Investigation of the contribution of homogeneous flame fronts to the formation of NOx in combustion chambers with promising fuel combustion schemes

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Abstract. Specifics of nitrogen oxides formation in conditions of partially mixed combustion in combustion chambers in the presence of diffusion and homogeneous flame fronts are studied. A NOx emission calculation procedure based on detailed kinetics, including all NOx formation mechanisms, is proposed. NOx emission values calculated using the complete detailed kinetics and kinetics containing only the Zel'dovich mechanism are compared. A methodology for estimating the effect of homogeneous flame fronts on NOx emission is proposed and verified. Under conditions of the model problem, a contribution of homogeneous flame fronts to total NOx emission is studied. Combustion conditions with a considerable contribution of homogeneous fronts to total NOx emission are shown.

1. Introduction

At present, an improvement of emission characteristics of combustion chambers for engineering systems retain its relevance, despite developments of environmentally friendly hydrocarbon fuel combustion layouts. Among methods aiming at a decrease in nitrogen oxide (NOx) emissions, the most promising are methods based on fuel combustion in premixed (homogeneous) fuel mixtures.

The occurrence of homogenization in combustion layouts complicates estimations of total NOx emission levels and requires a further improvement of prediction (analytical) models. This paper is devoted to studies the contribution of homogeneous flame fronts to total NOx emission produced by combustion chambers. The analysis of NOx formation on homogeneous fronts is aimed at an increase in accuracy of total NOx emission estimations due to a more adequate description in models the combustion pattern in combustion chambers with homogenization. This will provide data for further improvements of combustion systems.

At present, when estimating NOx emission in combustion chambers without preliminary fuel-air mixture homogenization that are widely used in a number of engineering systems, the contribution of homogeneous flame fronts is not taken into account in NOx emission calculations. This does not introduce a considerable error into emission estimates, because, in accordance with concepts proposed by V.R. Kuznetsov [1], nitrogen oxides are formed, mainly, in high-temperature areas near the stoichiometric surface \( z = z_s \), where \( z \) – recovered fuel concentration, and \( s \)-index characterizes its stoichiometric value.

To decrease NOx emissions with the aim of meeting strict environmental requirements to new advanced combustion chambers, the high-temperature areas have been noticeably reduced. This is the result of transition, in whole or in part, to combustion of homogeneous mixtures. For example, in advanced aircraft combustion chambers, e.g. in TAPS (Twin Annular Premix System), the diffusion
flame front can be completely absent in cruise modes of engine operation. In other modes, except for idling, the diffusion front is used as a pilot flame to support the main homogeneous combustion. As can be anticipated, the contribution of homogeneous fronts to total NOx emission can be considerable for this type of combustion chambers.

When developing an up-to-date model for estimating the level of NOx emission, a problem arises due to simultaneous occurrence of fuel combustion processes in different fronts and NOx formation processes. Under these conditions, the use of such simplified approaches as empirical equations for NOx formation rate or partial kinetic schemes where the NOx formation rate is described only by the Ya.B. Zel’dovich mechanism will not ensure a required accuracy. This conclusion is supported by results of solution the standard problem of normal flame front propagation. As a rule, NOx formation calculated with the use of the complete detailed mechanism exceeds NOx formation calculated by the Ya.B. Zel’dovich mechanism. In this paper, in simulation of NOx emission we use only complete detailed kinetic schemes or their modifications.

2. Numerical model and a unit under study
To simulate the NOx formation on homogeneous flame fronts, fundamentally different approaches distinguished by resolution levels of the flame front structure can be used. The most detailed description of physico-chemical processes inside the flame front with a detailed resolution of the front structure is provided by a direct numerical simulation with detailed kinetics of hydrocarbon fuel oxidation and nitrogen oxide formation. However, this approach is rather laborious. It requires considerable resources and is excessive for the purpose of preliminary estimations of homogeneous front contribution to NOx emission.

In this paper we use a more simplified approach based on ideas developed by V.R. Kuznetsov [1]. The very core of the approach is the fact that the problem of estimation the level of NOx emission during combustion can be divided into two problems to be solved independently. The first problem is calculation of flow characteristics in a unit under study: temperature and velocity fields, distribution of basic components and combustion products, turbulent flow characteristics using a simplified combustion model. The second problem is a direct estimation of NOx emission.

