The Effect of Temperature on the Emissions of Shale Gas Combustion in USA

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Abstract

The turbulent, non-adiabatic, and non-premixed combustion of shale gas and air in a cylindrical combustor is computationally investigated under the effects of equivalence ratio, wall temperature, fuel and oxide inlet temperatures. The results indicate that the mass fractions of NO come to the maximum values at 0.97, 1.03, and 1.03 equivalence ratios for Fayetteville, New Albany, and Haynesville. The rising equivalence ratio raises CO emissions for all the shale gas. The rearing oxide inlet temperature increases NO mass fractions up to 290 K for Fayetteville and 308 K for New Albany and Haynesville. It also enhances CO emissions. The escalating fuel inlet temperature boosts NO mass fractions. However, it reduces CO emissions at all the shale gas combustion. The ascending wall temperature uplifts both NO and CO mass fractions.

Keywords: Shale gas, Non-premixed combustion, Nitrogen oxide, Carbon monoxide.

ABD'de Kaya Gazı Yanmasının Emisyonları Üzerinde Sıcaklığın Etkisi

Öz

Silindirik bir yakıcıda kaya gazı ve havanın türbülanslı, adyabatik olmayan ve önkarışımsız yanması ekivalans oranı, duvar sıcaklığı, yakıt ve oksit giriş sıcaklıklarının etkileri altında hesaplamalı olarak incelenmiştir. Sonuçlar NO'in kütle kesitlerinin Fayetteville, New Albany ve Haynesville için 0.97, 1.03 ve 1.03 ekivalans oranlarında maksimum değerlerine ulaştığını göstermektedir. Artan ekivalans oranı tüm kaya gazları için CO emisyonlarını yükseltmektedir. Yükselen oksit giriş sıcaklığı Fayetteville için 290 K ve New Albany ve Haynesville için 308 K'e kadar NO kütle kesitlerini artırmaktadır. CO emisyonlarını da yükseltmektedir. Artan yakıt giriş sıcaklığı NO kütle kesitlerini artırmaktadır. Bununla birlikte, tüm kaya gazları yanmalarında CO emisyonlarını düşürmektedir. Artan duvar sıcaklığı hem NO hem de CO kütle kesitlerini yükseltmektedir.

Anahtar Kelimeler: Kaya gazı, ön karışımsız yanma, nitrojen oksit, karbon monoksit.

1. Introduction

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The expectations of high living standard, growing population, developing technologies, the usage of unproductive power consuming devices, the transformation in energy structure, regional conflicts, and the competition among countries raise energy need and strongly lead countries to search new energy sources. Moreover, the demand for electricity gradually rises because of electrical based services as transporting, heating and cooling, cooking, lighting, sanitation, information and communication [1]. The intensive energy producing systems mostly use coal, gas, nuclear materials, and hydraulic potential. However, the environmental reasons have forced countries to recede from coal and nuclear plants and put gas forward in the last decays [2].

There are different gas types as natural gas, shale gas, and synthesis gas (syngas). Natural and shale gases are extracted from the underground and shale rocks. Synthesis gas is produced from organic and inorganic sources as coal, tire, urban waste, biomass, and etc. Shale gas as un-conventional natural gas can decrease greenhouse gas emissions by low carbon energy. It also has a long mining life and production cycle compared with conventional natural gas. The reserve of shale gas in the world is plenty with 214.5 trillion cubic meters and 1.4 times of natural gas [2, 3].

The gas production from shale gas reservoirs with low matrix permeability, organic-rich deposition, and mineral-filled nature fracture clusters have begun to become crucial in the world energy supply in the last few years [4]. It is firstly extracted and commercialized with horizontal drilling and hydraulic fracturing methods by United States followed by China, India, Poland, South Africa, Australia, UK, and Ukraine. The largest shale gas resource of the world belongs to China planning the shale gas production of 80-100 billion m^3/year by 2020. Nevertheless, the extraction of shale gas by hydraulic fracturing causes the pollution of water, greenhouse gas emission by fugitive methane, hazardous health problems, and even earthquakes [5].

