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VALIDATION OF REDUCED MECHANISMS FOR NITROGEN CHEMISTRY IN NUMERICAL SIMULATION OF A TURBULENT NON-PREMIXED FLAME

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Abstract

In this paper, the formation of nitrogen pollutants in computational fluid dynamics simulation of turbulent non-premixed flame was modelled by coupling reduced nitrogen chemical reaction mechanisms with comprehensive combustion model.

Keywords: CFD-modeling, NO_x, combustion

INTRODUCTION

Development and application of comprehensive combustion models, advances in the science of NO_x reactions, and dramatic improvements in computer hardware have made a modelling of the NO_x chemical reaction processes a valuable tool in understanding NO_x emissions from combustion systems. Available detailed NO_x chemical kinetic mechanisms come from Miller and Bowman [1], Glarborg [2], Baulch [3-4], Dagaut [5], Glassman [6] and Kilpinen [7]. However, the development of an effective NO_x model requires simplification of such generalized reaction mechanisms, taking into account sufficient details to adequately describe the NO_x reaction process, to allow coupling with the turbulent mixing process in the CFD simulation of practical

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combustion systems. Consequently, reduced kinetic mechanisms can be typically used to describe the NO_x reaction processes, allowing the reduction of calculation time and making this time-consuming method more attractive for industrial applications [8-11]. This paper presents a review of modelling work performed at Department of Energy, Power Engineering and Environment regarding the prediction of NO_x formation in combustion of non-premixed methane-air flame. This modelling work has involved an approach that couples reduced NO_x reaction mechanisms with a detailed description of the combustion process, which are described in the following sections.

A joint solution of detailed CFD equations for turbulent flow, combined with NO_x reduced chemical reaction mechanisms was used for predicting NO_x formation in numerical simulation of turbulent, non-premixed, piloted methane-air jet diffusion flame. Combustion modelling was based on the steady laminar flamelet model [12], where stationary flamelet profiles and appropriate probability density function (PDF) tables were created in pre-processor step by using CSC solver. A detailed chemical reaction mechanism GRI Mech 3.0 for methane, which consists of 53 species and 325 elemental reactions and contains nitrogen chemistry, was used for methane oxidation. A conservative form of the discrete transfer radiation method – DTRM was applied for radiative heat transfer calculation.

COMBUSTION MODEL

For combustion prediction, a steady laminar flamelet model – SLFM [12-15] was employed. The instantaneous values of the species mass fractions and temperature are uniquely related in SLFM to the instantaneous values of mixture fraction as:

$$\rho \frac{\partial Y_i}{\partial \tau} - \rho \frac{\chi}{2} \frac{\partial^2 Y_i}{\partial Z^2} - \dot{\omega}_i = 0 \tag{1}$$

$$\rho \frac{\partial T}{\partial \tau} - \rho \frac{\chi}{2} \frac{\partial^2 T}{\partial Z^2} - \rho \frac{\chi}{2c_p} \frac{\partial T}{\partial Z} \frac{\partial c_p}{\partial Z} - \sum_{i=1}^{N_{spec}} \rho \frac{\chi}{2} \frac{c_{pi}}{c_p} \frac{\partial Y_i}{\partial Z} \frac{\partial T}{\partial Z} + \frac{1}{c_p} \sum_{i=1}^{N_{spec}} h_i \dot{\omega}_i - \frac{q_R}{c_p} = 0 \tag{2}$$

where t is time, Z is the mixture fraction, T is temperature, Y_i , $\dot{\omega}_i$, and h_i are the mass fraction, chemical reaction rate and specific enthalpy of species i, respectively, c_p is the specific heat coefficient, while q_r is the radiative heat gain/loss.

Mixture fraction is a scalar representing the mass fraction of all the elements that originate from the fuel stream. Various definitions of this scalar can be found in [12]. The scalar dissipation rate $\chi = \chi(Z)$ is an important variable and it is given in a parameterized form as:

$$\chi = \chi(Z) = \chi_{st} \frac{\exp\left\{-2\left[erfc^{-1}(2Z)\right]^2\right\}}{\exp\left\{-2\left[erfc^{-1}(2Z_{st})\right]^2\right\}} \tag{3}$$

For given values of the stoichiometric scalar dissipation rate parameter χ_{st} ($0 < \chi_{st} < \chi_{st,\ ext}$) the flamelet equations (Eqs (1) and (2)) are solved in the pre-processing step, using the CSC solver, until the stationary solutions are obtained.

