Numerical Modeling of Nonpremixed Turbulent Combustion

Luc Vervisch

Institut National des Sciences Appliquées de Rouen
LMFN / UMR CNRS 6614 / CORIA / FRANCE
vervisch@coria.fr

Abstract

Non-premixed turbulent flames control many practical applications of combustion. Studying these mechanisms has been the objective of numerous theoretical and experimental works, numerical simulation is also widely used to understand these flames. A brief review of numerical models for nonpremixed turbulent combustion is given. Since injection of liquid fuel is a common procedure in turbulent combustion devices operating in the non-premixed regime, we also discuss a methodology coupling the basic inputs of turbulent combustion closures with spray vaporization.

Introduction

Non-premixed (or diffusion) flames are observed in combustion systems where fuel and oxidizer are not perfectly premixed before entering the combustion chamber (eg. diesel engines, aeronautical combustion chambers, gas turbines and furnaces). There exist strong motivations for studying these turbulent flames:

- Many practical systems include liquid injection of the fuel, and therefore nonpremixed combustion.
- The development of new combustion technologies for aircraft engines, and more generally for gas turbines operating in the non-premixed regime, implies the accurate determination of the position in the flow where combustion starts and the control of pollutants emission. Collecting knowledge on nonpremixed turbulent flames is needed to addressed these crucial points.
- Nonpremixed flames and partially premixed combustion have an impact on some devices using premixed flames: In many of these chambers, the premixing of the reactants is not always complete at the molecular level and some partial premixing may be observed. Sometimes, partial premixing is even desirable to limit pollutant emissions (stratified charge engines).

In the systems where the reactants are supplied in separate streams, the entrainment of fuel and oxidizer by the large scales of the flow leads to incomplete mixing. The largest scales of the turbulence are linked to the geometry of the combustion chamber and to its physical size. After entrainment by these unsteady large scales, turbulent micromixing mechanisms, acting at smaller scales, bring fuel and oxidizer into contact in the reaction zone where product are formed and the heat is released. Accordingly, the modeling of nonpremixed turbulent flames requires a good understanding of simultaneous turbulent mixing and combustion processes.

Numerical studies may be organized into three groups:

- Direct Numerical Simulation (DNS). A full numerical simulation of the problem is the objective of DNS, where all the scales (time and length) are resolved from the smallest to the largest for a given synthetic problem. Indeed DNS cannot be used in real combustion chamber configurations, however, it is a tool of great interest to study in detail various properties of flames, whereas large scales effects are not included [1, 2, 3, 4, 5].
- Reynolds Averaged Navier Stokes (RANS) calculations [6, 7]. The turbulent signals (velocity, temperature, ...) are averaged and calculated from equations which rely on turbulence and turbulent combustion models. One of the main limitation of RANS is the lack of accuracy in capturing unsteady large scales mixing controlling many properties of combustion chambers.
- Large Eddy Simulation (LES) is an attractive tool since the large scale mixing between fuel and oxidizer is fully resolved and simulated [8, 9, 10, 11, 12]. Nevertheless, the complex coupling between micro-mixing and chemical reactions occurring at unresolved scales needs models (as in RANS).

Modeling strategies for non-premixed turbulent flames

Using RANS or LES, the modeling of turbulent diffusion flames relies on simplifying assumptions for both chemistry and transport. Depending on the simplifications made for these mechanisms, various approaches for laminar flames and models for turbulent flames are obtained. All these closures are based on a particular description of fuel / air turbulent mixing. Following fundamentals of diffusion combustion [13], the mixture fraction Z is usually chosen ; Z is a conserved scalar with $Z = 1$ in pure fuel and $Z = 0$ in the oxidizer stream. The two fields $\widetilde{Z}$ and $\widetilde{Z''^2}$ are the basic inputs of many models ; they describe the means (temporal in RANS or space filtered in LES) of Z and its fluctuations. Because $\widetilde{Z''^2}$ characterizes non-homogeneities in the mixing between the reactants, considerations about nonpremixed turbulent combustion regimes have shown that it is one of the control parameters of these flames [14]. We discuss the effect of spray on $\widetilde{Z''^2}$ in the subsequent section.

Turbulent combustion models may be organized into three groups (see table 1):

- Assumption of infinitely fast chemistry (mixed is burnt).
- Finite rate chemistry involving a coupling between diffusion and reaction similar to the one observed in laminar flames (flamelets assumption).
- Finite rate chemistry with a separated treatment of diffusion from reaction (CMC, pdf methodology), where diffusion is described via turbulent micro-mixing, while chemical source can be dealt with in exact and closed form (only for pdf).

These closures are summarized in table 1.

