Introduction

Combustion is a complex phenomenon that is controlled by many physical processes including thermo-dynamics, buoyancy, chemical kinetics, radiation, mass and heat transfers and fluid mechanics. This makes conducting experiments for multi-species reacting flames extremely challenging and financially expensive. For these reasons, computer modeling of these processes is also playing a progressively important role in producing multi-scale information that is not available by using other research techniques. In many cases, numerical predictions are typically less expensive and can take less time than similar experimental programs and therefore can effectively complement experimental programs [1].

The formation of NOx during a combustion process occurs in three ways. These are thermal NOx, fuel NOx and prompt NOx. Thermal NOx is formed from the reaction of molecular nitrogen with oxygen atoms in the burning air at high temperatures over 1800 °C. It was defined by Zel'dovich as $\text{N}_2 + \text{O} \rightarrow \text{NO} + \text{N}$, $\text{N} + \text{O}_2 \rightarrow \text{NO} + \text{O}$, $\text{N} + \text{OH} \rightarrow \text{NO} + \text{H}$ reactions. Fuel NOx results from oxidation of nitrogen's compounds and nitrogen in fuel. Prompt NOx is formed from the reaction of carbon and hydrocarbon radicals with molecular nitrogen in the burning air in fuel-rich conditions [2].

Thermal NO can be reduced by decreasing the flame temperature or limiting the oxygen concentration. The formation of NO in a combustion process in a gas turbine combustion chamber, is a very complicated problem due to many parameters that influence its formation process. These parameters include such as, fuel composition, excess air, preheating temperature, fuel to air ratio, inlet air temperature and velocity and combustion air swirl angle [2, 3].

In this paper the numerical calculation of the combustion process in a simple cylindrical combustor is a 2-dimensional problem that involves various options of inlet-air velocity, to predict NOx formation mechanisms. Effects of increased inlet-air velocity on NOx formation are examined. Numerical results show that NO formation mechanisms, decrease, with increasing inlet-air velocity. The simulation has been performed using the Computational Fluid Dynamics (CFD) commercial code ANSYS CFX release 15, including laminar flamelet model, for simulating the methane combustion mixing with air (none-premixed combustion) and predicting concentration of $(\text{CH} - \text{CH}_2 - \text{H}_2 - \text{OH})$. k-model was also investigated to predict the turbulent combustion reaction, which indicated the simulation results of velocities, temperatures and concentrations of combustion productions. A thermal and prompt NOx formation is performed for predicting NO emission characteristics. A comparison between the various inlet-air velocity, and their effects on NO emission characteristics and temperature fields are presented.

Key words: Computational Fluid Dynamics (CFD), Flamelet model, oxide of nitrogen, non-premixed combustion, turbulent combustion.
provided by the Flamelet library. This is in contrast to the standard Thermal NO PDF reaction that approximates O radical concentration from O2 concentration and temperature. There is no need to do this when running the Flamelet model since O is one of the components. 2- Prompt NO and methane PDF, so this reaction accounts for NO formation by the prompt NO mechanism [4].

For the reaction rates of thermal and prompt NO, the Arrhenius equation with temperature PDF was performed. PDF (probability density function) is a mathematical model that describes the probability of events occurring over time. This function is integrated to obtain the probability that the event time takes a value in a given time interval [4].

1. Governing equations

The numerical model of turbulent combustion is formulated from the Favre-averaged Navier-stokes equation together with turbulence and combustion models. Favre-averaged Navier-stokes equation can be expressed in Cartesian tensor notation as: [5]

\[
\frac{\partial \bar{\rho} \bar{u}_j}{\partial x_j} = 0, \quad (1)
\]

\[
\frac{\partial}{\partial x_j} (\bar{\rho} \bar{u}_j \bar{u}_i) = \frac{\partial \bar{P}}{\partial x_j} + \mu_{\text{eff}} \left( \frac{\partial \bar{u}_j}{\partial x_i} + \frac{\partial \bar{u}_i}{\partial x_j} \right). \quad (2)
\]

Where \( \mu_{\text{eff}} \) is effective viscosity given by:

\[
\mu_{\text{eff}} = \mu + \mu_t. \]

The eddy viscosity \( \mu_t \) is given by:

\[
\mu_t = PC_{\mu} \frac{k^2}{\varepsilon}. \]