The combustion/turbulence interaction is accomplished via the presumed beta probability density function (beta PDF) as:

$$\widetilde{Y}_i = \int_0^1 Y_i(Z, \chi_{st}) P(Z) dZ \tag{4}$$

$$\widetilde{T} = \int_0^1 T(Z, \chi_{st}) P(Z) dZ \tag{5}$$

where $\widetilde{Y}_i$ is a time-mean mass fraction of the species i and $\widetilde{T}$ is time-mean temperature.

The PDF approach requires two additional transport equations for the mean mixture fraction and its variance, which are calculated as:

$$\frac{\partial\left(\overline{\rho}\widetilde{Z}\right)}{\partial t} + \frac{\partial\left(\overline{\rho}\widetilde{u}_i\widetilde{Z}\right)}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\overline{\rho}\frac{\nu_t}{\sigma_t}\frac{\partial\widetilde{Z}}{\partial x_i}\right) \tag{6}$$

$$\frac{\partial\left(\overline{\rho}\,\widetilde{Z''^2}\right)}{\partial t} + \frac{\partial\left(\overline{\rho}\widetilde{u}_i\,\widetilde{Z''^2}\right)}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\overline{\rho}\frac{\nu_t}{\sigma_t}\frac{\partial\widetilde{Z''^2}}{\partial x_i}\right) + 2\overline{\rho}\frac{\nu_t}{\sigma_t}\left(\frac{\partial\widetilde{Z}}{\partial x_i}\right)^2 - 2.0\overline{\rho}\frac{\widetilde{\varepsilon}}{\widetilde{k}}\widetilde{Z}''^2 \tag{7}$$

By appropriately choosing the stoichiometric scalar dissipation rate χ_{st} parameters and by discretising the mixture fraction moments space, it is possible to calculate the flamelet profiles (Eqs 1 and 2) and to account for turbulence-chemistry interaction (Eqs 4 and 5) in advance, and to create, the so-called, PDF look-up tables for further interaction with CFD code [15].

The reduced reaction mechanisms for nitrogen chemistry

Hundreds of elementary reactions are involved in a detailed description of the formation and destruction of oxides of nitrogen in combustion systems. However, it is not currently feasible to use such detailed reaction mechanisms to model a turbulent reacting system in which large reaction kinetics schemes are coupled with the turbulent fluid dynamics [8]. Consequently, the present model for nitrogen chemistry based on reduced chemical reaction mechanisms was used in commercial CFD code FIRE^{TM} to describe the NO_x reaction process in combustion of hydrocarbon fuels.

NO_x represents a family of seven compounds: nitric oxide (NO), nitrogen dioxide (NO_2), nitrous oxide (N_2O), dinitrogen dioxide (N_2O_2), dinitrogen trioxide (N_2O_3), dinitrogen tetroxide (N_2O_4) and dinitrogen pentoxide (N_2O_5). As far as air pollution is concerned, NO, NO_2 and N_2O are the most important. However, combustion sources emit NO_x mostly in the form of NO, accounting for approximately 90-95% of total NO_x emissions. Thus, the formation of NO determines the total amount of NO_x in this study, while the presence and effects of other nitrogen oxides formed during combustion processes are neglected.

The formation of NO in the combustion processes is characterized by using the following transport equation for the NO mass fraction:

$$\frac{\partial(\bar{\rho}\tilde{Y}_{\mathrm{NO}})}{\partial t}+\frac{\partial(\tilde{u}_i\bar{\rho}\tilde{Y}_{\mathrm{NO}})}{\partial x_i}=\frac{\partial}{\partial x_i}\left(\bar{\rho}D_t\frac{\partial\tilde{Y}_{\mathrm{NO}}}{\partial x_i}\right)+\bar{S}_{\mathrm{NO}} \qquad (8)$$

where $\tilde{Y}_{\mathrm{NO}}$ is the mean mass fraction of NO and $\bar{S}_{\mathrm{NO}}$ is the mean turbulent source of nitric oxide.

The prediction of NO_x emissions may be decoupled from the generalized combustion model and executed after the flame structure has been predicted because total amount of nitrogen oxides formed in combustion are generally low and does not affect the flame structure. Moreover, the different time scales of major species and NO pollutants allow the decoupling of the two processes. NO_x reactions occur at much slower rates than the main heat release, and thus NO_x formation can be analyzed separately.

