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# The Effects of $CO_2$, $N_2$, and $H_2O$ Dilutions on NO Formation of Partially Premixed Synthesis Gas Combustion

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**Abstract.** One of the main methods to decrease NO emission during the combustion of gases is the use of diluents. This study is interested in the effects of $CO_2$, $N_2$, and $H_2O$ dilutions in the adiabatic, turbulent, partially premixed combustion of synthesis gas. The amounts of NO emissions are computationally determined. The results show that NO maximizes at 1.39 of equivalence ratio under humid burning air conditions. The best reductive effect on NO emissions indicates $H_2O$ dilution followed by $CO_2$ and $N_2$. The increase in the dilution rates gradationally reduces NO. The rising pressure enhances NO emissions with/without diluters. The increasing inlet air and premixed mixture temperatures raises NO.

***Keywords***: Synthesis gas, partially premixed, combustion, nitrogen oxide.

## *Kısmi Önkarışımlı Sentez Gazı Yanmasının NO Oluşumu Üzerinde $CO_2$, $N_2$ ve $H_2O$ Seyreltmelerinin Etkileri*

**Özet.** Gazların yakılmasında NO emisyonunu azaltmak için ana metodlardan biri seyrelticilerin kullanımıdır. Bu çalışma sentez gazının adyabatik, turbülanslı, kısmi önkarışımlı yanmasında $CO_2$, $N_2$ ve $H_2O$ seyreltmelerinin etkileri ile ilgilenmektedir. NO emisyonlarının miktarları hesaplamalı olarak saptanmıştır. Sonuçlar, nemli yakma havası şartlarında, NO'in, 1.39 ekivalans oranında maksimize olduğunu göstermektedir. NO emisyonları üzerinde en iyi azaltıcı etkiyi $CO_2$ ve $N_2$ tarafından takip edilen $H_2O$ seyrelticisi göstermektedir. Seyreltici oranlarındaki artış derecesel olarak NO'i azaltmaktadır. Yükselen basınç seyreltili veya seyreltisiz NO emisyonlarını artırmaktadır. Artan hava ve önkarıştırılmış karışım giriş sıcaklıkları NO'i yükseltmektedir.

***Anahtar Kelimeler***:, Sentez gazı, kısmi karışımlı, yanma, nitrojen oksit.

## 1. INTRODUCTION

Synthesis gas (syngas) is a product obtained by gasification process from coal, tire, biomass, or steam reforming from natural gas. It generally consists of different components as $H_2$, $CH_4$, CO, $CO_2$, $H_2O$, $N_2$, $H_2S$, $NH_3$, and COS depending on fuel source what it is derived of. Synthesis gas is utilized in industrial furnace and high efficiency gas turbines for power generation after post gasification process removing $H_2S$ and other unwanted contaminants. Its wide presence and appropriate combustion characteristics makes synthesis gas a conspicuous option among gas fuels [1, 2].

$NO_x$ emissions forming because of high temperature reactions of $N_2$ and $O_2$ in burning air and fuel also continue to be an environmental problem as a pollutant for synthesis gas combustion. $NO_x$ is the sum of mostly NO and $NO_2$ from greenhouse gases and countries take common

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precautions to reduce these gas releases [3]. $NO_x$ emerges during the combustion by three different ways called thermal, prompt, and fuel. Thermal $NO_x$ begins to be more effective by the reactions of nitrogen and oxygen at temperatures over 1300 °C and is defined by the reactions of $N_2 + O \leftrightarrow NO + N$, $N + O_2 \leftrightarrow NO + O$, $N + OH \leftrightarrow NO + H$. The reactions with nitrogen of both carbon and hydrocarbon derivatives form prompt $NO_x$ in fuel-rich areas. Finally, the oxidation of nitrogen and its compounds in fuel causes fuel $NO_x$ [4].

The partially premixed or diffusion combustion methods are largely preferred to obtain lower $NO_x$ and to get rid of flashback caused by high burning velocity of $H_2$ in combustion devices burning synthesis gases. Furthermore, the gas diluents as $N_2$, $H_2O$, and $CO_2$ are used to decrease flame temperature and $NO_x$ by adding to air, fuel or unburned fuel/air mixtures and also have effects on flame's stability, extinction, propagation, and fuel flammability [5, 6].