In this paper, the standard k-\( \varepsilon \) turbulence model has been used to model turbulent kinetic energy, \( k \) is one of the form:

\[
\frac{\partial}{\partial x_j} (\bar{\rho} \bar{u}_j \bar{k}) = \frac{\partial}{\partial x_j} \left( \frac{\mu_t}{\sigma_k} + \frac{\partial \bar{k}}{\partial x_j} \right) + G - \varepsilon. \quad (3)
\]

Where \( G \) is turbulence production due to strain and is given by:

\[
G = \mu_t \left( \frac{\partial \bar{u}_j}{\partial x_j} + \frac{\partial \bar{u}_i}{\partial x_i} \right). \]

The transport equation for the dissipation of turbulent kinetic energy is of the form

\[
\frac{\partial}{\partial x_j} (\bar{\rho} \bar{u}_j \varepsilon) = \frac{\partial}{\partial x_j} \left( \frac{\mu_t}{\sigma_{\varepsilon}} + \frac{\partial \bar{\rho} \varepsilon}{\partial x_j} \right) + C_{\varepsilon} \frac{\bar{\rho}}{k} G - C_{\varepsilon 2} \bar{\rho} \frac{\varepsilon^2}{k}. \quad (4)
\]

Where \( C_{\varepsilon 1}, C_{\varepsilon 2}, \sigma_{\varepsilon}, \sigma_k, \sigma_{\varepsilon} \) are the model constants.

2. Flamelet model of combustion

The flamelet concept for non-premixed combustion describes the interaction of chemistry with turbulence in the limit of fast reactions (large Damköhler number) [4]. The combustion is assumed to occur in thin sheets with inner structure called flamelets. The turbulent flame itself is treated as an ensemble of laminar flamelets that are embedded into the flow field. The Flamelet model is a non-equilibrium version of the classical «Burke-Schumann» limit [4]. It adds new details to the simulation of combustion processes compared to other common combustion models for the price of the solution of only two scalar equations in the case of turbulent flow. An arbitrary number of intermediates may be specified as long as their laminar chemistry is known. The main advantage of the Flamelet model is that even though detailed information of molecular transport processes and elementary kinetic reactions are included, the numerical resolution of small length and time scales is not necessary. This avoids the well-known problems of solving highly nonlinear kinetics in fluctuating flow fields and makes the method very robust. Only two scalar equations have to be solved independent of the number of chemical species involved in the simulation. Information of laminar model flames are pre-calculated and stored in a library to reduce computational time. On the other hand, the model is still restricted by assumptions like fast chemistry or the neglecting of different Lewis numbers of the chemical species [4].

According to the laminar flamelet concept studies, by Peters (1984) and by Bray and Peters (1994), a turbulent non-premixed flame is considered to be comprised of an array of laminar ones. A conserved scalar variable, the mixture fraction, is then introduced to describe the flame structure, with the thermochemical state variables and mixture fraction relationships obtained either from laminar flame measurements by Moss et al (1988) or by performing calculations of one-dimensional, adiabatic counter-flow laminar diffusion flames with a detailed chemical kinetic scheme, as a function of the strain rate [6,7]. Mean values of the thermochemical state variables, such as gas density, species concentrations and temperature, can then be evaluated using a joint probability density function (PDF) of the mixture fraction and strain rate, which is frequently decomposed into a product of presumed individual PDFs [6,7]. Peters (1984) presented an extensive review of flamelet approach for modelling turbulent combustion. By transformation of the physical coordinate into one with the mixture fraction and under the thin flame assumption, it was shown by Peters (1984) that in
the steady state, temperature $T$, and species mass fraction $Y_k$ are determined by the balance between diffusion and chemical reaction [6,7].

Under flamelet regime hypothesis [7], the species transport equation are simplified to:

$$\rho \frac{\partial Y_k}{\partial t} + \frac{\rho u_i}{2} \frac{\partial^2 Y_k}{\partial Z^2} = \omega_k.$$  \hspace{1cm} (5)

A detailed chemical mechanism (combustion of methane mixing with air) of 17 spices and 55 reactions was adopted in this numerical simulation.