In this work, the CFD solver was used in a "post-processing" step to solve NO transport equation, where a converged combustion flow field solution was first obtained before performing the prediction of NO formation. Consequently, the quality of the prediction of NO formation is highly dependent on the quality of the flame structure prediction.

The NO in methane flames is formed primarily by two separate reaction processes, thermal and prompt, in the gas phase. It follows that the source term, S_{NO} in Eq. (8), which represents the NO production, is calculated from these two predominant chemical mechanisms as:

$$S_{\mathrm{NO}} = M_{\mathrm{NO}}\left(\frac{dc_{\mathrm{NOthermal}}}{dt} + \frac{dc_{\mathrm{NOprompt}}}{dt}\right) \tag{9}$$

The thermal NO mechanism arises from the thermal dissociation and subsequent reaction of nitrogen and oxygen molecules in combustion air at relatively high temperatures in fuel-lean environment. The major factors that influence thermal NO formation are temperature, atomic oxygen, concentrations of nitrogen and residence time. This process is described by a set of chemical reactions known as the extended Zeldovich mechanism:

$$\mathrm{N_2} + O \overset{k_1}{\leftrightarrow} \mathrm{NO{+}N} \tag{10}$$

$$\mathrm{N} + \mathrm{O_2} \overset{k_2}{\leftrightarrow} \mathrm{NO{+}O} \tag{11}$$

$$\mathrm{N} + \mathrm{OH} \overset{k_3}{\leftrightarrow} \mathrm{NO} + \mathrm{H} \tag{12}$$

Using these three reactions, the net rate of NO formation can be calculated as:

$$\frac{dc_{\mathrm{NO}}}{dt} = k_{1f}c_{\mathrm{O}}c_{\mathrm{N_2}} + k_{2f}c_{\mathrm{N}}c_{\mathrm{O_2}} + k_{3f}c_{\mathrm{N}}c_{\mathrm{OH}} - k_{1b}c_{\mathrm{NO}}c_{\mathrm{N}} - k_{2b}c_{\mathrm{NO}}c_{\mathrm{O}} - k_{3b}c_{\mathrm{NO}}c_{\mathrm{H}} \tag{13}$$

where k_1, k_2, k_3 are the rate coefficients for positive reactions, while k_{1b}, k_{2b}, k_{3b} are for negative reactions. The rate coefficients for reactions (1-3) used in present model are based on the evaluation of Hanson and Salimian [17].

Using the quasi-steady assumption that the rate of consumption of free nitrogen atoms becomes equal to its formation rate, the expression for the overall rate of thermal NO formation process is given by:

$$\frac{dc_{\mathrm{NO}}}{dt} = 2k_{1f}c_{\mathrm{O}}c_{\mathrm{N_2}}\frac{\left(1 - \dfrac{k_{1b}k_{2b}c_{\mathrm{NO}}^2}{k_{1f}c_{\mathrm{N_2}}k_{2f}c_{\mathrm{O_2}}}\right)}{\left(1 + \dfrac{k_{1b}c_{\mathrm{NO}}}{k_{2f}c_{\mathrm{O_2}} + k_{3f}c_{\mathrm{OH}}}\right)} \tag{14}$$

Temperature and remaining unknown species concentrations are obtained from converged combustion code solution.

Prompt NO is formed much earlier in the flame than the thermal NO by chemical reactions between hydrocarbon fragments and atmospheric nitrogen in fuel-rich regions of the flames. The prompt NO formation is significant in most hydrocarbon fuel combustion conditions, such as low temperature and fuel-rich conditions.

The mechanism is initiated by the rapid reactions of hydrocarbon radicals, which arise from fuel fragmentation during combustion, with molecular nitrogen, resulting in the dissociation of the N_2 and in the formation of intermediates such as hydrogen cyanide (HCN):

$$\mathrm{CH_x} + \mathrm{N_2} \leftrightarrow \mathrm{HCN} + \mathrm{N} + \ldots \tag{15}$$

The model used in the present study to predict prompt NO concentration is calculated from the De Soete [16] global model as:

$$\frac{dc_{\mathrm{NO}}}{dt} = kfc_{\mathrm{O_2}}^{b} c_{\mathrm{N_2}} c_{fuel} \exp\left(-\frac{E}{RT}\right) \tag{16}$$

where c denotes the concentration, k is rate constant, E is the activation energy and b is the order of reaction for molecular oxygen. Values of k and E are experimental constants [18]. In the above equation f is an empirical function designed to account for the effect of various aliphatic hydrocarbon fuels and air/fuel ratio effects.