The method used for the energy production from any type of gases is the combustion process. Gas (fuel) and air (oxide) can be burned in a combustor as premixed, partially premixed, non-premixed, and etc. The heat energy emerged at the end of the combustion is converted to mechanic work or electricity energy in today's system. The combustion process also emits hazardous emissions to the environment as nitrogen oxides (NO_x), carbon monoxide (CO), sulfur oxides (SO_x), hydrocarbons (HC), volatile organic compounds (VOCs), ozone (O_3), soot and other particles except for carbon dioxide (CO_2) and water vapor (H_2O) because of generally incomplete combustion, high reaction temperature, fuel and oxide compounds. The detrimental emissions for the gas combustion are mostly seen as NO_x and CO. NO_x is composed by mainly NO and NO_2 and is responsible for respiratory system illness, smog and acid rains. CO as toxic gas causes mortal poisoning. CO and NO_x emissions of USA in 2017 are reported as 60109 and 10776 in thousands of tons [6-13].

NO_x emerges in three different ways as thermal, prompt, and fuel during combustion. Thermal NO_x arises at high temperature above 1300 ^oC with the oxidization of oxygen and nitrogen defined by Zeldovich mechanism. Prompt NO_x produces in that the formation rate of NO_x surpasses the oxidization rate of oxygen and nitrogen in the thermal way. Fuel NO_x occurs from nitrogen in fuel depending on temperature, nitrogen onset concentration in fuel and air, and stoichiometric ratio. CO forms from the reaction of carbon and oxygen during the incomplete combustion [12]. Non-premixed combustion examined in this study stands for the case in that fuel and oxide enter to a burner from separated ways and the oxidization process occurs by contacting and mixing of fuel and oxide at the inside of burner. Oxide can be oxygen or air.

The combustion phenomena for various types of gases are both numerically and experimentally investigated under different conditions as turbulent, laminar, adiabatic, non-premixed, premixed, and etc. for different types of combustors. It is seen that the studies of shale gas generally focus on the emissions and environmental effects of the extracting process of it. There is a gap for the combustion process, characteristics, and emissions of shale gas in the literature. Ozturk detected that increasing inlet pressure raise NOx, ascending humidity ratio reduces NOx, and rising flow rate decreases NO_x for non-premixed shale gas combustion [12]. Cohen and Winkler determined shale gas to have lower greenhouse gas emissions than coal in the electricity generation [14]. Vargas et al. concluded the shale gas 3 (58% CH4 - 20% C2H6 - 12% C3H8 - 10% CO2) has higher laminar burning velocity than shale gas 1 and 2 [15]. Gebhardt indicated the compound of Polish shale gas is probable for usage by comparing to American gases [16].

In this study, NO and CO emissions of turbulent, non-premixed and non-adiabatic combustion of shale gas in a cylindrical combustor are numerically investigated at different wall temperature, fuel and oxide inlet temperatures, and equivalence ratios by ANSYS software.

2. Materials and Methods

The combustion process including the cases of thermo dynamics, heat and mass transfer, radiation, chemical kinetics, fluid mechanics is both numerically and experimentally studied. Numerical method is preferred more by researchers for the combustion phenomenon because it is easier to handle, cheaper, and consumes less time. The computational fluid dynamics (CFD) is a finite volume method solving numerically the problems of fluid mechanics, various reactions, heat and mass transfer, combustion, and etc. It can be used for the numerical calculations of rates, reactions, flame, temperatures, mass and mole fractions, products or emissions during the combustion of fuel and oxide in a burner.

Fluid Flow (Fluent) in ANSYS as a CFD software utilized in this study analysis and solves the equations of the problem defined by mathematical models under the determined boundary conditions, solution methods and controls on the meshed geometry of a system. The calculations of non-premixed combustion for simplification and faster solutions are carried out on a 2D model of the cylindrical combustor. The mesh of 2D field of the combustor consists of 12261 nodes and 12000 elements. The meshed combustion field is illustrated in Fig. 1 [12].
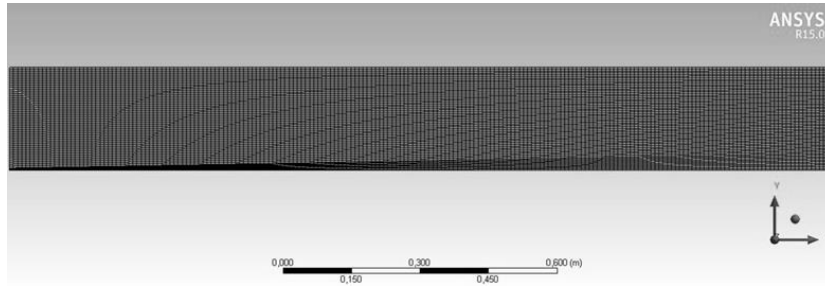
Fig. 1. The meshed combustion field of the combustor