The simplified energy equation is:

$$\rho \frac{\partial T}{\partial t} + \frac{\rho u_i}{2} \frac{\partial^2 T}{\partial Z^2} = \frac{1}{C_p} \sum_{k=1}^{N} h_k \omega_k.$$ \hspace{1cm} (6)

Where $Z$ is mixture fraction, $\chi_i = 2D_i (VZ)^2$ (laminar scalar dissipation), $\omega_k$ is the chemical source term, $C_p$ is the mean mixture specific heat, $D$ is thermal diffusivity which is equal to: $D = \lambda / \rho C_p$, where $\lambda$ is thermal conductivity, $L_k = D / D_k$ is the Lewis number of the $k$-th species and $D_k$ is the diffusion coefficient of species $k$.

An external program in ANSYS CFX called CFX RIF (representative interactive flamelet), solves these equation to obtain a laminar flamelet table, which is integrated using a Beta PDF to generate the turbulent flamelet library [4, 8].

This library provides the mean species mass fraction as functions of mean mixture fraction $\tilde{Z}$ and variance of mixture fraction $\tilde{Z}^2$ and turbulent scalar dissipation rate $\tilde{\chi}$ [4, 8]:

$$Y_i = Y_i(\tilde{Z}, \tilde{Z}^2, \tilde{\chi}_{\text{tot}}).$$ \hspace{1cm} (7)

On the other hand 2 transport equation are solved in the CFD code, the first gives mixture fraction:

$$\frac{\partial \tilde{Z}}{\partial t} + \frac{\partial (\rho u_i \tilde{Z})}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \left( \mu + \frac{\mu_t}{\sigma_z} \right) \frac{\partial \tilde{Z}}{\partial x_j} \right).$$ \hspace{1cm} (8)

And the second gives the mixture fraction variance:

$$\frac{\partial \tilde{\chi}}{\partial t} + \frac{\partial (\rho u_i \tilde{\chi})}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \left( \mu + \frac{\mu_t}{\sigma_z^2} \right) \frac{\partial \tilde{\chi}}{\partial x_j} \right) + 2 \frac{\mu_t}{\sigma_z} \left( \frac{\partial \tilde{Z}}{\partial x_j} \right)^2 - \rho \tilde{\chi}.$$ \hspace{1cm} (9)

The turbulence dissipation scalar is modelled by:

$$\tilde{\chi} = C_{\chi} \frac{\tilde{Z}}{k} \tilde{Z}^2.$$ \hspace{1cm} (10)

The fuel properties are specified by the product gases in the downstream level. For turbulent flames, the mean scalar variables are computed from the laminer flamelet relation of the mixture fraction and the scalar dissipation rate by integration over a joint probability density function as: [6]

$$\tilde{\phi} = \int_{0}^{\infty} \int_{0}^{\infty} \tilde{\rho}(Z, \chi) P(Z) P(\chi) dZ d\chi.$$ \hspace{1cm} (11)

The assumption of statistical independence leads to

$$P(Z, \chi) = P(Z) P(\chi)$$

Ass suggested by peter (1984) [7].

3. Nox modelling

The formation of NO is a slow process which kinetically rate limited. Unlike other species the mean value of NO can not be obtain from flamelet library using equation (11) [9].

When modeling NOx formation in methane/air combustion, the thermal NO and prompt NO are taken into account. In the simulation process, we solve the mass transport equation for the NO species, taking into account convection, diffusion, production and consumption of NO and related species. This approach is completely general, being derived from the fundamental principle of mass conservation. For thermal and prompt NOx mechanisms, only the following NO species transport equation is needed: [10]

$$\rho \frac{\partial Y_{NO}}{\partial t} + \rho u_i \frac{\partial Y_{NO}}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \rho D \frac{\partial Y_{NO}}{\partial x_j} \right) + S_{NO}.$$ \hspace{1cm} (12)

The source term $S_{NOx}$ is to be determined for different NOx mechanism.

4. Thermal NO

The thermal NO mechanism is a predominant source of NOx in gas flames at temperatures above 1800 K. The NO is formed from the combination of free radical O and N species, which are in abundance at high temperatures. The two-step mechanism, referred to as the Zeldovich mechanism, is thought to dominate the process [4].

$$O + N_2 \rightarrow k_1 \rightarrow NO + N \quad (R-1)$$

$$N + O_2 \rightarrow k_2 \rightarrow NO + ON \quad (R-2)$$

In sub or near stoichiometric conditions, a third reaction may be important:
When this step is included with the first two, it is referred to as the extended Zeldovich mechanism.