In the following relation for correction factor f, n is the number of carbon atoms in the fuel and Φ is the equivalence ratio.

$$f = 4.75 + 0.082n - 23.2\phi + 32\phi^2 - 12.2\phi^3 \tag{17}$$

The combustion process typically takes place in a turbulent environment, which requires special consideration when predicting NO concentrations. Therefore, incorporating the effects of the turbulent fluctuations on presented NO pollutant reaction process is very important. Time–mean reaction rates of NO cannot be calculated from the time-mean value of temperature because the relationship among NO kinetic rates and temperatures are highly nonlinear. The presumed probability density function (PDF) approach was used to account for effects of turbulent fluctuations on the kinetic rates of NO, integrating the kinetic rates with respect to fluctuating temperature:

$$\overline{S}_{\mathrm{NO}} = \int_0^1 P(T) S_{\mathrm{NO}}(T)\, dT \tag{18}$$

where $P(T)$ is the probability density function of the normalized temperature T, S_{NO} is the instantaneous NO source. For the PDF of the temperature, a beta function is given by:

$$P(T)=\frac{T^{\alpha-1}(1-T)^{\beta-1}\,dT}{\int_0^1 T^{\alpha-1}(1-T)^{\beta-1}\,dT}=\frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)}T^{\alpha-1}(1-T)^{\beta-1} \tag{19}$$

where Γ is given by:

$$\Gamma(z)=\int_0^\infty e^{-t}t^{z-1}dT \tag{20}$$

The parameters α and β depend on the mean value of the temperature from the main combustion calculation and its variance.

$$\alpha=\tilde{T}\left[\frac{\tilde{T}(1-\tilde{T})}{\widetilde{T''^2}}-1\right] \tag{21}$$

$$\alpha=\left(1-\tilde{T}\right)\left[\frac{\tilde{T}(1-\tilde{T})}{\widetilde{T''^2}}-1\right] \tag{22}$$

The temperature variance is calculated in post-processor step by solving the variance transport equation as:

$$\frac{\partial}{\partial t}\left(\bar{\rho}\widetilde{T''^2}\right)+\frac{\partial}{\partial x_i}\left(\bar{\rho}\tilde{u}_i\widetilde{T''^2}\right)=\frac{\partial}{\partial x_i}\left(\bar{\rho}\frac{\nu_t}{\sigma_t}\frac{\partial\widetilde{T''^2}}{\partial x_i}\right)+2\bar{\rho}\frac{\nu_t}{\sigma_t}\left(\frac{\partial\tilde{T}}{\partial x_i}\right)^2-2.0\bar{\rho}\frac{\tilde{\varepsilon}}{\tilde{k}}\widetilde{T''^2} \tag{23}$$

Numerical simulation

The presented reduced reaction mechanisms for nitrogen chemistry were implemented through user functions in commercial CFD code FIRE^{TM} and numerically tested and investigated for turbulent methane-air jet diffusion flame (Sandia flame D), experimentally investigated by Barlow & Frank [19]. The burner configuration is shown in Fig. 1.

The burner is placed in a co-flow of air and the flame is stabilized by a pilot jet. A stream of fuel is injected through the inner tube, while a pilot stream is injected through the outer tube surrounding it and the co-flow of air is injected outside of the pilot, as illustrated in Fig. 1. The fuel is the mixture of 25% methane and 75% air by volume. The bulk velocity of the fuel jet is 49.6 m/s and the temperature is 294 K. The annular pilot burns a mixture of C_2H_2, H_2, air, CO_2 and N_2 having the same equilibrium state as methane/air mixture at Z =

0.27, with temperature 1880 K. The bulk velocity of the pilot is 11.4 m/s. The air co-flow temperature is 291 K, and the velocity is 0.9 m/s.

