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Prediction of NOx in premixed high-pressure lean methane flames with a MMC-partially stirred reactor

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Abstract

The multiple mapping conditioning (MMC) method is used to extend the stochastic PDF approach to the flamelet regimes of premixed combustion. MMC permits for a desired degree of flamelet-like conditions while reflecting the fluctuating nature of turbulent flames and preserving the integrity and universality of the chosen mixing model. The model is implemented in the context of the partially stirred reactor (PaSR), which is therefore generalised to have a wider range of applicability. A stochastic formulation of original MMC is deployed, where mixing of particle scalar values is conditioned on a Markovian reference variable which emulates an implied particle position relative to a flame. The model interactions with the reference variable are controlled through the flamelet localness parameter, Λ, which is also related to the ratio of diffusive to convective time scales. The model is implemented in a Monte Carlo numerical scheme using detailed GRI3.0 chemical kinetics without adjustments of kinetic coefficients. Predictions of NOx emissions are validated against experimental data for a lean premixed high-pressure combustor in which reactions fall between the flamelet and distributed regimes. There is good agreement between model predictions and experimental data.

Keywords: Multiple mapping conditioning; Probability density function; Flamelet; Turbulent premixed combustion; Combined reactors

1. Introduction

The great attraction of probability density function (PDF) models [1] is that, unlike many other turbulent combustion models, species chemical source terms appear in closed form and do not require additional modelling. It can therefore be

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argued that PDF models are generally not constrained to specific turbulent combustion regimes. However, the PDF model equations introduce an unclosed conditional scalar dissipation term, and in the context of a Monte Carlo numerical scheme that term is modelled via a mixing operation. The predictive ability of PDF methods for the non-premixed combustion regime is well established [2]. Conversely, their applicability for premixed flames with high Damköhler numbers has been questioned [3] on the basis of the existence of flamelet regimes. Laminar flamelet models (LFM) [4,5] assume that the turbulent flame is comprised of locally one-dimensional laminar flamelets. LFMs are economical for engineering applications as the laminar flames can be precomputed for subsequent use in turbulent flow simulations [6]. While the LFM represents a rigorous limit for cases when the Karlovitz number approaches zero, realistic premixed flames can possess flamelet features and simultaneously involve strain, stretch, curvature and possible local extinctions. Modelling of these phenomena may be suited to PDF methods which are generally better at handling more distributed flames. There is a large volume of literature dedicated to asymptotic studies of flamelets disturbed by non-uniform fluid flows [4,7–10]. Due to the nature of asymptotic analysis, these works are necessarily limited to studies on small perturbations of laminar flamelets.

In light of the issues mentioned above, several methods have been suggested for accommodating the flamelet regime within the context of PDF models. For example, Pope and Anand [11] and Haworth [12] model the joint velocity-progress variable PDF with embedded premixed structures to account for the tight reactive–diffusive coupling in the flame front and a conventional mixing model for the distributed reaction regime. Such approaches result in a model for both the flamelets and distributed reaction regimes. Klimenko and Pope [13] replace conventional (and conservative) mixing with competitive mixing to emulate the invasion conditions in turbulent premixed flames in the flamelet regime and demonstrate how the propagation speed can be made consistent with existing experimental data [14]. Zoller et al. [15] propose a model for the corrugated flamelet regime which combines the BML approach and a flame surface density closure, with a premixed LFM applied when the reaction progress variable reaches unity.

It is the aim of the present work to incorporate flamelet features into the PDF methodology with the aid of the multiple mapping conditioning (MMC) model [16,17]. MMC is a PDF model which uses independent reference variables with links to physical parameters of the flow to enforce localness in the mixing model. In the context of premixed flames the enforcement of localness is used to avoid mixing between burned and unburned particles across the flame front. Pope [18] introduces the shadow position mixing model (SPMM), which makes use of alternative, *shadow* trajectories of notional particles. SPMM is an MMC-type model which allows the free selection of a localisation parameter and is expected to be efficient in emulating joint scalar-velocity statistics. In the current paper we introduce an MMC model which follows the original stochastic formulation [16]. In the suggested model the reference variable represents an *implied* particle position with respect to the flame front, which has some conceptual resemblance to the use of reference variables in SPMM. Using *implied* position only permits the simulation of flamelet-like conditions and does not account for spatial transport.

The breadth of model validation data for premixed turbulent flames is relatively limited when compared to the availability of data for non-premixed turbulent flames. This shortage is gradually being addressed through high quality experiments such as those for the Sydney piloted premixed jet burner(PPJB) [19] and the Cambridge stratified swirl burner [20], as well as experimental [14] and DNS [21] premixed databases. A number of RANS-PDF and LES-PDF modellers (e.g. Refs[22–27]) have made contributions by validating against these and other experimental databases but once again the body of modelling research is relatively limited when compared to that for non-premixed combustion.

Combustion in a partially stirred reactor (PaSR) is an alternative platform for validation of PDF models. The turbulence is assumed to be statistically homogeneous and isotropic, so that turbulence–chemistry interactions can be investigated without the need for CFD. The PaSR tends to a plug flow reactor (PFR) in the limit of slow mixing and to a perfectly stirred reactor (PSR) in the limit of very fast mixing. An early example of a stirred tank reactor which incorporates mixing, flow-through and reaction is found in Levenspiel and Spielman [28]. The work of Correa [29,30] on premixed methane combustion and Chen [31] on non-premixed hydrogen combustion establishes the PaSR as a tool for analysis of turbulence–chemistry interactions and as a test bed for PDF models. For example, a PaSR is used by Bender et al. [32] to study the coupling of chemistry and turbulent mixing for both detailed and reduced chemical kinetics, and a projection scheme is introduced for mixing models to be used with the intrinsic low dimensional manifold (ILDM) method [33]. As well as being a basis for model development, the PaSR is an important model in itself with application to gas turbine combustors and other chemical reactors. Cannon et al. [34] use a PDF-PaSR model to predict carbon monoxide (CO) and nitric oxide (NOx) emissions for a range of lean and stoichiometric

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