Accounting for spray vaporization using SDM

Liquid fuel injection is one of the most common procedures in devices where non-premixed turbulent flames are utilized. Although much works have been devoted to gas-phase turbulent combustion modeling, relatively few studies have focused on the bridges between the turbulent combustion models and the feeding of the reaction zones through droplets vaporization. Indeed, turbulent combustion closures have been essentially developed in the context of an initially gaseous fuel that was more or less mixed with air before reacting. When the fuel is initially in a liquid phase, the three-dimensional spatial distribution of the gaseous reactants depends on complex interactions between the breakdown of the liquid sheets, the vaporization of the liquid, turbulent mixing, and, the combustion itself. Consequently, it is interesting to estimate whether the very basic ingredients of gaseous turbulent combustion modeling need some adjustments to treat the particular case of liquid fuel injection. To this end, Direct Numerical Simulation (DNS) can be used to illustrate how vaporization effects might need to be included in turbulent combustion models to properly account for the properties of the mixing between air and evaporating fuel. Then, a sub-model coupling non-premixed turbulent combustion models with spray need to be proposed [31].

When vaporization occurs, due to the local sources of fuel, the mixture fraction Z is not a conserved scalar, resulting in additional unclosed terms appearing in the transport equations for $\widetilde{Z}$ and $\widetilde{Z''^2}$. In RANS or LES, the liquid phase is usually described using a Lagrangian technique and the sources of fuel, leading to mean sources of $\widetilde{Z}$, are estimated on an Eulerian mesh from fuel droplets tracked in the Lagrangian frame. However, the vaporization source terms found in the budget of $\widetilde{Z''^2}$ are generally neglected in the Eulerian context of the modeling. Consequently, so far the direct effects of spray vaporization on the fluctuations of mixture fraction are not included in most turbulent combustion models.

In a recent investigation of spray turbulent mixing using numerical simulations of an oxidizer gas laden with vaporizing droplets [32], it was observed that the main characteristics of micro-mixing are modified according to the characteristic vaporization time of the liquid. For instance, the mixture fraction spectrum and the small scale mixture fraction dissipation rate are sensitive to the local sources of fuel, leading to an influence of the vaporization time on the characteristic fuel / air mixing time. Accordingly, one may expect $\widetilde{Z''^2}$ to be sensitive to vaporization through the neglected source terms. First, we have used direct numerical simulation to study these sources.

DNS was shown to be useful for studying flows laden with particles [33]. DNS with particles can be extended to the case of vaporizing droplets, with a two-way coupling between the dispersed phase

	Chemistry	Transport	Laminar flames	Turbulent Combustion models
(1)	**Infinitely Fast**		$Y_i = Y_i(Z)$	**Presumed PDF** $\overline{P}(Z)$
	One-step	$Le_i = 1$	[15]	[6]
	Multi-step	$Le_i = 1$	[16]	$\overline{Y}_i = \int_0^1 Y_i(Z)\overline{P}(Z)dZ$
	One-step	$Le_i \neq 1$	$Y_i = Y_i(Z(Z_L))$ [17]	
(2)	**Finite rate**			**Flamelets** (Diffusion+Reaction)
	One-step	$Le_i = 1$	Asymptotic analysis $Y_i = Y_i(Z,\chi)$ [13]	Library of laminar flames and presumed PDF $\overline{P}(Z,\chi)$ $\overline{Y}_i = \int_Z \int_\chi Y_i(Z,\chi)\overline{P}(Z,\chi)dZd\chi$ [18] Density of Flame Surface Σ $\overline{\dot{\omega}}_i = \dot{m}_i\Sigma$ [19]
	One-step	$Le_i \neq 1$	Asymptotic analysis [20] [21]	
	Multi-step	$Le_i \neq 1$	Counter flow calculations $Y_i = Y_i(Z,\chi)$ [22]	Library of laminar flames $\overline{Y}_i = \int_Z \int_\chi Y_i(Z,\chi)\overline{P}(Z,\chi)dZd\chi$ [23]
(3)	**Finite Rate**			**PDF** (Micro-mixing) + (Reaction)
	Multi-step	$Le_i = 1$	Diffusion and Mixing [26]	CMC [24, 25] PDF-GENERATOR [27, 28, 29] PDF transport equation, [30]

Table 1: Modeling strategies for non-premixed turbulent flames may be classified in three groups: (1) When the chemistry is infinitely fast, Y_i the mass fraction of the species and temperature are given via the mixture fraction Z (non-reactive conserved scalar) and by the modified mixture fraction Z_L for non-unity Lewis numbers ($Le_i \neq 1$). To account for local fluctuations, use is made of a presumed form for $\overline{P}(Z)$ the probability density function (pdf) of Z. (2) Under the assumption that turbulent flames may be viewed as a collection of laminar flamelets, asymptotic analysis brings a description of laminar flames parametrized with the mixture fraction and its dissipation rate $\chi = D \mid \nabla Z \mid^2$. The consumption rate of species per unit of flame surface $\dot{m}_i$ is also readily obtained. Then, either a presumed form for the joint pdf $\overline{P}(Z,\chi)$ or a transport equation for the density of flame surface Σ are used to estimate $\overline{Y}_i$ or mean burning rates $\overline{\omega}_i$. (3) Studies of diffusion provide the guideline to develop closures for turbulent micro-mixing needed when using approaches based on one-point pdf. The Conditional Moment Closure (CMC), PDF-Generator techniques or the transport equation for joint pdfs involve micro-mixing closures, while chemical source terms appear in a closed form and may be treated using a detailed chemistry.