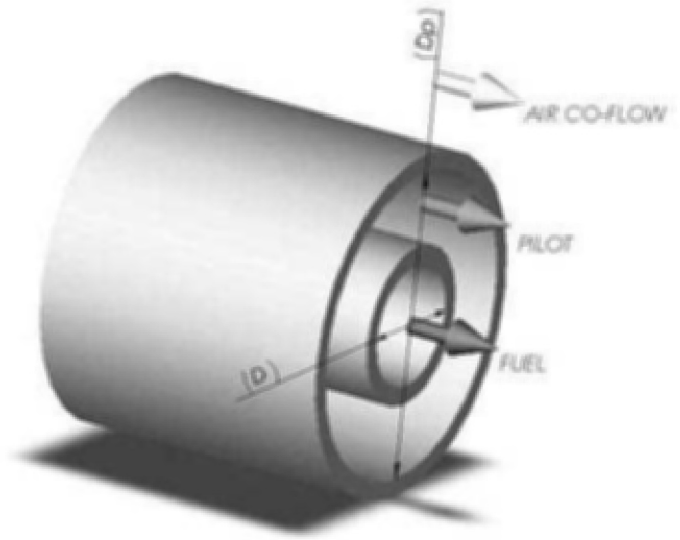

Fig. 1. Burner configuration

The 3D steady-state simulations were performed using the AVL's CFD package FIRE^{TM}, which uses conventional numerical methods and a differencing schemes for a completely arbitrary mesh, and can solve a large computational meshes required for simulating practical combustion devices. The simulation was performed using a computational mesh with 338 400 cells, which are refined towards the inlets and axis.

The methane-air reaction mechanism was taken into account via the SLFM model. Stationary flamelet profiles and appropriate probability density function (PDF) tables were created in a pre-processor step by using CSC solver. The detailed chemical reaction mechanism GRI Mech 3.0 for methane, which consists of 53 species and 325 elemental reactions and contains nitrogen chemistry, was used for the calculation of flamelet profiles in pre-processor step. Turbulent flows were modelled using the standard k-ε turbulence model, which quantifies turbulence in terms of its intensity k and its rate of dissipation ε. The model constant $C_{\varepsilon 2}$ in turbulent kinetic energy dissipation rate transport equation was adjusted to $C_{\varepsilon 2} = 1.8$ instead the standard value in order to obtain the correct spreading rate. The radiative heat transfer was calculated using the discrete transfer method, where the radiative properties are modelled as the weighted sum of grey gases. Reduced reaction mechanisms were used in a post-processing mode, to model nitrogen chemistry, which have little effect on the flow field and the flame structure, as described in the previous section.

RESULTS AND DISCUSSION

The numerical predictions of NO obtained by NO reduced mechanisms for the turbulent non-premixed jet diffusion flame are compared with the results obtained by SLFM and with the experimental data. The experimental measurements of Barlow and Frank (1998) are obtained for axial profile and radial profiles at different locations, which are provided in the web site [19].

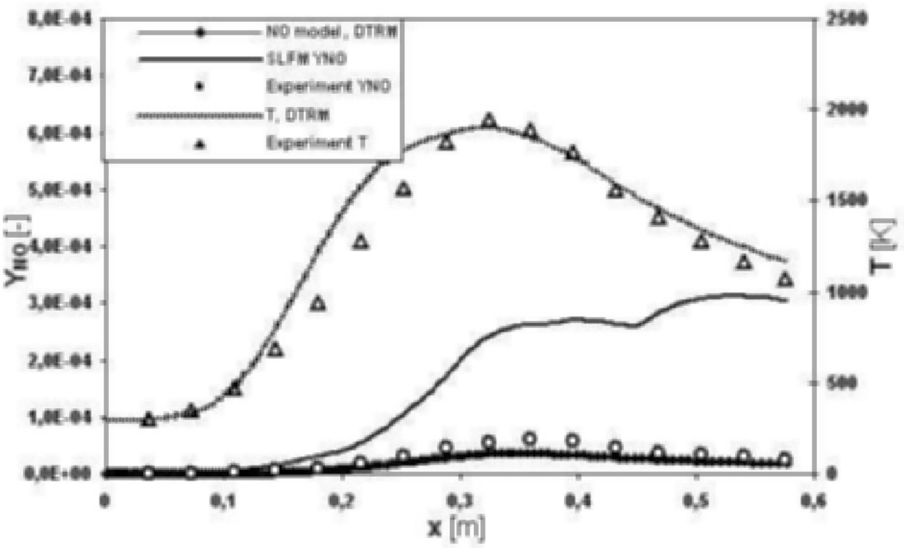

Fig. 2. Axial profiles of mean temperature and NO mass fraction

Figure 2 compares the temperature and NO mass fraction profiles with experimental data along axis symmetry of the burner for Sandia flame D. The predicted NO mass fraction profile obtained by NO reduced reaction mechanism is in good agreement with the experimental data, while NO mass fraction profile calculated by SLFM is over-predicted.