The name of thermal is used because the reaction rate of the first reaction has very high activation energy due to the strong triple bond in the N2 molecules, and thus sufficiently fast only at high temperature [11]. The first reaction is the rate-limiting step of the thermal NO formation.

The rates of each of these three reactions are expressed as:

\[ k_1 = 1.8 \times 10^4 \exp(-318 k J/mol^-1)/(RT) cm^3/(mol.s) \]
\[ k_2 = 6.4 \times 10^9 T \exp(-26 k J/mol^-1)/(RT) cm^3/(mol.s) \]
\[ k_3 = 3.8 \times 10^{13} \]

For the rate of formation of NO one obtains according to the reactions (1-3):

\[ \frac{d[NO]}{dt} = k_1[O][N_2] + k_2[N][O_2] + k_3[N][OH]. \]

(13)

Because

\[ \frac{d[NO]}{dt} = k_1[O][N_2] - k_2[N][O_2] - k_3[N][OH]. \]

(14)

And the Nitrogen atoms can be assumed to be in quasi-state (first reaction in step (2) and (3), i.e. \( d[N]/dt \approx 0 \)), one obtain for the NO formation:

\[ \frac{d[NO]}{dt} = 2k_1[O][N_2]. \]

(15)

Thus it can be seen that NO can be minimized by decreasing \([N_2]\), \([O]\) or \(k_1\) (i.e. by decreasing the temperature) [11].

When using the Laminar Flamelet model, almost always the O radical concentration can be taken without further assumptions from the solution because the model predicts it directly [4].

5. Promp NO (Fenimore mechanism)

The mechanism of prompt or Fenimore NO was postulated by C.P. Fenimore(1979), who measured \([NO]\) above a hydrocarbon flat flame and noted that \([NO]\) did not approach zero as the probe approached the flame from the downstream side, as the Zeldovich mechanism predicts [11]. The additional mechanism that is promptly producing \([NO]\) at the flame front is more complicated than thermal NO, because the prompt NO results from the radical CH, which was previously considered to be an unimportant transient species that is generated through a complex reaction scheme shown in Fig. 1. The CH which is formed as an intermediate at the flame front only, reacts with Nitrogen of the Air, forming hydrocyanic acid(HCN), which reacts further to NO [11].

Hydrocarbon radicals can react with molecular to form HCN, which may be oxidized to NO under lean flame conditions.

\[ CH + N_2 \rightarrow HCN + N \]
\[ HCH + O_2 \rightarrow NO + \ldots \]

The complete mechanism is very complicated. However, De Soete (also Peters and Weber, 1991) proposed a single reaction rate to describe the NO source by the Fenimore mechanism, \(S_{NO,prompt}\)

\[ S_{NO,prompt} = W_{NO}k_{prompt}[O_2]^{1/2}[N_2][fuel]\]

\[ k_{prompt} = A_{prompt} \exp(-T_{A,prompt}/T) \]

\(w_{NO}\) and W denote molar mass of mixture, respectively. The Arrhenius coefficient depends on fuel (De Soete, 1974) proposed the following values if the methane as is the fuel:

\[ A_{prompt} = 6.4 \times 10^6 [1/s] \]
\[ T_{A,prompt} = 36510[K] \]

![Fig. 1. Mechanism of the oxidation of C1- and C2-hydrocarbons (Warnatz 1981a, 1993)](image-url)
6. The domain of simulation and its simple geometrical parameters

The simple symmetry 2D model of our domain of simulation, with the fuel inlet (methane) and oxidizer inlet (air) is shown in fig. 2. Methane and air are entered in the domain separately. The symmetrical geometrical sizes of the domain are on XY system of coordinate, where X=1.8 meters and Y=0.225 meters. The model was meshed for simulating in a hexahedrons meshing method, with 9935 total number of nodes, and 8075 total number of number of elements that are shown in fig.3.