and the carrier phase. The simulations correspond to a full DNS of the carrier phase, however the flow inside the drops is not resolved. The droplets are local sources of fuel, properties of which are calculated in a Lagrangian context, whereas the compressible Navier Stokes Equations are solved in the Eulerian context. In addition to the basic limitations of DNS [34, 4], the accurate treatment of the two-way coupling between the two phases imposes new restrictions, and the range of applicability of our simulations is limited to dilute sprays. These problems involving a dilute spray mimic situations that may be observed for instance in aeronautical or rocket engines at a particular stage of the combustion process [35]. To address other regimes of two-phase combustion where the flow inside the drops needs to be resolved, a different DNS technique tracking the liquid interface should be followed [36].

With this new DNS tool, it is possible to study different mixing problems where the fuel is initially in a liquid phase. The generic configuration of homogeneous turbulence was retained, and the DNS data were probed to understand the vaporization terms found in the transport equation for $\widetilde{Z''^2}$. The results confirm that those terms cannot be dropped or large errors may exist in the evaluation of $\widetilde{Z''^2}$.

These vaporization sources are closed when the joint statistics of the Eulerian source of fuel $\dot{W}_v$ and of the mixture fraction is known. DNS studies of the joint probability density function of $\dot{W}_v$ and Z suggest the introduction of the conditional mean source of fuel in the modeling of the fuel vapor sources. Conditional Moment Closure (CMC) has been introduced to model turbulent flames [24]. In CMC the control parameters of flames (e.g. species, temperature) are described via their conditionally averaged quantities. For nonpremixed flames a natural conditioning variable is the mixture fraction Z. Mean values are then obtained at each Eulerian point by integrating the conditioning quantities weighted by the probability density function of the mixture fraction. Using different modeling assumptions, the same type of procedure is utilized in Steady Laminar Flamelet (SLF), where the mixture fraction Z and its dissipation rate χ are the control parameters of conditional mean values describing flamelets [18] (table 1). Along the same lines, a possible route to model the vaporization terms in the equation for $\widetilde{Z''^2}$ consists of introducing the conditional mean value of the vaporization source of fuel $\left(\overline{\dot{W}_v \mid Z^*}\right)$, the conditioning quantity being also the mixture fraction. Once the statistical properties of Z are known through its presumed probability density function (pdf) [37] or via a Monte Carlo solution [30], all unclosed terms related to vaporization sources are directly evaluated from the conditional mean source of fuel.

In this spirit, a closure is proposed for $\left(\overline{\dot{W}_v \mid Z^*}\right)$, that is derived from a single droplet vaporizing in a given volume. In the proposed Single Droplet Model (SDM), the control parameter of the conditional vaporization source of fuel are quantities obtained in RANS or LES from the Lagrangian solution of the disperse phase, e.g. the mean vaporization rate of fuel, the mean diameter of the droplets, the mean spray density, and, the mean diameter of the droplets at injection in the combustion chamber.

Usually, in RANS or LES calculations of complex flows including spray, the mean source of fuel in the equation for $\widetilde{Z}$ results from the Lagrangian procedure. This mean source can also be evaluated from the conditional mean source $\left(\overline{\dot{W}_v \mid Z^*}\right)$, therefore, when coupled with the full numerical solution, to be consistent the new closure must also reproduce the mean source of fuel that was already provided in the Lagrangian context. To fulfill this condition, an additional parameter is dynamically determined in SDM, then the sources in the system of equations for $\widetilde{Z}$ and $\widetilde{Z''^2}$ describing mixing are fully closed.

The accuracy of this novel Single Droplet Model (SDM) is compared against the DNS data, and encouraging results are shown. Because SDM is combined with the statistics of the mixture fraction to provide the vaporization sources, it appears as a generic closure that can be incorporated in turbulent combustion models invoking the Steady Laminar Flamelet assumption [18], it can also be coupled with presumed Probability Density Function (PDF) modeling [29], Conditional Moment Methods [24], or, PDF calculations [30, 38]. Depending on the vaporization of the liquid phase, SDM is then expected to contribute to the approximation of the level of mixture fraction fluctuations $\widetilde{Z''^2}$.

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