The dimensions of the combustor, the wall temperature, and the inlet flow rates and temperatures of shale gas and air are depicted in Fig. 2. If it is not given any different condition in the text, the wall temperature of the combustor is 300 K, the pressure is 1 Atm, the equivalence ratio (ER) of fuel/air is 1 respectively.
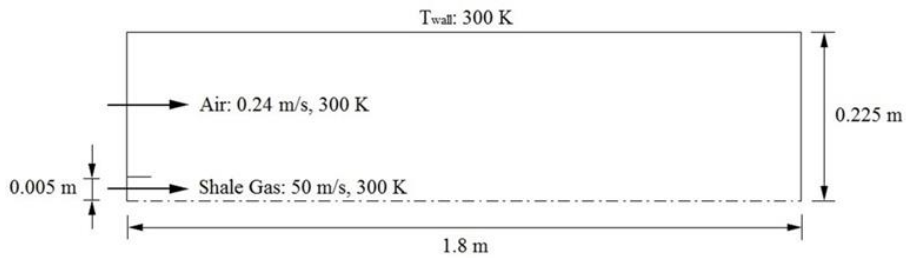

Fig. 2. The inlet temperatures and rates of fuel and oxide for the cylindrical combustor [12]

Shale gases used as fuel in the calculations are extracted from several field sources of Fayetteville, New Albany, and Haynesville regions of USA. The average values of the gas compositions of the fields are given in Table 1.

*Table 1. The shale gas compositions used in the numerical calculations [17]*

Regions	CH_4	C_2H_6	C_3H_8	CO_2	N_2
Fayetteville	97.3	1	0	1	0.7
New Albany	89.875	1.125	1.125	7.875	0
Haynesville	95	0.1	0	4.8	0.1

The following models and properties for the solutions are adjusted in the setup: Energy – On, Viscous Model – k-epsilon (2 eqn), k-epsilon model – standard, Near-Wall Treatment – Standard Wall Functions, Radiation Model – P1, Species Model – Non-Premixed Combustion (Inlet Diffusion, Chemical Equilibrium, Non-Adiabatic are selected), NO_x Model – On (Thermal, Prompt and N2O Intermediate are selected). Fuel (shale gas) and Oxide (air) ratios and flow rates for the complete combustion and other cases of non-premixed are separately entered in the section of Fuel and Oxide at Boundary tab of PDF Table.

The mass fraction of NO_x is evaluated in the terms of the mass fraction of NO at the outlet of the combustor in this study. Furthermore, NO can be used in the place of NO_x that is the sum of mass fractions of NO and NO_2 because there is mostly a difference of 10^{-3} between NO and NO_2 mass fractions.

