a transport equation for the joint pdf of scalars. We will assume here that a combustion model based on a presumed pdf shape for the mixture fraction is used, although the methodology can also be readily applied to transport pdf models. The instantaneous temperature, T, and molar fraction of a species i, x_i, may be related to mixture fraction, z. Then, the mean value of the absorption coefficient–Planck function correlation may be easily determined as follows:

$$\overline{\kappa_\nu I_{b\nu}} = \int_0^1 \kappa_\nu(T(z), x_i(z)) I_{b\nu}(T(z)) \mathrm{pdf}(z) \mathrm{d}z \quad (3)$$

The mean absorption coefficient in the first term on the right of Eq. (2) is determined similarly, while the second term is much more difficult to evaluate, as stated in the introduction. In fact, in contrast to the absorption coefficient and the Planck function, which depend only on local properties of the medium, the radiation intensity depends on properties along the direction of propagation of radiation.

In order to account for the absorption coefficient – radiation intensity correlation, and relax the OTFA, the joint pdf of the absorption coefficient and the radiation intensity would be needed. Alternatively, since the absorption coefficient may be related to the mixture fraction, the joint pdf of the mixture fraction, z, and radiation intensity is also adequate. The pdf of mixture fraction is often assumed to be expressed by a beta function or by a clipped Gaussian distribution [7]. Moreover, experimental data suggest that the pdf of the radiation intensity is also approximately Gaussian [17], at least in regions where flame intermittency is not significant. Here, we will assume that the shape of the joint pdf (z,I) is a two-dimensional clipped Gaussian distribution. This allows the mean radiative absorption term to be computed as follows

$$\overline{\kappa_\nu I_\nu} = \int_0^\infty \int_0^1 \kappa_\nu(T(z), x_i(z)) I_\nu \mathrm{pdf}(z, I_\nu) \mathrm{d}z\, \mathrm{d}I_\nu \quad (4)$$

The term $\overline{\kappa'_\nu I'_\nu}$ may be evaluated similarly. Definition of the joint pdf(z,I) requires knowledge of the first two moments of z and I along with the correlation coefficient between z and I. While the first two moments of z are generally available from the combustion model, and the mean value of the radiation intensity is obtained from the solution of Eq. (2), two additional equations are needed to determine the variance of I and the correlation coefficient. A model is proposed in [16] for the determination of these two unknowns. Here, we will focus on the assessment of the assumption of the shape of the joint pdf.

3. Test case and computational details

A free jet diffusion flame, Sandia flame D, is used to investigate the problem under consideration [18]. Detailed experimental data for this flame are available in [19]. Mean temperature radial profiles at distances of $x/d = 30$, 45 and 60 fuel nozzle diameters from the burner exit are displayed in Fig. 1 (d stands for the fuel nozzle

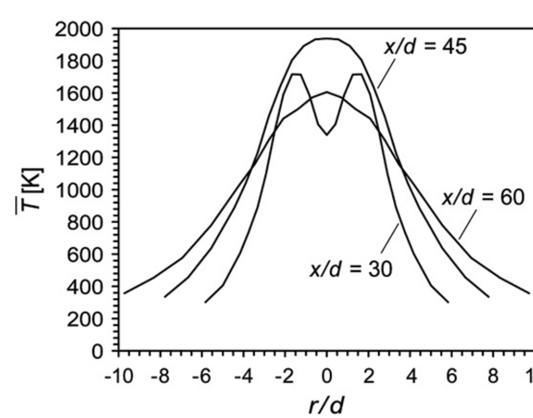

Fig. 1. Mean radial temperature profiles of Sandia flame D (data from [19]).