The mean temperature and NO mass fraction profiles along the flame axis obtained with and without radiation modelling are shown in Fig. 3. The adiabatic calculation over-predicts the peak temperature values, while non-adiabatic values (with DTRM) are in better agreement with the experimental

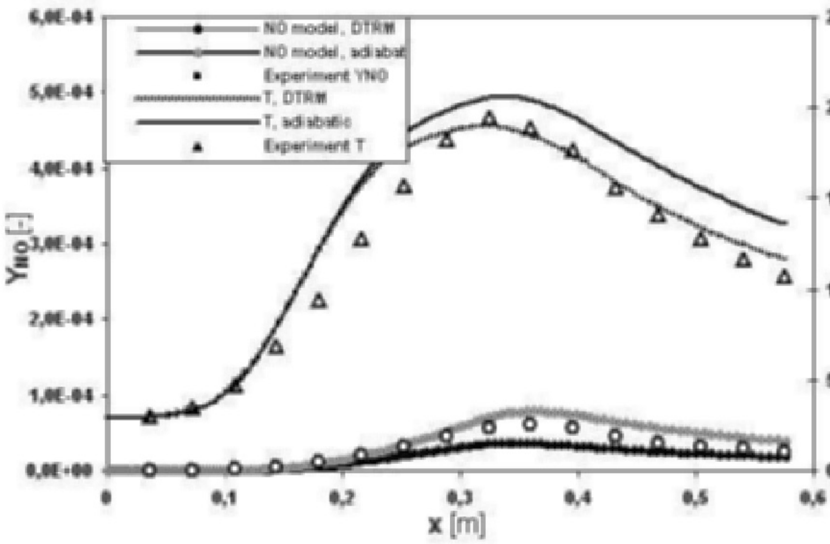

Fig. 3. Axial profiles of mean temperature and mean NO mass fraction

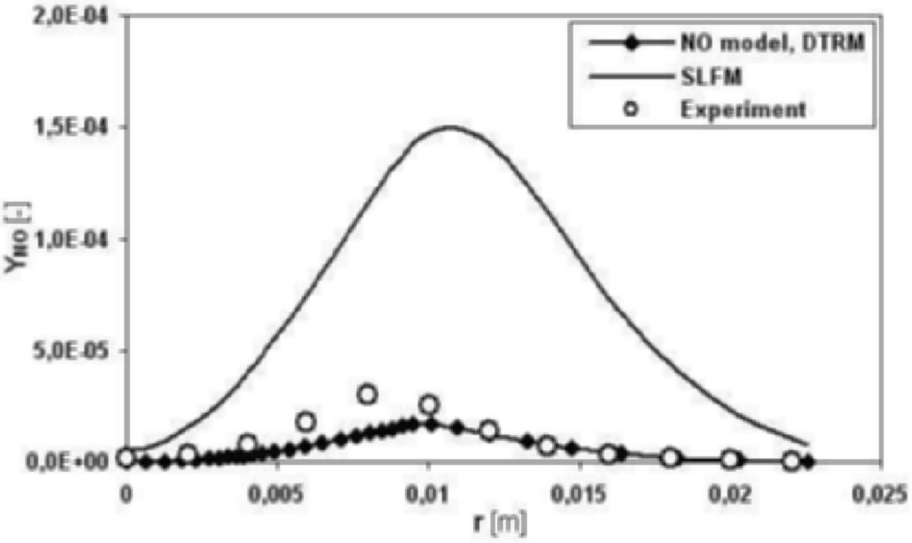

Fig. 4. Radial profiles of mean NO mass fraction at axial distance r/d=15

data, indicating the importance of radiation modelling for the present flame. A similar behaviour is observed with NO mass fraction profile in the case when radiation was not included, while in the non-adiabatic case the NO mass fraction profile is slightly under-predicted. The calculated NO mass fraction profiles show similar trends with the calculated temperature profile, where the temperature maximum corresponds to the peak of the NO concentration.