Many studies are interested in the production methods of synthesis gas from different sources. There have been a few studies to investigate the combustion and emission characteristics of premixed or non-premixed synthesis gases under different conditions in literature. Park and Kim detected that $H_2O$ and $CO_2$ dilutions are more effective than $N_2$ to reduce $NO_x$ emissions [7]. Parka et al. concluded the increased pressure raises $NO_x$ emissions and fuel side $N_2$ dilution reduces $NO_x$ for coal based synthesis gas [8]. Williams et al. found oxygen up to 22% in $CO_2$ is beneficial to decrease $NO_x$ [9]. Huang et al. determined the preheating air causes higher $NO_x$ but lower CO emissions [10]. Tian et al. detected the rising $N_2$ dilution in dry and humid burning air fades $NO_x$ in dry and humid burning air at a non-premixed combustor and its effect rises with humidification of air [11]. Tran et al. showed $CO_2$ dilution lowers the adiabatic flame temperature and laminar burning velocity for syngas/air mixture [12]. Giles et al. found $CO_2$ and $H_2O$ are more effective than $N_2$ in reducing NO and the most effective is $H_2O$ diluent in airstream for counter-flow diffusion flames [13]. Chan et al. determined $CO_2$ dilution lower flame temperature and increases the specific heat of the premixed methane/air mixture [14]. Zhang et al. concluded the increasing $CO_2$ dilution reduces the temperature and $NO_x$ [15].

In this study, the mass fractions of NO emitted at the end of partially premixed combustion of synthesis gas derived from waste tires are computationally determined with dilution effects of $CO_2$, $H_2O$, and $N_2$ mixed in the upstream air under different equivalence ratio, pressure, inlet air and premixed fuel/air temperatures by ANSYS software.

## 2. MATERIALS AND METHODS

The numerical calculations for evaluating NO mass fractions at the end of partially premixed synthesis gas/air combustion are realized in ANSYS R15.0. Fluent in ANSYS is the computational fluid dynamics software that is used to model turbulence, flow, chemical reactions, heat transfer, aerodynamics, hydrodynamics, combustion, etc. It reaches a solution by solving the equations related to the phenomena under defined conditions on meshed field of a physical model created in Fluent. Moreover, computational fluid dynamics software for investigating the combustion case are preferred more by researchers because of its cheaper, easier manipulation, and lesser time consumption with respect to experimental way.

The meshed field of co-axial combustor used for burning synthesis gas/air mixture is given in Figure 1. The mesh of 2D model of the chamber consists of 11800 elements and 12076 nodes. The composition of synthesis gas derived of waste tires is 24% $CH_4$, 51.8% $H_2$, 16.9% CO, and 7.3% $CO_2$ [16].

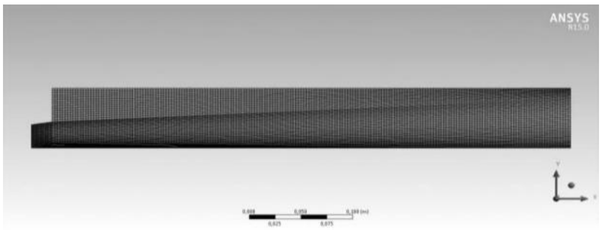


**Figure 1.** The meshed chamber of co-axial combustor.

The inlet flow rates and temperatures of premixed shale gas/air and air with the dimensions of the co-axial burner are illustrated in Figure 2. If not mentioned any different condition in the text, the premixed shale gas and air enters by 30 m/s rate at 300 K as the upstream air enters into the combustor by 10 m/s rate at 600 K. The air includes humidity at the rate of 1.5%. The diluents of $CO_2$, $H_2O$, and $N_2$ to examine the dilution effects on NO emissions during the combustion are added to the upstream air at changing ratios from 0 to 30%.

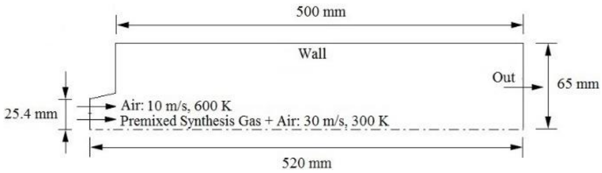


**Figure 2.** The dimension of co-axial combustor and the inlet flow rates and temperatures [17].

The following model and property options under Fluent Setup are selected for the solutions of partially premixed combustions:

- Viscous Model – k-epsilon (2 eqn), k-epsilon model – standard, Near-Wall Treatment – Standard Wall Functions
- Species Model – Partially Premixed Combustion (Premixed Model – C Equation, Chemical Equilibrium, Adiabatic, and Flame Speed Model – Zimont)
- $NO_x$ Model – On (Thermal, Prompt, and $N_2O$ Intermediate are selected)
- The inlet flow rates, inlet temperatures, and equivalence ratios are entered from Zone of Boundary Conditions, Prompt Tab of $NO_x$ Model and Boundary tab of PDF Table by changing Fuel (shale gas-air mixture) and Oxide (air) ratios for the complete combustions and others.

