Numerical Simulation on NO_x Emission in Liquid Fuel Spray Flames

Yasamin Khazraii, Keyvan Daneshvar, and Hossein PoorkhademNamin

***Abstract*—The present study is concerned with numerical simulating of NO_x emission in turbulent liquid fuel spray flames using thermal and fuel models. The influence of fuel spray angle and inlet air temperature on the emission of nitric oxide is investigated. Numerical simulation of two phase flow and combustion modeling for pollutants formation are done with Fluent 6.32 software. The conservation equations of mass, momentum and energy in the turbulent flow field were solved in conjunction with the $k-\varepsilon$ turbulence model. The formation of thermal NO from molecular nitrogen was modeled according to the extended Zeldovich mechanism. Fuel-based *NO* was modeled assuming that all the nitrogen in the fuel is released as hydrogen cyanide (HCN), which then further reacts forming nitric oxide NO or molecular nitrogen N_2, depending on the local combustion conditions. The results show that by increasing in spray angle NO_x emission increases. When the spray angle increases, the contact between fuel and air will raise and also the air-fuel mixing increases. Therefore with increasing in the mentioned spray angle, a more perfect combustion happens and the maximum flame temperature increases. Also, the concentration of NO_x which is affected by maximum temperature increased. . The results reveal that fine droplet sprays lead to higher NO_x emission.**

***Index Terms*—Liquid Fuel, NO_X emission, numerical modeling, spray angle**

I. Introduction

Combustion processes, usually lead to production of pollutants to the environment. In optimization of these processes not only the combustion efficiency and reduction fuel consumption, but also the environment and reducing certain pollutants should be considered. For this purpose, extensive researches have been done to save energy and achieve high efficiency and control and reduce pollution caused by combustion. A significant proportion of major air pollutants are produced from the combustion of liquid fuel. Liquid fuel is widely used in the boilers, industrial furnace and gas turbines combustion chambers.

Sulfur oxide, carbon monoxide, soot and nitrogen oxides are most important contaminants which spread in the liquid fuel flames. Produced pollution by nitrogen oxides has remained harmful effects on human health and the environment and also play an important role in the formation of acid rain, chemical smog and ozone layer hole [1].

Liquid fuels are categorized to light and heavy fuels depending on the amount of carbon. Liquid fuel burners are usually non-premixed and the fuel and oxidizer are mixed in the combustion chamber. Gas fuels are widely categorized as premixed or non-premixed. In premixed burner smaller and stronger flame is produced, in comparison with the non-premixed type. Flame adiabatic temperature is higher and radiation heat transfer and also the rate of the formation of nitrogen oxides are increased. But in non-premixed type, flame is taller, the temperature at the center of flame and NO_x production are reduced [2]. Although the chemical processes of the both premixed and non-premixed combustion are the same but additional physical processes regarding to the non-premixed combustion (evaporation and mixing) are needed. For example, overall mixing can be stoichiometric, but there are some areas in combustion chamber with large or low amount of fuel. This aspect of the non-premixed combustion can cause to more complex formation of pollutants [3].

The numerical simulation of liquid fuel combustion is a challenging task. In addition to the difficulties inherent to gas-phase combustion, namely the need to model turbulence, combustion and radioactive heat transfer, liquid fuel combustion presents other complex phenomena. These include the atomization, spray combustion and soot formation, among others. A few numerical studies on liquid fuel combustion have been published in the literature. The detailed modeling of combustion characteristics and *NO* formation in spray combustion systems is strongly sensitive to atomization of the jet liquid fuel, droplets fuel spray evaporating and mixing of fuel and oxidizer [4-6]. Speed, angle and pattern of fuel spray can be controlled by the burner nozzle. Very extensive researches have been done for the effect of the nozzle design, working conditions and fuel properties on the combustion characteristics and on spraying the hydrocarbon fuels [7-9]. Most conducted research has focused on the nozzles used in the combustion gas turbines and boilers. In liquid fuel combustion in the gas turbine, there is the problem of the formation of soot and NO_x emissions and physical phenomena such as fuel atomization or evaporation, droplets dispersion, structure of spray and mixing with air, have widely effected on combustion [10]. In the past, research was often performed based on techniques and methods, to improve combustion efficiency and quality of atomization. Improvement of the burner efficiency requires the study of spray nozzle characteristics. Recently, most research is focused to review and to study spray characteristics such as length of segregation, spray angle and droplet size and distribution in the burner nozzle [11-12]. The

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purpose of this paper is the prediction of *NO* emission from turbulent liquid fuel spray flames by using fuel and thermal *NO* mechanisms and the investigation of the effect of spray angle on *NO* formation predicted by the above mentioned two mechanisms. In addition, the influence of air inlet temperature and spray droplet size on NO_x emission is investigated.