The radial profiles of NO mass fraction at axial location x/d = 15 are given in Fig. 4. The agreement between the NO mass fraction profile predicted by the reduced NO reaction mechanisms and the measurements is fairly good, while NO concentrations predicted by SLFM are more than several times over-predicted.

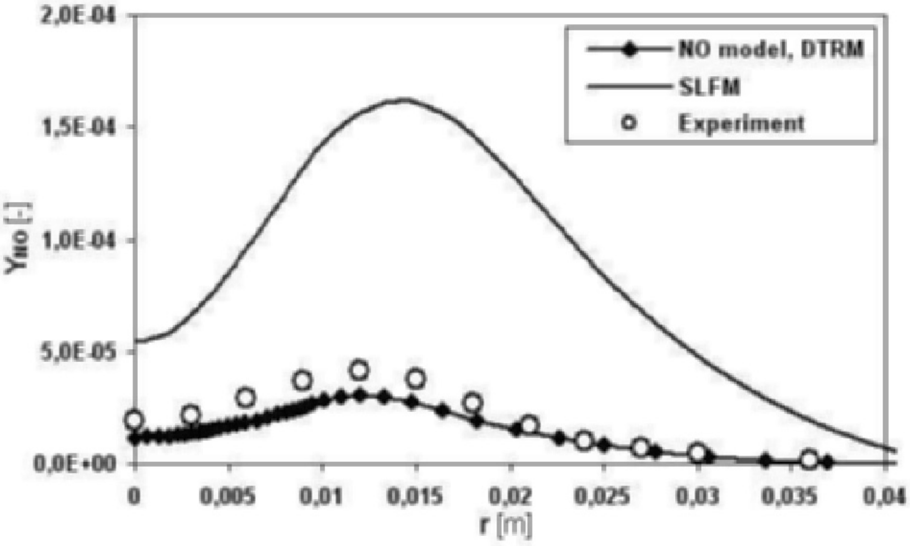

Fig. 5. Radial profiles of mean NO mass fraction at axial distance r/d=30

The radial profiles of mean NO mass fraction are shown in Figs 5-8. The predicted NO mass fraction profiles obtained by NO reduced reaction mechanism are again in fairly good agreement with the experimental data, including the magnitude and radial positions corresponding to peak value. The radial profiles of NO mass fraction obtained by SLFM, also as in the case of axial profile, are over-predicted.

It is noticeable that NO formation calculated by SLFM is clearly over-predicted, making this model inadequate to predict important aspects of the flame as NO concentrations, while using the reduced chemical mechanisms for nitrogen chemistry leads to a significant improvements showing a good agreement with the measurements.