3. Results and Discussion

The mass fractions of NO at different equivalence ratios are given in Fig. 3a. The maximum NO mass fractions of Fayetteville, New Albany, and Haynesville occur at the equivalence ratio of 0.97, 1.03, and 1.03 respectively. The highest NO belongs to New Albany shale gas and is 0.00269 kg NO/kg. Thermal NO formation has a bigger effect in total NO emissions of New Albany and Haynesville according to Fayetteville shale gas combustion because of high reaction temperatures over 2000 K. The combustion is actually carried out with %20 excess air to reduce the emissions and provide a better combustion in practice. It corresponds to roughly ER=0.8. NO emissions for Fayetteville, Haynesville, and New Albany at ER=0.8 are 0.000385, 0.00086, and 0.0012 kg NO/kg. CO mass fractions of the non-premixed combustions of shale gases are depicted in Fig 3b. The ascending equivalence ratio raises CO mass fractions for all the shale gases as expected. The rising equivalence ratio enhances fuel ratio and reduces air in the combustor. Thus, CO rises as the result of incomplete combustion. The highest CO emerges at Fayetteville combustion. There is a difference of %52 between Haynesville and Fayetteville at ER=1. For ER=0.8, CO emissions of New Albany, Haynesville, and Fayetteville are 0.0071, 0.01025, and 0.0201 kg CO/kg. The maximum reaction temperatures are illustrated in Fig. 3c. The order of maximum reaction temperature from the highest to the lowest is New Albany, Haynesville, and Fayetteville. The maximum reaction temperature of New Albany is 2048 K. The absent air reduces reaction temperatures in the rich fuel areas because of the incomplete combustion. The difference between the maximum reaction temperatures of Fayetteville and Haynesville is %3 with 68 K.
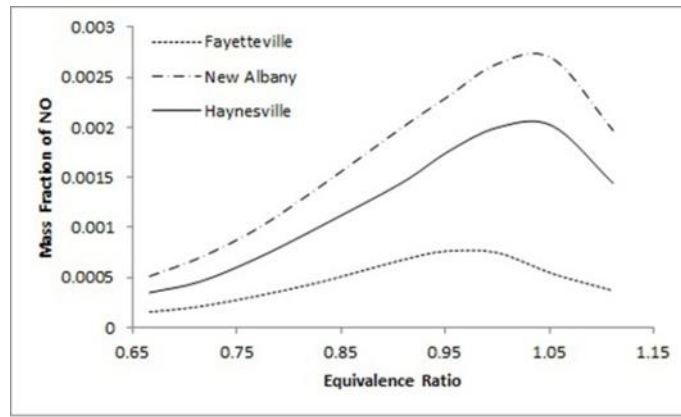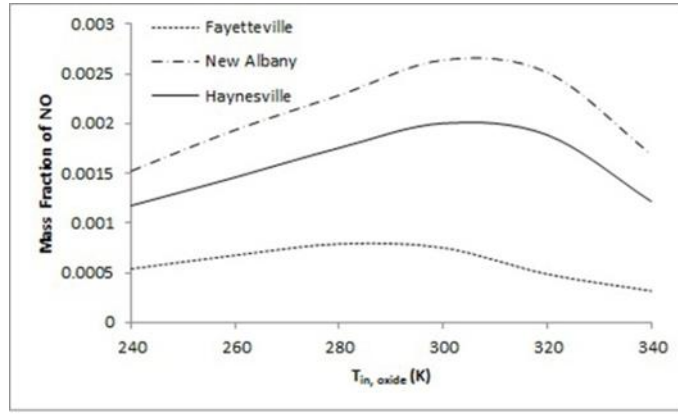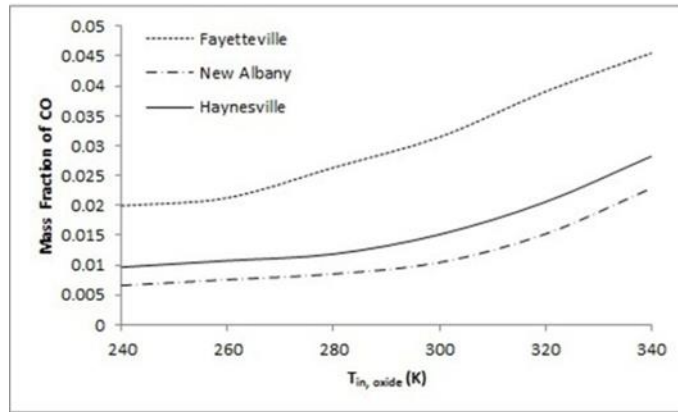
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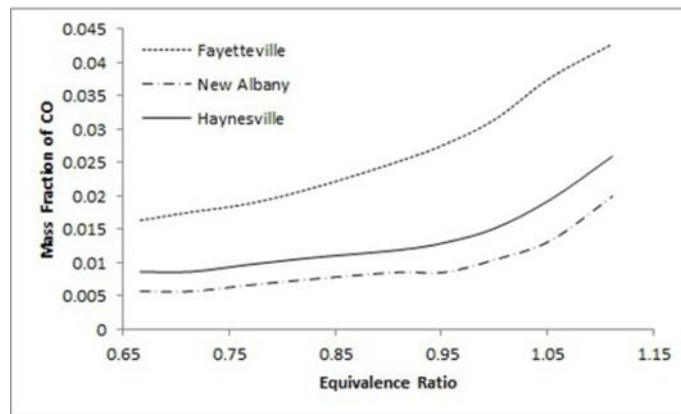
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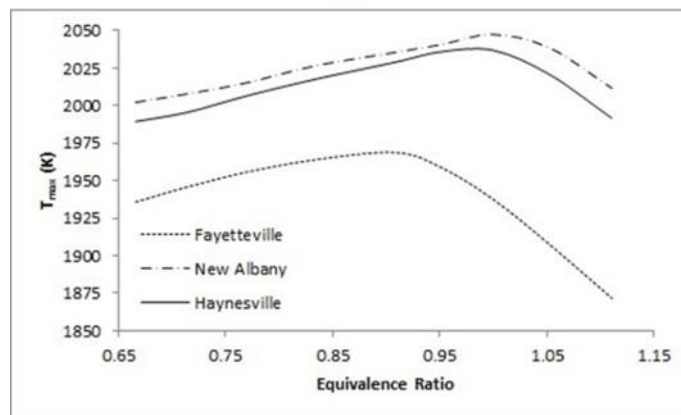
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Fig. 3. The mass fractions and maximum reaction temperatures at different equivalence ratios: (a) NO mass fraction, (b) CO mass fraction [12], (c) Maximum reaction temperatures