II. Governing Equation

A standard $k-\varepsilon$ turbulence model is widely used in turbulent combustion simulation and is used to describe turbulent flow. For turbulent flow, the two-dimensional equations of continuity, momentum, turbulent kinetic energy, *k*, and the dissipation rate, ε in the physical flow domain can be expressed in the tensor form as follows:

$$\frac{\partial \overline{u_i}}{\partial x_i} = 0 \tag{1}$$

$$\overline{u}_j \frac{\partial \overline{u_i}}{\partial x_j} = -\frac{1}{\rho}\frac{\partial \overline{p}}{\partial x_i} + \nu \frac{\partial^2 \overline{u_i}}{\partial x_j \partial x_j} - \frac{\partial \tau_{t_{ij}}}{\partial x_j} \tag{2}$$

$$u_j \frac{\partial k}{\partial x_j} = \tau_{t_{ij}} \frac{\partial u_i}{\partial x_j} - \varepsilon + \frac{\partial}{\partial x_j}\left[\nu + \nu_t / \sigma_k \frac{\partial k}{\partial x_j}\right] \tag{3}$$

$$u_j \frac{\partial \varepsilon}{\partial x_j} = C_{\varepsilon 1}\frac{\varepsilon}{k}\tau_{t_{ij}}\frac{\partial u_i}{\partial x_j} - C_{\varepsilon 2}\frac{\varepsilon^2}{k} + \frac{\partial}{\partial x_j}\left[\nu + \nu_t / \sigma_\varepsilon \frac{\partial \varepsilon}{\partial x_j}\right] \tag{4}$$

where

$$\tau_{t_{ij}} = \overline{u_i' u_j'} \tag{5}$$

$$\nu_t = C_\mu k^2 / \varepsilon \tag{6}$$

where ν_t is the kinematic turbulent viscosity and τ_t is the Reynolds stress. The $k-\varepsilon$ model empirical coefficients have the following values[11]:

$C_{\varepsilon 1} = 1.44, C_{\varepsilon 2} = 1.92, C_\mu = 0.09, \sigma_k = 1.0,$ and $\sigma_\varepsilon = 1.3$

III. Two Phase Flow Modeling

In many practical combustion processes, fuel is solid or liquid and during the combustion, firstly the fuel is converted to the gas phase and then is burned by oxidation gas. Liquid fuel combustion is usually done by injecting liquid fuel into the gas phase combustion environment. Turbulence within the liquid flow is created inside the injector. This turbulent fluid flow gets out of the nozzle in the form of complex mix of strings and then crushes into small drops and appears as dense clouds of droplets that launches through the gas into the flame zone. Heat transfer to drop, increases the vapor pressure and therefore the fuel evaporates into the gas, so burning of gas phase is began. Non-premixed flame surrounds the group drops or droplets and eventually fuel vapor burns. This set of processes is called combustion spray. By assuming that spherical particles of liquid fuel is dispersed in the gas phase and their hits due to their quick evaporation is negligible, in the Lagrangian System, continuity and energy conservation equations governing to the particles, are written as follows:

$$\frac{dd_p}{dt} = -\frac{C_b}{2d_p}\left(1 + 0.23\,\mathrm{Re}^{1/2}\right) \tag{7}$$

$$\frac{dT_p}{dt} = \frac{6k\left(2 + 0.6\,\mathrm{Re}^{1/2}\,\mathrm{Pr}^{1/3}\right)\left(T_\infty - T_P\right)}{\left(\rho_P d_p^2 C_{P,P}\right)} \tag{8}$$

In (7), d_p is drop diameter C_b is evaporation constant which is function of physical properties of the environment and fuel that is determined as follows:

$$C_b = \frac{8k}{\rho_l C_p}\ln\left[1 + C_p / L\left(T_\infty - T_P\right)\right] \tag{9}$$

In this equation k and C_p are thermal conductivity coefficients and the specific heat in constant pressure for gas mixtures, respectively. T_∞ , T_p and L are gas temperature, the drop temperature and the latent heat of vaporization of fuel respectively. By using (7), the particle diameter change rate, after reaching to the boiling temperature, and from (8) the temperature change rate of the fuel particles can be calculated [14].