$NO_x$ emissions are evaluated in terms of NO concentration at the out because NO can be utilized in the place of $NO_x$ consisting of NO and $NO_2$ owing to an order difference of $10^{-3}$ mostly between mass fractions of NO and $NO_2$.

## 3. RESULTS AND DISCUSSION

The increment of temperature in the combustion chamber always causes to the rise of NO formation at the end of combustion. Figure 3 and 4 represent the contours of temperatures in the co-axial combustor as the equivalence ratio equals to 1 and 1.4. It is seen that there is a difference of 1215 K between the maximum temperatures of ER=1 and 1.4.

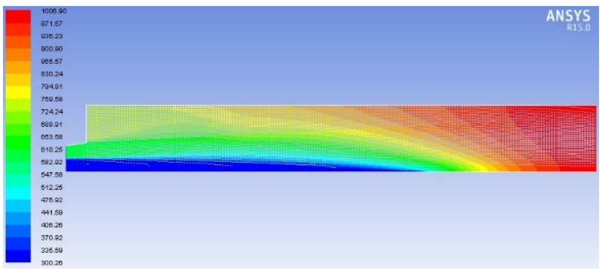


**Figure 3.** The contours of temperatures during the combustion of synthesis gas at ER=1.

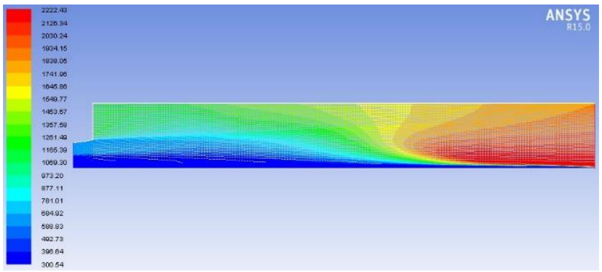


**Figure 4.** The contours of temperatures during the combustion of synthesis gas at ER=1.4.

NO mass fractions arising at the end of partially premixed combustions of synthesis gases/air at various equivalence ratios (ER) are illustrated in Figure 5. NO roughly reach to the maximum at 1.39 of the equivalence ratio of premixed synthesis gas/air for the all. The highest NO value as 0.000141 kg NO/kg belongs to the synthesis gas/air combustion with non-dilution as expected. It is respectively followed by $N_2$, $CO_2$, and $H_2O$ diluted combustions toward to the lowest. It is seen that $H_2O$ dilution indicates the best reductive effect on NO. The difference between NO of the combustion without dilution and 15% $N_2$, $CO_2$, and $H_2O$ diluted ones is 13.4%, 14.8%, and 24.8% at ER=1.39. The decrease of the burning air amount in the combustor with rising fuel side equivalence ratio raises causes the incomplete combustion and the descending reaction temperature drops NO emission after a certain point of ER.