![Fig. 2. The 2D symmetrical domain of simulation and its geometrical parameters](image)

![Fig. 3. The 2D hexahedral mesh for simulation of combustion](image)

7. Information about the numerical simulation

In this paper, the numerical simulation was performed, in 5 various velocity of air, at the inlet of the domain. All the information about these various simulation are shown in table 1.

| 5 various cases and the related informations for the simulation of combustion for predicting NO |
|---------------------------------|------|------|------|------|------|
| Case 1 | Case 2 | Case 3 | Case 4 | Case 5 |
| Fuel | CH4 | CH4 | CH4 | CH4 | CH4 |
| Oxidizer | O2 | O2 | O2 | O2 | O2 |
| Inlet velocity of air (m/s) | 0.5 | 1 | 1.5 | 2.5 | 4 |
| Inlet velocity of methane (m/s) | 80 | 80 | 80 | 80 | 80 |
| Pressure (atm) | 1 | 1 | 1 | 1 | 1 |
| Temperature of fuel (K) | 300 | 300 | 300 | 300 | 300 |
| Temperature of oxidizer (K) | 300 | 300 | 300 | 300 | 300 |
| Reynolds number | 1.45×10^3 | 2.79×10^3 | 4.13×10^3 | 6.81×10^3 | 1.1×10^4 |
| Mach number | 7.41×10^{-4} | 1.43×10^{-3} | 2.11×10^{-3} | 3.49×10^{-3} | 5.54×10^{-3} |
| Turbulent model | k- | k- | k- | k- | k- |
All of 5 cases of simulation was simulated in ANSYS CFX solver. The convergence criteria in this simulation was at the MAX residual type with the $10^{-4}$ residual target. The physical timescale for this combustion simulation was 0.003[s]. All the simulation were converged successfully with solving the mass and momentum (U, V, W momentums), heat transfer (energy), turbulence (k-), mass fraction of NO, mixture fraction including mean and variance, temperature variance for predicting oxide of Nitrogen. The case 1 was converged in 927th iteration, the case 2 was converged in 527th iteration, and the case 3 was converged in 442th iteration, the case 4 was converged in 386th iteration and the last case means case 5 was converged in 330th iteration.

It is clear that, all of the convergence iterations are different from another, it means the maximum iteration is for case 1 and the minimum for case 5. This can be a good and useful subject for the future works to discuss.

8. Results and discussion of simulation

The results of the simulation are presented in fig. 4 for distributing and predicting of NO concentrations and mass fractions for 5 various cases with various for inlet-air velocity.

In fig. 5 the temperature field and counters are presented for predicting temperature distributing during the formation of oxides of Nitrogen for 5 various cases with various for inlet-air velocity.

Fig. 4. Distribution and mass fraction fields of NO for the 5 various air-inlet velocity
The contour and fields of NO distributions in fig. 4 and temperature fields and contours in fig. 5 show that, with increasing the air-inlet velocity in the domain of combustion area, the concentration of NO and temperature will decrease. This means that, the maximum concentration of NO in case 1 is 0.00039897% which means 3.6594ppm, which gives the maximum temperature about 2115.6 K at the air-inlet velocity equal to 0.5 m/s. also the results in fig. 4 and fig. 5, show that the maximum concentration of NO in case 2 is 0.000353% (3.53 parts per million) and the maximum temperature is 2091.9 K, at the air-inlet velocity equal to 1 m/s. The results in case 3 says that, at the air-inlet velocity equal to 1.5 m/s, the maximum concentration of NO is 0.00030729% (3.0729ppm) which has a maximum temperature of 2090.6 K. In case 4 the air-inlet velocity is 2.5 m/s and so the results in this case says that the maximum concentration of NO is 0.00027005% (2.7005 ppm) which gives the maximum temperature of 2085.4 K. And the results in case 5 says the the maximum concentration of NO is 0.00023304% (2.3304 ppm) which gives the maximum temperature of 2077.3 when the air-inlet velocity is 4 m/s.

All the results in NO concentration in various air-inlet velocities, shown in a graph in fig. 6, which describes variance or changing of concentrations of NO along the X direction of our domain of combustion area.

