



Modelling nitrogen oxide emissions in turbulent flames with air dilution: Application to LES of a non-premixed jet-flame



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ABSTRACT

The aeronautical industry faces the challenge of designing new engines with a better specific fuel consumption while decreasing pollutant emissions such as nitrogen oxide (NO). To this aim, many Computational Fluid Dynamics (CFD) models have been developed to predict NO emissions. Most of these models are based on a simplified description of the nitrogen chemistry, while few of them attempt to take into account the whole NO chemistry and its interactions with carbon oxidation. This article presents a new model, called NOMANI (Nitrogen Oxide emission model with one-dimensional MANifold), which predicts NO emissions from all chemical processes present in detailed mechanisms and which is well suited to aeronautical burners. To have a good estimation of the NO mass fraction produced in the flame front and in the burnt gases, two progress variables are used. The first one is built from major carbon species, and once carbon chemistry is completed the NO mass fraction is used as a second progress variable with possibility of accounting for dilution by secondary air. This modeling is first assessed thanks to a phenomenological study based on the nitrogen chemistry under dilution by fresh air. The model is then applied and validated in highly resolved Large-Eddy Simulations (LES) of the TNF Sandia Flame D.

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1. Introduction

Large-Eddy Simulations (LES) is a very promising tool in the design chain of aeronautical combustion chambers, because it provides access to unsteady flow features, essential to the description of scalar mixing and turbulent combustion. The major challenge in combustion LES is due to the large spectrum of turbulent and chemical scales, the stiffness of the chemical reactions and the high number of involved species, which imply that the reaction zones cannot be fully resolved and must be modeled. A related issue in the modeling of pollutant emissions arises from the fact that nitrogen oxide (NO) production involves several chemical processes. Most of them have to be taken into account to get accurate predictions of NO emissions in different regions of the flame.

In this paper, a strategy is proposed to compute NO in turbulent flames, on a detailed chemical mechanism chosen; the mechanism is a given input of the model that is not the focus of the study. Here the methane–air GRI-3.0 [1] is used as the reference.

The NO production processes have been intensively investigated in the past, and they can be grouped into two families that evolve with two different characteristic times. The first one corresponding to the prompt NO combines all processes that have the

same characteristic time scale as carbon chemistry. The second major part of the NO production occurs once the exothermic reactions are completed, featuring much larger characteristic time scales. For fuels having no nitrogen atoms in their composition, the prompt NO production in the flame front area is known as the Fenimore mechanism [2]. The prompt NO results from the coupling between the nitrogen and carbon chemistry and has been extensively investigated. Recent works [3–5] highlighted the role of the NCN pathway in the prompt NO formation. Many authors [6,7] have emphasized the importance of evaluating the prompt NO for rich mixtures, even if the temperature remains moderate, *i.e.* $T < 1100$ K. The burnt gas zone combines all the other chemical processes, which produce 90% or more of NO mass fraction. These mechanisms include the Zeldovich mechanism, and those *via* N_2O and NNH [8–12].

The prediction of NO formation in gas turbines is an active research field due to its environmental impact [13]. In the exhaust of combustion chambers, NO is always far from its equilibrium state, because the residence time of these devices is small compared to the time scale needed by NO to reach its equilibrium value [14]. Prompt NO may therefore be significant within the aeronautical context, moreover dilution of burnt gases by secondary air also impacts NO levels.

Numerous RANS (Reynolds Averaged Navier Stokes) and LES models for NO emissions exist. Most of them, which have been

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validated by comparison with experimental data, consist in the solving of a transport equation for the nitrogen oxide mass fraction. This equation needs to be closed since the nitrogen oxide production rate depends on pressure, enthalpy and all species mass fractions of the mixture. Several strategies have been investigated to close the transport equation of the nitrogen oxide mass fraction.

Löffler et al. [15] developed a model that is coupled with a RANS approach. Applying quasi-steady-state (QSS) approximation for intermediate species leads to a linear equation system. It is then possible to close the NO balance equation, but this assumption fails in the flame front; hence, this model is limited to NO produced in the burnt gases. In the flame front, where prompt NO is produced, radicals are not at the equilibrium, and due to the QSS assumption, the model cannot track the prompt NO. As a result, Löffler closure is well suited to predict NO levels for configurations where the prompt NO stays negligible, mostly situations where the equivalence ratio stays below 0.75.

A second approach to close the transport equation of the nitrogen oxide mass fraction is to resort to PDF and Conditional Moment Closure (CMC) methods to handle detailed chemistry in the simulation of turbulent flames [16–19].

An alternative to QSS, PDF and CMC models is the tabulated chemistry approach, which takes into account complex chemistry effects at low cost and complexity. The first tabulated model of nitrogen oxide emission in RANS calculations is presented by Bradley et al. in 1998 [20]. It is dedicated to the prediction of prompt NO formation in lean mixtures. The model consists in solving a transport equation for NO mass fraction, the source term being extracted from a laminar look-up table as a function of a progress variable, which is the normalized temperature. Bradley et al. also proposed to replace the normalized temperature by the NO mass fraction, but stressed that this progress variable is poorly coupled to the temperature field.