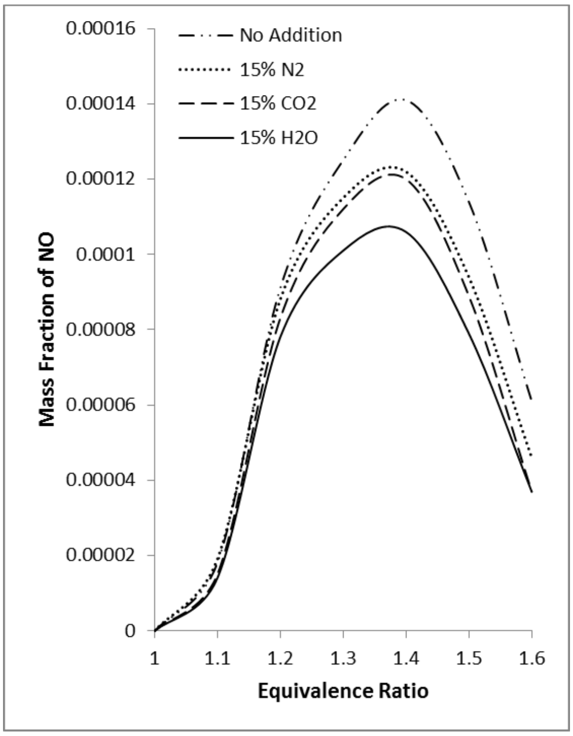


**Figure 5.** The mass fractions of NO at different equivalence ratios.

The mass fractions of NO with no dilution and the diluted combustions at ER=1.4 is given for different dilution rates in Figure 6. The increase of addition rates for $N_2$, $CO_2$, and $H_2O$ in the upstream burning air gradationally decreases NO emissions. The best effect for NO attenuation is provided at $H_2O$ dilution following by $CO_2$ and $N_2$. At 10% of addition rate, the reduction rates of NO for $N_2$, $CO_2$, and $H_2O$ additions are 8.5%, 9.2%, and 17.7% respectively.

$N_2$ dilution reduces flame temperature, flame speed, thermal diffusivity and high temperature regions in the combustion chamber. It lowers NO emissions. $CO_2$ addition indicates more chemical effects than $H_2O$ [11, 18]. The addition of $CO_2$ in the upstream air raises heat capacity of mixture and decreases combustion rate, reaction kinetics, flame speed, and flame temperature by causing a reductive effect on mixture concentration [14]. $H_2O$ has the high heat holding capacity and drop the reaction temperature, burning velocity, and NO [5].

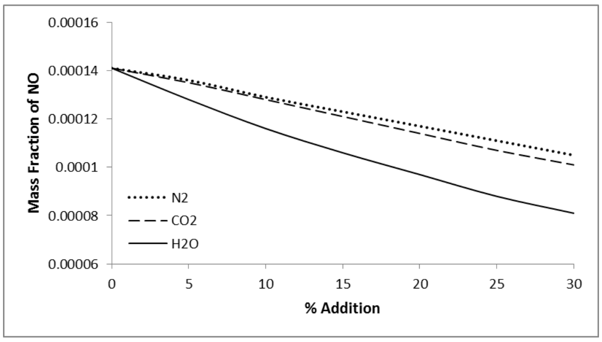


**Figure 6.** The mass fractions of NO at different $N_2$, $CO_2$, and $H_2O$ addition rates.

The pressure effect on NO mass fractions for 15% dilution rate at ER=1.4 is indicated in Figure 7. The pressure gauge is absolute. The pressure has an ascender effect on NO. NO emissions especially become crucial in the combustion chambers of vehicle's engines and combustion systems running at high pressures. NO for non-addition, 15% $N_2$, 15% $CO_2$, and 15% $H_2O$ dilution rates between 0 and 10 Atm increase 68.7%, 56.9%, 44.6%, and 56.6%. NO with 15% $N_2$, $CO_2$, and $H_2O$ additions diminish 18.9%, 26.4%, and 30.2% in turn at 10 Atm pressure.

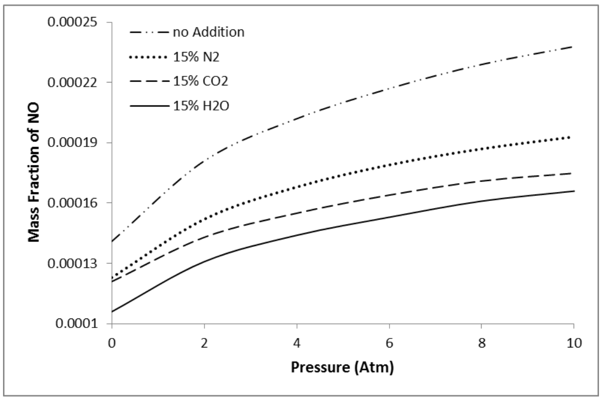


**Figure 7.** The mass fractions of NO at different pressures.

The effect of air inlet temperature at upstream on NO is given in Figure 8. The increase of air inlet temperature raises the reaction temperature and rates in the combustion chamber and the rising temperature causes NO to rise as well. NO increment between 500 and 800 K is 97.6%, 120.5%, 123.3%, and 110.6% for no addition, 15% $N_2$, 15% $CO_2$, and 15% $H_2O$ addition rates. The decrease rates for NO at 800 K temperature for 15% $N_2$, $CO_2$, and $H_2O$ additions is 6.7%, 9.1%, and 21.7% respectively.