The effect of air (oxide) inlet temperature on the emissions of NO and CO is represented in Fig 4a and 4b. The fuel inlet and wall temperatures are constant at 300 K. NO emissions of New Albany and Haynesville rise up to 308 K and begin to decreases after that temperature. This case for Fayetteville roughly occurs at 290 K. The reason of the NO decrement after a certain inlet temperature value of oxide can be because warmer oxide does not adequately mix with fuel owing to the wrapping effect created by warmer oxide around fuel flowing at 300 K in the center of the combustor. The increment ratios for New Albany, Haynesville, and Fayetteville are %42, %41, and %31 between 240 K and maximum NO temperatures. The ascending oxide inlet temperature enhances CO emissions for all the shale gas combustions. The increments between 240 and 340 K are %128, %192, and %247 for Fayetteville, Haynesville, and New Albany respectively. The maximum reaction temperatures indicated in Fig 4c act similar as NO emissions because there is a crucial relation between the temperature and NO. The highest values of the maximum reaction temperatures are approximately 1956, 2039, and 2049 K for Fayetteville, Haynesville, and New Albany.
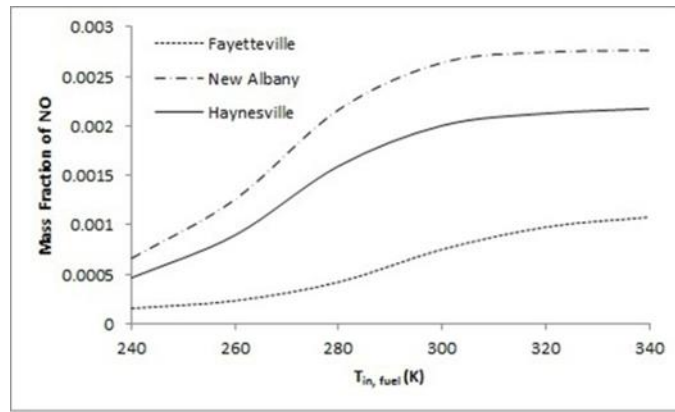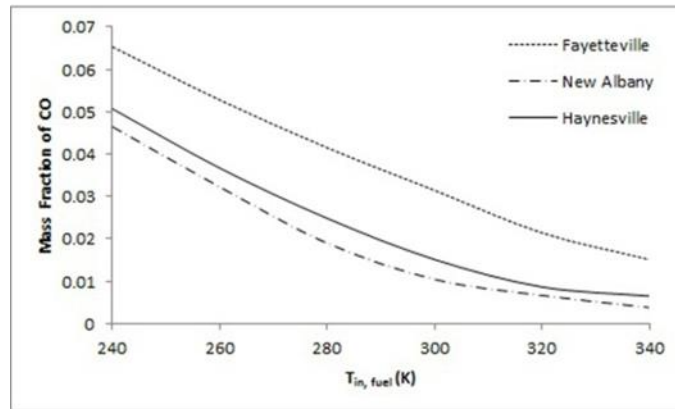
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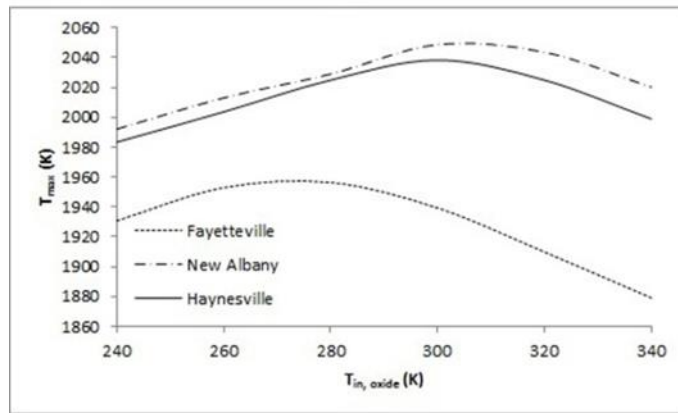
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Fig. 4. The mass fractions and maximum reaction temperatures at different oxide inlet temperatures: (a) NO mass fraction, (b) CO mass fraction, (c) Maximum reaction temperatures