To solve the first problem, the commercial STAR-CCM + version 13.02 software developed by Siemens PLM Inc. is used. As a model, a cylindrical combustion chamber with d = 150 mm and L = 2d is studied in this work. Fuel in this model is supplied to the combustion chamber through a tube (10 mm in diameter) along the combustion chamber axis. Air is fed through a coaxial annular channel with OD=72 mm. The computational domain is a 30° sector having approx. 4 500 000 computational cells. Turning angle of air and fuel flow is 45° relatively to the combustion chamber axis. All calculations of flow and combustion in this combustion chamber are carried out for combustion of fuel (methane) in the following conditions: p = 1 atm, \(T_{\text{air}} = 600^\circ\text{K}\) и \(T_{\text{fuel}} = 300^\circ\text{K}\). In the initial basic operation mode of the combustion chamber model, air flow is \(G_{\text{air}} = 153.3\) g/s, and fuel flow– \(G_{\text{fuel}} = 4.5\) g/s. In the above-listed conditions, residence time is \(\tau_0 = 20\) ms. For the chosen layout for reagents feeding and the level of operating parameters we can anticipate an implementation of mixed diffusion-homogeneous combustion in the model.

Two series of calculations are carried out in this study. In the first series of calculations, residence time in the combustion chamber, \(\tau\), is variable from 20 to 5 ms. This variation is provided by an increase in flow rates of reagents. Air and fuel flow rates at the combustion chamber inlet vary proportionally (when changing the flow rates, fuel-to-air ratio is constant and equals to \(\varphi = 0.5\)):

\[
G_{\text{air}}^{\tau} = G_{\text{air}}^{0} \frac{\tau_0}{\tau}, \quad G_{\text{fuel}}^{\tau} = G_{\text{fuel}}^{0} \frac{\tau_0}{\tau}.
\]

In the second series of calculations for 8-ms residence time, a version is studied when a portion of fuel is fed through a central tube and the remaining fuel is supplied as homogeneous mixture with air.
to the combustion chamber through an annular channel. If we introduce \( f \) - parameter that varies in the course of the study, characterizes the degree of homogenization, and is equal to a fuel portion used in formation of homogeneous mixture with air, fuel and mixture flows supplied to the combustion chamber through the central tube and the annular channel will be expressed, respectively, as:

\[
G_{\text{fuel}}' = (1 - f) \cdot G_{\text{fuel}}^{\text{hom}}, \quad G_{\text{air}}' = C_{\text{air}}^{\text{hom}} + f \cdot G_{\text{fuel}}^{\text{hom}}
\]

The Realizable Two-Layer K-Epsilon turbulence model is used in the calculations. For modeling of combustion, the superposition of the Turbulent Flame-Speed Closure model and the diffusion model (PPDF model) are used for combustion simulation [2]. Chemical kinetics in the first problem formulation is modeled by the adiabatic chemical equilibrium model with the following composition of components: CH4, CO, CO2, H, H2, H2O, N2, O, O2. The velocity of turbulent flame propagation is calculated using the Zimont model. The Guelder correlation is used for calculations of laminar flame propagation velocity.

![Figure 1](image-url)

**Figure 1.** Temperature distributions in the combustion chamber for three homogenization values.

Figure 1 shows the calculated data for the temperature distribution in the combustion chamber found by solution of the first problem. They illustrate the behavior of temperature fields in case of fuel redistribution between the central tube and the outer homogeneous mixture supply channel. Temperature fields are shown for three values of homogenization: diffusion combustion \((f = 0)\) and 40\% and 80\% fuel supply to the combustion chamber as a part of homogeneous mixture. The solid line in Fig. 1 shows the position of \( z = z_s \) stoichiometric surface.

As can be seen in Fig. 1, an increase in fuel mixture homogenization leads to a reduction in the stoichiometric surface and, as a consequence, a decrease in high-temperature areas, that according to present-day well-known ideas, contributes to a decrease in NOx emission. An increase in the homogenization degree also leads to an additional beneficial effect - an improvement of the temperature field uniformity at the combustion chamber outlet.