The changing in temperature and NO concentration in various cases in this simulation are clear, which mean that the minimum temperature is 2077.3 K with the minimum of NO concentration, 2.3304 ppm, in case 5 which has the most greater air-inlet velocity, which is 4 m/s and the maximum temperature in this study is 2115.6 K. and NO concentration is 3.6594ppm for the case 1 which has the most smaller air-inlet velocity which is 0.5 m/s.
Conclusion

1. All of this combustion simulation was performed on ANSYS CFX released 15.
2. Laminar flamelet model is an appropriate method for predicting the various kind of fuel with the minor species such as (CO-H), but it is not recommended for predicting the formation of NO and those who related to simulating of emission characteristic, because in flamelet model the transport equation are not solve for the formation of NO.
3. Thermal and prompt modeling of Nox are the best solution to predict Nox and its characteristic of formation during the various condition of the problem.
4. In this paper we tried to show the effect of various velocity of air at the inlet of domain, on formation of NOx and variance of temperature in these conditions. It is clear that the most optimized option, is the case 5, which had a large amount of velocity compared to the other cases. The results showed that the percentage of NO and minimal temperature field was in case 5.
5. Decreasing the temperature and oxide of Nitrogen is one of the interesting and complicated problem for combustion engineers. There are a lot of methods to decrease them such as the regulation of humidity of air, the regulation of temperature of fuel or preheating air entering the area or domain of the combustion, design the swirlers for ensuring the turbulent combustion and adjust the emission characteristics, and design the dilution holes for cooling system of gas turbine combustion chambers including decreasing formation of oxide of Nitrogen.

References


Масуд Хаджинанд. Моделирование влияния входной скорости воздуха на образование оксидов азота в метановоздушном горении без предварительного смешивания

Выполнено численное моделирование горения воздушной смеси метана без предварительного смешивания потоков. Целью этой статьи является предоставление информации о влиянии скорости воздуха на входе на выбор оксидов азота в выхлопных газах для простого типа камеры сгорания. Показано влияние повышенной скорости воздуха на входе на формирование NOx. Численные результаты показывают, что NO механизмы формирования снижаются с ростом скорости воздуха на входе. Моделирование было выполнено с использованием программы для вычислительной гидродинамики (CFD) ANSYS CFX выпуска 15, в том числе laminar flamelet модель для моделирования горения смешанных метана с воздухом (без предварительного смешивания) и прогнозирования концентрации (CH2-CH=CH2 O=CH CO=CO2 O=O2 H=H2 O=O2 H2O=H2O2 OH). К- модель была также исследована для прогнозирования турбулентной реакции горения, в которой указаны результаты моделирования скоростей, температуры и концентрации продуктов сгорания. Тепловое и быстрое NOx формирование осуществляется для прогнозирования эмиссионных характеристик оксидов азота. Представлено сравнение между различными скоростями воздуха на входе и их влияние на NO эмиссионных характеристик и температурных полей.

Ключевые слова: вычислительная гидродинамика (CFD), flamelet модель, оксид азота, горение без предварительного смешивания, турбулентное горение.

Масуд Хаджинанд. Моделирование влияния входной швидкости повітря на утворення оксиду азоту в метановоздушному горінні без попереднього змішування

Виконано чисельне моделювання горіння повітряної суміші метану без попереднього змішування потоків. Метою цієї статті є надання інформації про вплив швидкості повітря на вході на викид оксидів азоту у вихлопних газах для простого типу камери згорання. Показано вплив підвищеної швидкості повітря на вході на формування NOx. Чисельні результати показують, що NO механізми формування зменшуються з ростом швидкості повітря на вході. Моделювання було виконано з використанням програми для обчислювальної гідродинаміки (CFD) ANSYS CFX випуску 15, в тому числі laminar flamelet модель для моделювання горіння змішування метану з повітрям (без попереднього змішування) і прогнозування концентрації (CH2-CH=CH2 O=CH CO=CO2 O=O2 H=H2 O=O2 H2O=H2O2 OH). К- модель була також досліджена для прогнозування турбулентної реакції горіння, в якій вказано результати моделювання швидкостей, температури і концентрації продуктів згорання. Теплове і швидке NOx формування здійснюється для прогнозування емісійних характеристик оксидів азоту. Представлено порівняння між різними швидкостями повітря на вході та їх вплив на NO емісійних характеристик і температурних полів.

Ключові слова: обчислювальна гідродинаміка (CFD), flamelet модель, оксид азоту, горіння без попереднього змішування, турбулентне горіння.