IV. Combustion Modeling

In this study chemical formula for gasoline is assumed to be $C_{16}H_{29}$ and one step Magnussen-Hiertager model with eddy dissipation is used for combustion modeling [15]. In this simulation firstly, the liquid fuel converts into a gas type and then combustion is performed. Evaporation of fuel particles is started when the particles temperature reaches to the boiling temperature, and will be continued until all their mass becomes finish. Gas fuel is done in one step and according to the selected Magnussen-Hiertager combustion model; the effective factor to the reaction rate is the flow dynamics. Chemical reaction between oxygen and gasoline is written as follows:

$$C_{16}H_{29} + 23.25O_2 \longrightarrow 16CO_2 + 14.5H_2O \tag{10}$$

V. Nitrogen Oxide Modeling

To estimate *NO*, the solution of the mass transport equation (Y_{NO}) is required. This equation is solved after determining the main flow field and their main species. Mass transport equation for *NO* is written as follows, which includes influence convection term, production and consumption of *NO*.

$$\rho\frac{\partial Y_{NO}}{\partial t} + \rho u_i \frac{\partial Y_{NO}}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\rho D \frac{\partial Y_{NO}}{\partial x_i}\right) + S_{NO} \tag{11}$$

where source term (*S*) in this equation is calculated according to three forms mechanism *NO*: thermal *NO*, prompt *NO* and fuel *NO*. Since in liquid fuels combustion the amount of prompt *NO* compared with the other two types are almost neglected, in this study only thermal *NO* and fuel *NO* are calculated. Thermal *NO*, which is formed at high temperatures by nitrogen oxidation contained in combustion air, is expressed using developed Zeldovich mechanisms [14].

$$O + N_2 \xleftrightarrow{k_{\pm 1}} NO + N \quad (12)$$

$$N + O_2 \xleftrightarrow{k_{\pm 2}} NO + N \quad (13)$$

$$N + OH \xleftrightarrow{k_{\pm 3}} NO + H \quad (14)$$

where k_+ and k_- are reaction forward and backward Constants. Assuming that consumption rate of free nitrogen atoms is equal to its production rate; *NO* concentration is obtained from following equation:

$$\frac{d[NO]}{dt} = 2k_{+1}[O][N_2]\frac{\left(1-\frac{k_{-1}k_{-2}[NO]^2}{k_{+1}[N_2]k_{+2}[O_2]}\right)}{\left(1+\frac{k_{-1}[NO]}{k_{+2}[O_2]+k_{+3}[OH]}\right)} \quad (15)$$

Constants of value of equilibrium reaction rate in the above equations are obtained in the [17]. Considering that the formation rate of *NO* is much lower than the original hydrocarbon oxidation rates, more thermal *NO* is formed after completing combustion. In above equation, concentrations of N_2 and O_2 are determined by combustion calculation and the radical concentration for *[O]* and *[OH]* is obtained from the following relations [18].

$$[O] = 36.64T^{1/2}[O_2]^{1/2}\exp\left(\frac{-27123}{T}\right) \quad (16)$$

$$[OH] = 2129T^{-0.57}\exp\left(\frac{-4595}{T}\right)[O]^{1/2}[H_2O]^{1/2} \quad (17)$$

Therefore some source term in the part of the (11) is calculated from Zeldovich mechanism as follows:

$$S_{NO,th} = M_{NO}\frac{d[NO]}{dt} \quad (18)$$

In which M_{NO} is molecular mass of *NO* gas.

NO production fuel is a very complex phenomenon and it is strongly dependent to the flame stoichiometric, local combustion characteristics and initial concentration of the nitrogen compounds. Because of heating and evaporation of fuel droplets and nitrogen-containing radicals such as *HCN*, *CN* and *NH*, nitrogen-containing compounds are decomposed, which can be converted to NO_x. Considering that nitrogen cyanide (*HCN*) is predominant radicals, accepted mechanism for the formation of fuel *NO* is include of the formation of HCN from nitrogen in the fuel, and then performance of two oxidation reactions to get *NO* and combination with some part of *NO* and formation of N_2[19].

$$HCN \xrightarrow{+O_2} NO \quad (19)$$

$$HCN \xrightarrow{+NO} N_2 \quad (20)$$

Reaction rates of these two related based on measurements in De Soete work [18] are expressed as follows:

$$R_1 = A_1 X_{HCN} X_{O2}^{a} \exp\left(\frac{-E_1}{RT}\right) \quad (21)$$

$$R_2 = A_2 X_{HCN} X_{NO} \exp\left(\frac{-E_2}{RT}\right) \quad (22)$$

In the above equations, X is mole fraction and $A_1 = 3.5\times10^{10} 1/s$, $A_2 = 3\times10^{12}$, $E_1 = 67000 cal/mol$ and $E_2 = 60000$