### 3. Calculations of NOx emission

For the second problem or calculations of NOx emission, the approach proposed in [3] for CO emission modeling is used. By analogy with [3], to find the mass fraction of \( Y_{\text{NOx}} = Y_{\text{NO}} + Y_{\text{NO2}} \cdot \frac{\mu_{\text{NO}}}{\mu_{\text{NO2}}} \) (where: \( Y_{\text{NOx}} \) and \( Y_{\text{NO}} \), \( \mu_{\text{NO}} \), \( \mu_{\text{NO2}} \), and \( \mu_{\text{NO2}} \) - mass fractions and molecular weights of NO2 and NO, respectively), the following equation is used:
\[
\frac{\partial(\rho \bar{Y}_{NOx})}{\partial t} = \nabla(\rho \bar{U} Y_{NOx}) = \nabla(\rho D_{y} \nabla \bar{Y}_{NOx}) + \bar{\rho} Y_{NOx}^{front} \mathbf{s}_{i} \nabla \bar{c} - \bar{c} \bar{\rho} \bar{W}_{NOx}
\]

where \( t \) - time, \( \rho \) - density, \( \rho_{c} \) - density of initial mixture components, \( \mathbf{U} \) - velocity vector, \( c \) - progressive variable, \( \bar{\tau} \) and \( \bar{\tau} \) - means Reynolds and Favre averaging, respectively.

Right side of Eq. (1) contains the terms responsible for NOx formation. First term: \( \bar{\rho} Y_{NOx}^{front} \mathbf{s}_{i} \nabla \bar{c} \) is the rate of NOx formation on homogeneous flame fronts. According to [3], an abrupt change in NOx content, \( Y_{NOx}^{front} \), is found from the solution of the steady flamelet model with a scalar dissipation value, \( N \), equal to its critical value: \( N = N_{cr} \).

The second term, \( \bar{c} \bar{\rho} \bar{W}_{NOx} \), represents the rate of NOx formation in areas downstream from homogeneous flame fronts, where: \( W_{NOx} = W_{NCE} + W_{ND} \cdot \mu_{NCE} / \mu_{ND} \cdot W_{NCE} \), and \( W_{ND} \) - production rates of NO2 and NO, respectively.

For the calculation of \( W_{NOx} \) we use a modified steady flamelet model [4] derived by simplifying the unsteady flamelet model:

\[
\frac{\partial Y_{i}}{\partial t} = N \frac{\partial^{2} Y_{i}}{\partial \xi^{2}} + W_{i}
\]

The key point of simplifications of the above unsteady model (2) consists in its conversion into a steady model with respect to a part of components in the reaction mixture. This approach is a result of the fact that, as a rule, dissipative processes and processes of chemical transformation for the majority of components are balanced. In this case, the unsteady term in equations for these components can be neglected. The balance of these processes is violated for NO component with the characteristic time of NO formation, \( t_{NO} \), much longer than residence time in the combustion chamber, \( \tau \). Therefore, we have:

\[
\begin{cases}
N \cdot \frac{\partial^{2} Y_{NO}}{\partial \xi^{2}} + W_{i} = 0, & i \neq NO \\
\frac{\partial Y_{NO}}{\partial t} = N \cdot \frac{\partial^{2} Y_{NO}}{\partial \xi^{2}} + W_{NO}
\end{cases}
\]

Using the asymptotic estimate of the unsteady term in the equation for NO: \( \partial Y_{NO} / \partial t \approx Y_{NO} / \tau \), the unsteady equation of NO formation is reduced to an ordinary differential equation. A simplified system of equations (3), written with account of the above asymptotic approximation, has a limit solution. When \( t_{NO} >> \tau \), nitrogen oxides are practically not produced. Consequently, System (3) admits further simplification:

\[
\begin{cases}
N \cdot \frac{\partial^{2} Y_{i}}{\partial \xi^{2}} + W_{i} = 0, & i \neq NO \\
Y_{NO} = 0
\end{cases}
\]

It is worth noting that in deriving Eq. (4), no restrictions are imposed on the kinetic scheme structure. Therefore, when solving the asymptotic system of equations (4) and calculating the rate of NOx formation (\( W_{NOx} \)), it becomes possible to use a detailed kinetic scheme for methane (\( CH_{4} \)) oxidation and nitrogen oxide formation [5].
The nitrogen oxide emission index \( EINO_x \) is calculated on the basis of the following algorithm. In every cell of the computational domain, the value of scalar dissipation averaged over the turbulent liquid is calculated from known values of turbulent energy \( k \), dissipation of turbulent energy \( \varepsilon \), recovered fuel concentration \( z \), and its pulsation \( \sigma^2 \): 
\[
N = (k \cdot \sigma^2)/(\varepsilon \cdot \gamma),
\]
where \( \gamma \) - intermittency [1]. Based on a known \( N \) -value, \( W_{\text{Sch}} \) is calculated by solving the system (4). \( W_{\text{Sch}} \) is averaged using the Airy-Gauss probability density function (pdf). [1]. Final calculation of \( EINO_x \) is based on the following formula:
\[
EINO_x = \frac{\int \gamma \rho W_{\text{Sch}} dV}{G_{\text{fuel}}},
\]
where integration is carried out in the overall computational domain. For comparison, the same algorithm is used to calculate \( EINO_x^{\text{Zel}} \) but only the Ya. B. Zeldovich’s mechanism is chosen in the kinetic scheme [5]. The additional nitrogen oxide formation due to an abrupt change in concentration on homogeneous flame fronts is calculated by the formula:
\[
\Delta EINO_x^{\text{front}} = \frac{\int \gamma \rho Y_{\text{NOx}}^{\text{front}} s_1|\vec{v}| dV}{G_{\text{fuel}}},
\]