The escalating fuel inlet temperature increases NO mass fractions given in Fig 5a. The rank from the highest to the lowest is New Albany, Haynesville, and Fayetteville. The increment slopes of NO mass fractions decrease a bit after 290 K for Fayetteville and 308 K for New Albany and Haynesville. There is an increment of %320, % 370, and %575 for New Albany, Haynesville, and Fayetteville respectively between 240 and 340 K. On the contrary, the rising fuel inlet temperature reduces the mass fractions of CO because of fuel burning better in Fig 5b. New Albany combustion has lower CO emission. The difference of 100 K at fuel inlet temperature causes the decrement of %76, %87, and %91 for Fayetteville, Haynesville, and New Albany. The effect of the rearing fuel inlet on the maximum reaction temperatures is illustrated in Fig. 5c. It uplifts the maximum reaction temperatures for all the shale gases because of fuel combusting more effective. Nevertheless, the growing reaction temperature raises thermal NO mass fractions as well. The augmentation at the maximum reaction temperature for an increment of 100 K in the fuel inlet temperature is 102 K (%5), 117 K (%6), and 173 K (%9) for New Albany, Haynesville, and Fayetteville.
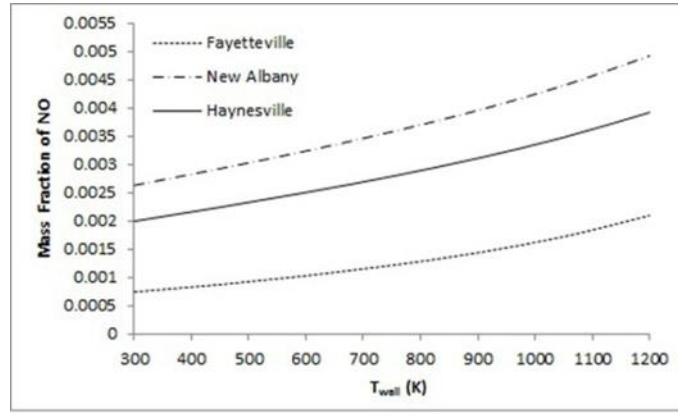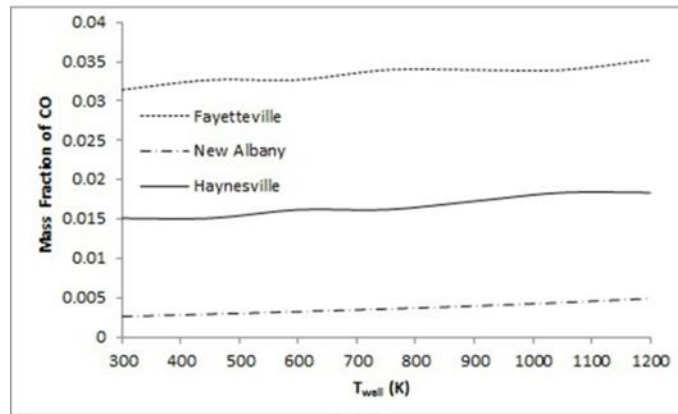
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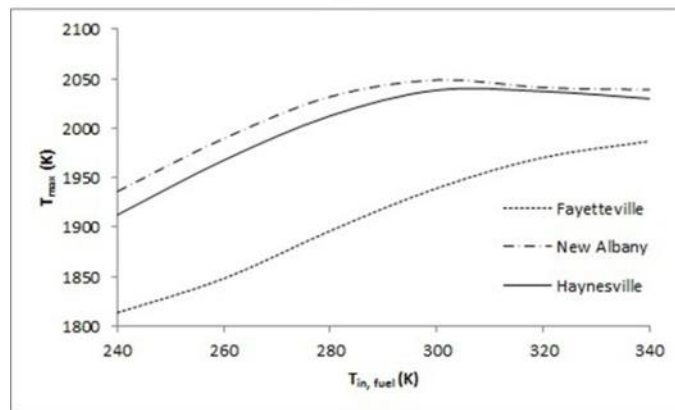
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Fig. 5. The mass fractions and maximum reaction temperatures at different fuel inlet temperatures: (a) NO mass fraction, (b) CO mass fraction, (c) Maximum reaction temperatures