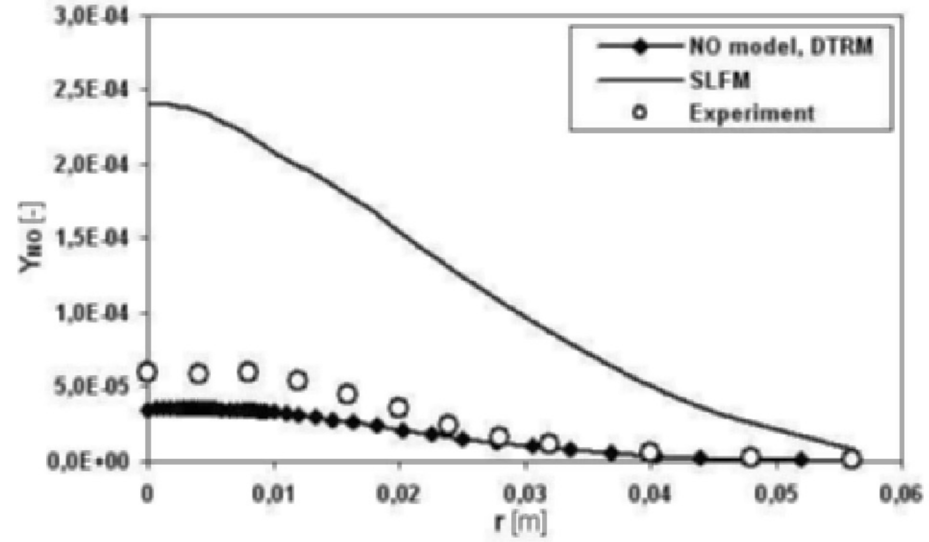

Fig. 6. Radial profiles of mean NO mass fraction at axial distance r/d=45

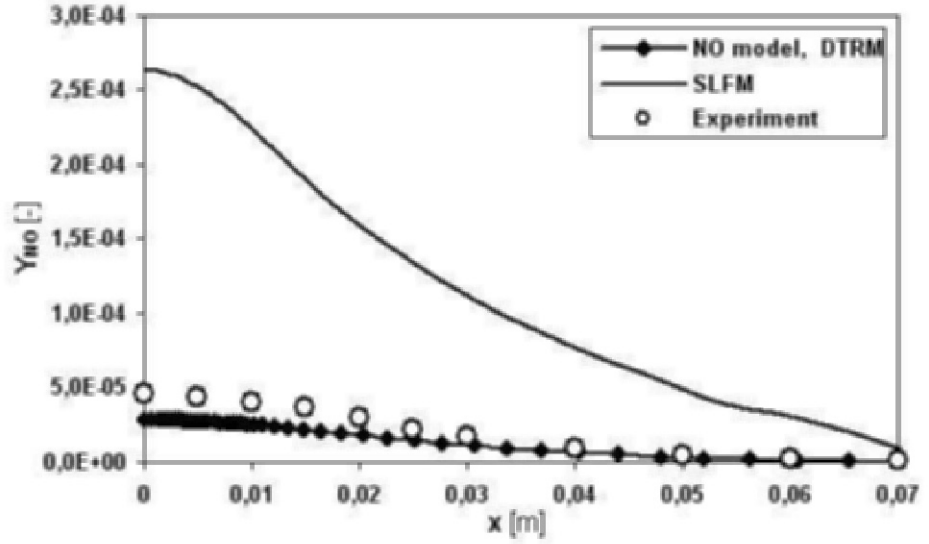

Fig. 7. Radial profiles of mean NO mass fraction at axial distance r/d=60

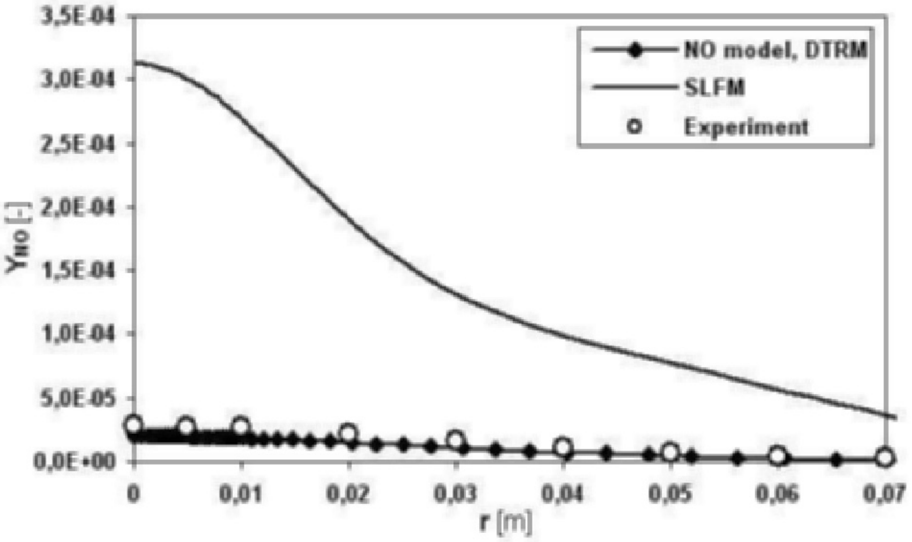

Fig. 8. Radial profiles of mean NO mass fraction at axial distance r/d=75

CONCLUSION

In this paper, reduced chemical reaction mechanisms for nitrogen chemistry were applied to Sandia National Laboratories Flame D, turbulent non-premixed methane-air flame. The NO formation was predicted in the post-processing mode using converged solution of pre-calculated flame structure. Two chemical kinetic processes, thermal and prompt NO, were used to predict NO pollutant emissions. The numerical results of NO formation have been presented in detail and compared with the results obtained by SLFM and with experimental data. The overall agreement between predictions of NO formation, obtained by reduced mechanisms for nitrogen chemistry, and measurements are good, while NO formation calculated with SLFM is over-predicted quite severely. It has been shown that the results obtained with reduced mechanisms provide a significant improvement over the SLFM nitric oxide results.

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