Figure 2 shows calculated data. As can be seen, \( EINO_x \) calculated from the complete detailed kinetics considerably exceeds \( EINO_x^{\text{Zel}} \) in the analyzed operating conditions. Therefore, the kinetic schemes used in a number of models for estimating the NOx emission, which include only the Zel'dovich mechanism, are baseless. As evident, this problem formulation leads to a noticeable underestimation of emission. In practice, it is advisable to use a complete detailed mechanism in combination with all known mechanisms of nitrogen oxide formation.

**Figure 2.** EINOx as a function of residence time (a) and homogenization (b).

The calculated data in Fig. 2a show that NOx formation on homogeneous flame fronts is weakly time dependent. To explain this effect, let’s study a closed surface surrounding the homogeneous front, and take the integral of \( \rho \vec{U} Y_{\text{Sch}} \) over this surface. Because of \( Y_{\text{NOx}} = 0 \) at the homogeneous front inlet and \( Y_{\text{NOx}} = Y_{\text{NOx}}^{\text{front}} \) at its outlet, the integral over the closed surface transforms simply into an
integral over the flame front surface. In view of the approach used in estimations of \( \Delta EINO_x^{front} \), \( Y_{NOx}^{front} \) is not dependant on residence time, \( \tau \), and \( \bar{p} \bar{U} \) is proportional to fuel flow, \( G_{\text{fuel}} \). It follows that:

\[
\int \bar{p} Y_{NOx}^{front} \nabla \hat{c} \cdot \hat{n} \, dV = \int \bar{p} \bar{U} Y_{NOx}^{front} \, dS \sim G_{\text{fuel}}.
\]

The second problem under study is the effect of mixture homogenization (\( f \)) on NOx formation. As can be seen from Fig. 2b, \( EINO_x \) decreases with an increase in the degree of homogenization as found by Ya.B. Zel’dovich and other mechanisms. As above mentioned, NOx production on homogeneous fronts is almost unchangeable with time and the degree of homogenization. Consequently, its relative contribution increases with an increase in \( f \) parameter.

4. Conclusions
Specifics of nitrogen oxides formation in conditions of partially mixed combustion in combustion chambers in the presence of both diffusion and homogeneous flame fronts are studied. As a result of the completed studies, the role of homogeneous flame fronts in formation of a part of nitrogen oxides in conditions of partially mixed combustion is demonstrated. For the model conditions, the effect of residence time and partial homogenization degree on nitrogen oxides formation is found. It is shown that nitrogen oxides formation on homogeneous flame fronts is not residence time dependent, while total NOx emission decreases with a decrease in residence time. It is revealed that an increase in partial homogenization of mixture in the course of combustion as well as a reduction in residence time results in a noticeable effect of homogeneous fronts on total NOx emission. The analysis of findings shows that in calculations of NOx emission produced by combustion chambers with partial homogenization (e.g. TAPS), it is necessary to take into account the effect of homogeneous flame fronts on NOx formation, that will contribute to an increase in accuracy of emission estimates.

References
[1] Kuznetsov V R, Sabel’nikov V A 1990 Turbulence and Combustion (Hemispfere Publishing Corporation)
[2] STAR-CCM+ Documentation Version 13.02 2018 Siemens PLM Software inc.
[3] Wegner B, Gruschka U, Krebs W, Egorov Y, Forkel H, Ferreira J, Aschmoneit K 2010 CFD Prediction of Partload CO Emissions using a Two-Timescale Combustion Model Proceedings of ASME Turbo Expo GT2010-22241
[4] Goltsev V F, Shchepin S A 2016 Analysis of the flamelet model for calculation of emissions of pollutants by combustors HighTemperature 54 No 4 pp 541-546
[5] Miller J A, Bowman C T 1989 Mechanism and Modeling of Nitrogen Chemistry in Combustion Prog. Energy Combust. Sci 5 p 287