Considering that *NO* is produced in the reaction (19), and is used in reaction (20), source term from *NO* fuel in (11) is obtained from the following equation:

$$S_{NO} = (R_1 - R_2)\frac{M_{NO}}{RT} \quad (23)$$

VI. Numerical Calculation

The numerical simulations were carried out using commercial CFD software Fluent 6.32 [19] that uses the finite volume method to solve the governing equations. Solid model creation and grid generation were conducted using Gambit 2.2. First order upwind scheme is used to model the convective terms of the governing equations. The pressure velocity coupling is resolved using SIMPLE algorithm. The convergence criterion is satisfied when the residuals of all the variables are less than 10^{-5}.Dimension of computational mesh, is very effective on accuracy of results in the numerical calculations and on performance time. Although by increasing the number of nodes in mesh generation and computational field, the accuracy of results is increased, but much more time and memory are needed. In this study, the area near the entrance and walls that the flow properties changes are higher, smaller meshes are selected. Computing meshes in the combustion chamber is shown in Fig.1. Results have shown that applying the smaller meshes than 150*400 cells cannot make results better and this matter proved the mesh-independent solution.

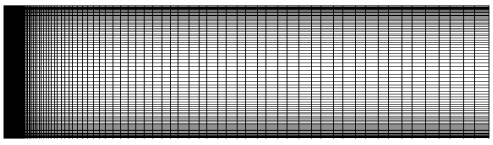


Fig. 1. Computational mesh in solution domain

VII. Boundary Condition

Numerical simulations are performed for a cylindrical spray combustor of internal diameter 10 cm and length 180 cm. The size range of the fuel droplets in spray is chosen to be in the range of 50 to 100 μm. The furnace boundary conditions are given in Table I.

VIII. Results and Discussion

The flow streamline pattern inside the furnace, for the present numerical solution is shown in Fig.2. As shown in

Fig.3, the vortex flow and backflow are informed near the furnace wall and entrance expansion area.

TABLE I: FURNACE BOUNDARY CONDITIONS

Fuel Mass flow Rate(Kg/h)	Inlet Air Mass flow Rate(Kg/h)	Equivalence Ratio	Inlet Air Temperature(*K*)	Chamber Wall Temperature(*K*)
2.12	48	0.66	300	750

Temperature contours in the combustion chamber for different fuel spray angles of 45o, 60o and 80o degree is shown in Fig.3 Increasing the fuel spray angle, the maximum temperature is increased. At spray angle of 45^o, 60^o, 80^o degree, maximum temperature are increased up to 1442 K, 1466 K, 1592 K respectively.

In Fig.4 the effect of the fuel spray angle on the temperature at the central axial of furnace is shown. Results show that with increasing the fuel spray angle, the amount of maximum temperature in the central axial furnace is also increased. By increasing the fuel spray angle, the time of staying particles inside the combustion chamber is increased. Due to extension of flame surface, axial velocity of particles is reduced and therefore the location of occurrence of maximum temperature in the central line of furnace with increasing the angle of fuel spray is closer to the input area.

In Fig.5 NO_x Contour based on ppm has been shown for three fuel spray angle 45^o, 60^o and 80^o. It should be note that in the fluent software the output of NO_x concentration are given based on mass or mole ratio or mole concentration not in terms of ppm, which is common in the industry. An empirical function is defined and therefore the fluent software can determine the amount of NO_x, in terms of ppm instead of mass or mole ratio.

The effect of spray angle on the NO_x emissions on the central axial furnace is shown in Fig.6. The results show that NO concentration along the axis is firstly increased from the burner to a maximum and then after slightly decreasing, remains constant almost to the end of the furnace. Three spraying angles comparison show that with increasing the angle of spraying, NO_x concentration is increased near the fuel nozzle. Fuel injection at low spray angles causes to longer flame length, thus the location of occurrence of maximum NO_x moves to farther distance in furnace from the input area.