The effect of the wall temperature of the combustor on the NO and CO emissions is depicted in Fig 6a and 6b. The ascending wall temperature in non-adiabatic combustion increases NO mass fraction because of the rising reaction temperature. The augment ratio between 300 and 1200 for NO mass fractions of New Albany, Haynesville, and Fayetteville is %86, %96, and %86. It also raises CO mass fractions somewhat. The highest CO value with 0.0333 kg CO/kg on average belongs to Fayetteville shale gas combustion. It can also be commented that the rising at both NO and CO mass fractions indicates a tendency toward poor or incomplete combustion. It is seen in Fig 6c that the increasing wall temperature enhances the maximum reaction temperature of the combustion. The increment of 900 K at the wall temperature causes to the elevation of 81 K, 84 K and 95 K for New Albany, Haynesville, and Fayetteville respectively.

The combustion systems burned gas and other fuels in heating devices, engines, and power plants emerges somehow the hazardous emissions as NO, CO, SO and the other pollutants. The undesired emissions are able to be withdrawn nearly to the proper limits by the ways as humid combustion air, exhaust gas re-circulation, water injection, low sulphur gas, liquid shower, compressed air, catalytic reduction, and etc [12].

(a)

(b)
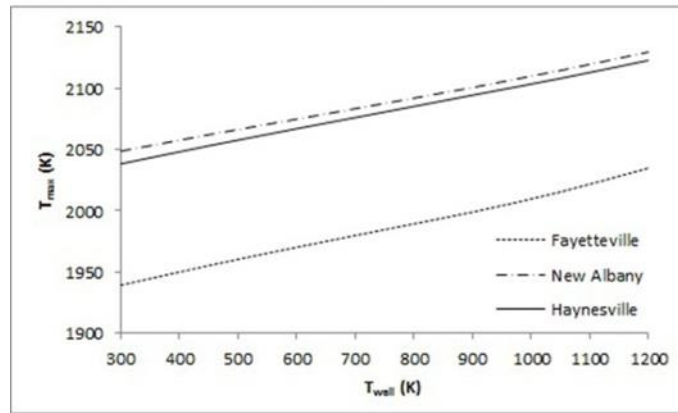
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Fig. 6. The mass fractions and maximum reaction temperatures at different wall temperatures: (a) NO mass fraction, (b) CO mass fraction, (c) Maximum reaction temperatures

4. Conclusion

The NO and CO emissions of turbulent, non-premixed, and non-adiabatic combustions of shale gases extracted from several regions of USA are numerically investigated and the alterations of mass fractions of NO and CO with the variations of oxide and fuel inlet temperatures, wall temperatures and equivalence ratios are computationally determined in this study. The following results are obtained:

- NO mass fractions of Fayetteville, New Albany, and Haynesville reach to the maximum at the equivalence ratios of 0.97, 1.03, and 1.03 respectively. The highest NO belongs to New Albany with 0.00269 kg NO/kg. The rising equivalence ratio increases CO mass fractions for all the shale gases. The rank of maximum reaction temperatures from the highest to the lowest is New Albany, Haynesville, and Fayetteville.

- NO mass fractions of New Albany and Haynesville arrive to the maximum value at 308 K and begin to decreases after that temperature under the effect of rising oxide inlet temperature. It is approximately 290 K for Fayetteville. The increasing oxide inlet temperature uplifts CO emissions for all the shale gas combustions. The maximum reaction temperatures for Fayetteville, Haynesville, and New Albany nearly come to the highest values at 1956, 2039, and 2049 K respectively.

- The rising fuel inlet temperature escalates NO mass fractions. The order from the highest to the lowest NO value is New Albany, Haynesville, and Fayetteville. The enhancing fuel inlet temperature decreases CO mass fractions. It raises the maximum reaction temperatures at all the shale gases combustions.

- The enhancing wall temperature ascends NO mass fractions. It also uplifts CO mass fractions a bit. The highest CO emission belongs to Fayetteville with 0.0333 kg CO/kg on average. The escalating wall temperature rears up the maximum reaction temperatures of the combustions.

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