A mathematical analysis of chemistry reduction is proposed in the Intrinsic Low-Dimensional Manifold (ILDM) concept, which was introduced in 1992 by Maas and Pope [21]. It is based on the analysis of the local time scales of the chemical system in a phase space. The evolution of the system is decomposed in characteristic times associated with eigenvalues of the Jacobian matrix of the species reaction rates. Through this analysis, Maas and Pope shed light on the existence of a manifold. The evolution along this manifold corresponds to the slowest processes, and the evolution outside the manifold is with fast relaxation times, bringing the mixture composition onto the manifold. Because of this property, it is possible to consider only the low-dimensional manifold instead of working in the high dimensional phase space. Maas and Pope [21] shown that a 1D or a 2D manifold provides accurate results for a system at high temperature, *i.e.* for a progress variable that is closed to its equilibrium value.

Nafe and Maas [22] studied the nitrogen chemistry with the ILDM concept. They found that nitrogen chemistry adds one characteristic time, so that the dimension of the tabulated manifold has to be increased by one. To overcome this difficulty, they decomposed the kinetics into carbon and nitrogen chemistries. Nitrogen chemistry is considered as frozen during carbon oxidation. Under this assumption, the computation of nitrogen oxide is provided by the transport of an extra progress variable, which is NO itself. The drawback of this method comes from the decoupling of the flame reaction zone from the NO production. As a result, it is mostly dedicated to configurations where the prompt NO is negligible.

Since 2007, new approaches based on tabulated flamelets appeared for NO. They are based on canonical combustion problems, as homogeneous reactors or one-dimensional premixed or diffusion flames [23–25]. These approaches are successful to predict the heat release and some species that evolve with the same

characteristic time as the progress variable. For species evolving differently from the usual progress variables, however, standard flamelet models may fail. Nitrogen chemistry and the progress variable Y_c , usually based on major species Y_{CO} , Y_{CO_2} and Y_{H_2O} , feature different characteristic time scales. These differences are illustrated in Fig. 1 where strong variations in NO are observed in burnt gases for a very small variation in Y_c . Due to this property, nitrogen oxide cannot be tabulated as a single function of Y_c .

To improve the capability of tabulated chemistry for predicting the slow evolution of NO, Godel et al. [26] and van Oijen et al. [27] suggested to include nitrogen species in the progress variable composition. This approach is very attractive but the filtered density function of this unique progress variable is very different from the classical progress variable based on CO and CO₂. This is due to the fact that a unique progress variable has to describe the evolution of the chemical system over very different time scales. When using presumed-conditional moment closures, this implies to modify the modeling of the unmixedness factor of the progress variable [28]. Another solution is proposed by Ihme et al. [29], who also discussed a closure based on tabulated chemistry; the NO formation rate is then approximated by adopting a linear scaling of backward reaction rates tabulated versus temperature, pressure and enthalpy. This model also assumes that all species are in steady state, except NO. Three chemical pathways are then considered: prompt NO, N₂O and thermal. Ketelheun et al. [30] compare the Bradley's formalism with the Ihme's formalism used in a premixed regime. Both of these models provided comparable results.

The work of Zöllner et al. [31] shows that the linear approximation is not suitable when the complexity of the chemical kinetics is increased. Due to some species, NO₂ for instance, strong non-linear dependencies exist. To ensure an efficient closure of NO reaction rate, Zöllner et al. integrate the full mechanisms, tabulating nitrogen chemistry with adiabatic and isobaric Perfectly Stirred Reactors (PSR). The NO mass fraction is used as a progress variable for the nitrogen chemistry. Some PSR are computed for the range of equivalence ratios (or mixture fractions) that are encountered during the CFD computation. Their compositions are constructed from the equilibrium state at the considered mixture fraction and temperature, but all nitrogen species are set to zero except the N₂ mass fraction. During the PSR computation only the nitrogen species evolve. According to the authors this approach is accurate for flames where moderate NO concentrations are present.

Introducing the tabulation of relaxation times as a function of perturbation amplitudes, Vervisch et al. [32] present a new model for the emission of thermal NO. This relaxation is tabulated as a function of equivalence ratio, pressure, temperature and dilution mass fraction. This method provides good results when NO is close

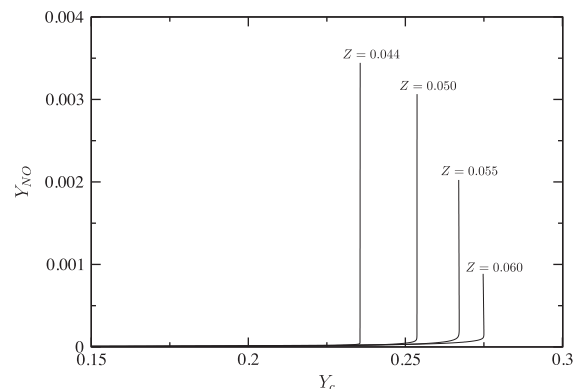


Fig. 1. Evolution of Y_{NO} in a 1D unstretched premixed methane/air flame as a function of the progress variable $Y_c = Y_{CO} + Y_{CO_2} + Y_{H_2O}$ for various mixture fractions Z .

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