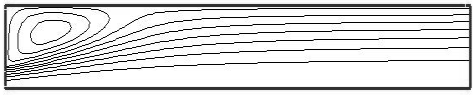
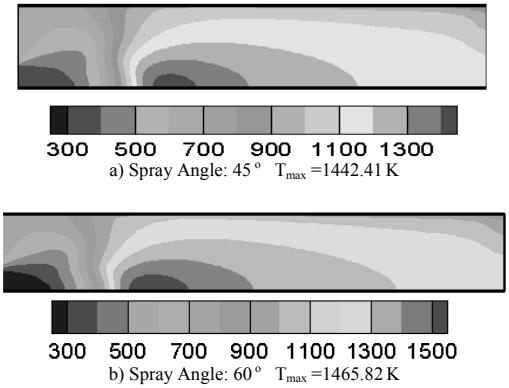


Fig. 2 Stream lines inside the combustion chamber



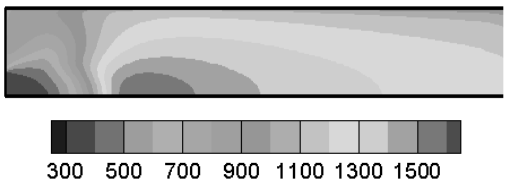


Fig. 3. Temperature contours in combustion chamber for different fuel angles

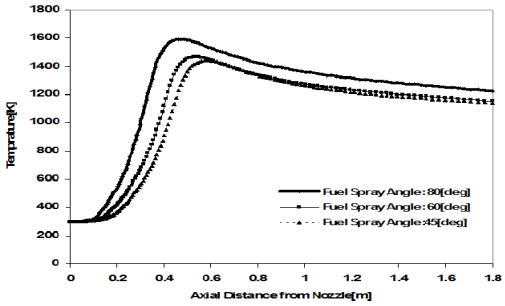


Fig. 4. Effect of fuel angle on the temperature profiles on the central axial of furnace

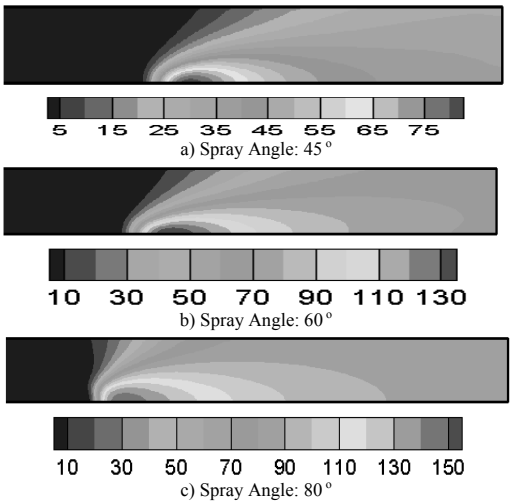


Fig. 5. NO_x contour [ppm] at different fuel spray angles inside the combustion chamber

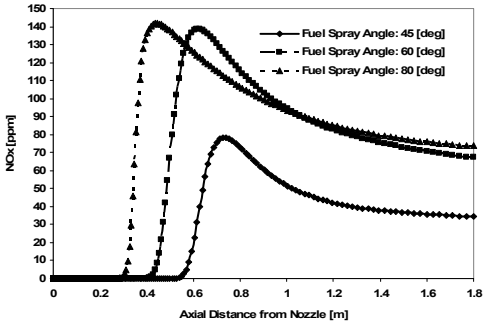


Fig. 6 .Effect of fuel spray angle on the NO_x concentration of in the central axial of furnace

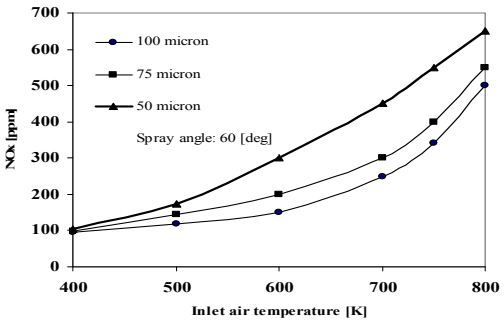


Fig. 7. Effect of inlet air temperature and fuel droplet size on NO_x concentration output

The effect of inlet air temperature and initial fuel droplet size on NO_x concentration output is shown in Fig.7. It can be seen that, as expected, an increase in inlet air temperature, led to increasing the NO_x concentration output, whilst an increase in spray droplet size decreases NO_x concentration. This occurs because smaller droplets evaporate and burn more quickly than larger ones. Comparing the results of the three droplet sizes (50, 75and 100 microns) reveals that for small fuel drops, the effect of inlet air temperature on NO_x concentration is linear.

CONCLUSION

computational results for the pollutant emissions resulting from combustion of liquid fuels are evaluated. Numerical simulations are done using fluent software version 6.32. Regarding to the existence of nitrogen in liquid fuels, the concentration of *NO* gas are calculated using two methods of thermal *NO* and fuel *NO* mechanisms. Increasing the fuel spray angle causes to increase NO_x in furnace output. Numerical results also show that on the central axial furnace, NO_X gas concentration is in maximum value. an increase in inlet air temperature, led to increasing the NO_x concentration output, whilst an increase in spray droplet size decreases NO_x concentration.

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