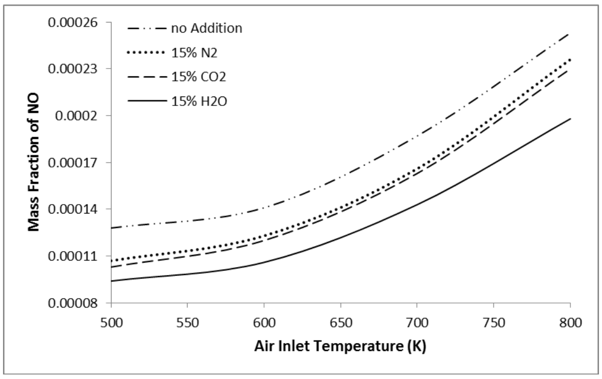


**Figure 8.** The mass fractions of NO at different air inlet temperatures.

The effect of inlet temperature of premixed synthesis gas/air mixture on NO emissions is presented in Figure 9. The rising inlet temperature of premixed mixture enhances the reaction temperature and implicitly NO emission as the upstream air inlet temperature does. NO increment between 250 and 325 K is 15.5%, 18.1%, 19.2%, and 17.7% for no addition, 15% $N_2$, 15% $CO_2$, and 15% $H_2O$ dilution rates. NO decrement with 15% dilutions at 325 K is 24.1% for $H_2O$ and approximately 12.7% for $N_2$ and $CO_2$.

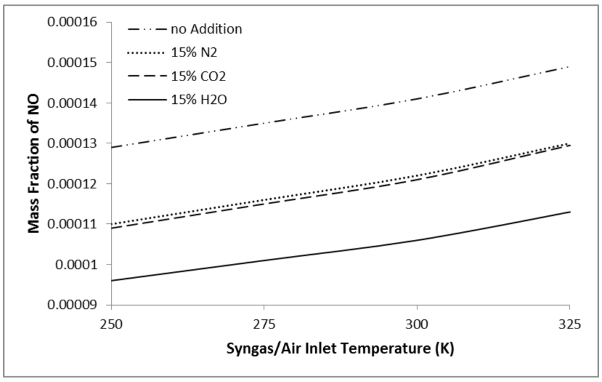


**Figure 9.** The mass fractions of NO at different synthesis gas/air inlet temperatures.

## 4. CONCLUSION

The hazardous NO emissions of adiabatic, turbulent, partially premixed combustion of humid air and synthesis gases are computationally investigated at different equivalence ratios, pressures, and inlet temperatures of upstream air and premixed gas/air under the dilutive effects of $N_2$, $CO_2$, and $H_2O$ added into the upstream burning air. The following results are obtained:

- NO emission is the maximum at ER=1.39. To decrease NO formation, equivalence ratio needs to be diminished to 1 or lower values. The best reductive effect on NO emission is realized by $H_2O$ addition followed by $CO_2$ and $N_2$. $H_2O$ and $CO_2$ can be given to the combustion chamber by dissociating from the exhaust gases. The difference between NO of the combustion without dilution and 15% $N_2$, $CO_2$, and $H_2O$ diluted ones is 13.4%, 14.8%, and 24.8% at ER=1.39.
- The increase in dilution rates of $N_2$, $CO_2$, and $H_2O$ in the upstream air reduces NO. NO emission with 10% $N_2$, $CO_2$, and $H_2O$ additions decreases 8.5%, 9.2%, and 17.7% in turn. The appropriate dilution ratios must be adjusted by taking consideration the reaction temperatures and system efficiency.
- The pressure increases NO emissions under all the combustion conditions with/without dilution. NO amount at the end of combustion with 15% $N_2$, $CO_2$, and $H_2O$ addition into the upstream air decreases 18.9%, 26.4%, and 30.2% respectively at 10 Atm pressure.
- The rising air inlet temperature enhances NO emissions. The increment tendency in NO formation with the air inlet temperatures above 600 K is higher than that of previous temperature values. The inlet air can be heated by exhaust gases for providing the better combustion and ignition. NO decreases 6.7%, 9.1%, and 21.7% with 15% $N_2$, $CO_2$, and $H_2O$ additions at 800 K.
- The increasing inlet premixed synthesis gas/air temperature uplifts NO amount. NO increases 15.5%, 18.1%, 19.2%, and 17.7% for the combustion without addition and with 15% $N_2$, $CO_2$, and $H_2O$ additions between 250 and 325 K of the inlet temperature. The inlet temperature of premixed synthesis gas/air can be hold at 300 K.

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