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***Journal of Scientific and Engineering Research*, 2018, 5(11):256-264**

Research Article

ISSN: 2394-2630
CODEN(USA): JSERBR

A Computational Evaluation for Hazardous Emissions of Non-premixed Shale Gas Combustion

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Abstract Two dimension numerical investigation of the non-premixed combustion of shale gas and air in the cylindrical combustor is carried out to determine the emissions of nitrogen oxides and carbon monoxide. Moreover, the effects of inlet temperature, flow rate, pressure, equivalence ratio, and humidity ratio over the emissions are investigated in this study. Based on the results, Increment of inlet temperature raises NO_x and reduces CO mass fractions. The maximum values of NO_x mass fractions of Fayetteville, Marcellus, Haynesville, and New Albany occurs at 0.98, 0.915, 1.03, and 1.03 equivalence ratios respectively. Rising humidity ratio of the burning air reduces NO_x and lightly uplifts CO mass fractions. Ascending inlet pressure grows up NO_x and mitigates CO mass fractions. Increasing inlet flow rate lowers NO_x and slightly enhances CO mass fractions.

Keywords Shale gas, combustion, nitrogen oxides, carbon monoxide

1. Introduction

Industrial progress, competition among countries, growing population and developing countries cause to the increase in energy demand in the last decay. Energy for vehicles, heating systems, industries and power plants is mostly obtained by combustion of carbon based fuels as gases, coals, oils, etc. Efficient combustion systems that produce energy by low fuels and emit less air pollutant have gained importance because of the effects of hazardous combustion emissions over human's health and environment [1].

The main gas pollutants emerging at the end of combustion because of incomplete combustion, high temperature, and fuel ingredient are nitrogen oxides (NO_x), sulphur oxides (SO_x), carbon monoxide (CO), hydrocarbons (HC), ozone (O_3), and volatile organic compounds (VOCs) [2-5]. NO_x consisting of mainly NO and NO_2 causes diseases of respiratory system and is responsible for smog and acid rains with SO_x (SO, widely SO_2) [6, 7]. HC constitutes the irritation at eye, nose and throat [2]. CO is a toxic gas and a reason for mortal poisoning. Finally, O_3 and VOCs lead to respiration illness as asthma and allergic symptoms [8, 9]. Total emissions of CO, NO_x, SO_2, and VOCS of USA in 2017 are determined as 60109, 10776, 2815, and 16232 in thousands of tons respectively [10]. World Health Organization has reported that seven million people die every year because of polluted air and ambient air pollution is the reason for the death of 4.2 million people in 2016 [11].

Shale gas consists of methane, heavy hydrocarbons (ethane, propane), carbon dioxide, nitrogen, hydrogen sulfide, and water. Shale gas has firstly begun to be extracted from shale rocks by horizontal drilling and hydraulic fracturing in USA. It is estimated that there is 100-year supply and shale gas will be %50 of total gas production by 2035 in USA. India, China, South Africa, UK, Poland, etc. are commercially about to evaluate their own shale gas resources. From environmental point of view, water polluted by hydraulic fracturing process, more greenhouse gas emitted by fleeing methane, and earthquake jeopardy caused by all extracting process stand as important issues [12, 13].

There are many studies over the combustion characteristics, the reduction of emissions, and emissions of natural gases under the conditions of laminar, turbulent, adiabatic, non-adiabatic, premixed, non-premixed, etc. in the literature. It is also seen that the compositions of some natural gases are close to the compositions of shale gases and researchers mostly focus on the emissions and environmental effects of the extracting process of shale gas. Vargas et al. determined adiabatic flame temperatures and laminar burning velocities in the combustion of several shale gas mixtures [13]. Cohen and Winkler detected the emission intensity between 0.31 tCO_2/MWh and 0.59 tCO_2/MWh at electricity production from shale gas in South Africa [14]. Chang et al. found the greenhouse gas emissions of shale gas to be lower than those of coal-fired electricity [15]. McTaggart-Cowan et al concluded that nitrogen addition descends NO_x emissions and ethane addition ascends it in high-pressure non-premixed natural gas combustion [16]. Zahedi and Yousefi determined the addition of N_2 or CO_2 to the mixture decreases NO emissions and the increasing initial pressures grows up NO emissions in pre-mixed laminar methane-air combustion [17]. Silva et al. studied on CO and CO_2 mass fractions in the emissions and temperature distributions for turbulent non-premixed combustion of natural gas in a cylindrical chamber [18]. Jerzak et al. concluded propane addition into natural gas increases CO concentration and causes a slight NO_x rise in the combustion gas [19]. Hayashi et al. emphasized NO_x ascends with pressure increment and high temperature in non-premixed gas combustion [20]. Boushaki et al. revealed that increasing equivalence ratio decreases NO_x emissions, oxygen enrichment reduces CO emissions, and the flame temperature enhances NO_x emissions for turbulent non-premixed methane combustion in a swirl burner [21]. Jerzak et al. concluded that the addition of CO_2 to natural gas rise CO emissions and leads to a reduction in NO_x and the combustion temperature [22]. Mctaggert-Cowan et al. extrapolated nitrogen addition to natural gas reduces the emissions of nitrogen oxides, particular matter, hydrocarbons, and carbon monoxide without affecting the performance and efficiency of a direct-injection engine [23].

In this study, air pollutant NO_x and CO emissions of turbulent, non-premixed and non-adiabatic combustion of shale gas in a cylindrical burner are numerically determined under the effects of inlet pressure, temperature, flow rate, humidity ratio, and equivalence ratio by ANSYS software.

2. NO_x and CO Formation

The formation of NO_x occurs in the three ways called as thermal NO_x, prompt NO_x, and fuel NO_x in a combustion process. Thermal NO_x largely forms from nitrogen of the burning gas oxidizing with air via the thermal mechanism (Zeldovich) in the combustion chamber at high temperature over 1300 ^oC. Prompt NO_x rapidly comes into existence when the formation rate of nitrogen oxides surpasses the oxidizing rate of nitrogen defined in thermal NO_x in rich mixture region especially. Fuel NO_x emerges from nitrogen in the fuel composition and generally depends on temperature, stoichiometry, the onset concentration of nitrogen in fuel/air mixture, etc. CO mostly arises from the join of carbon and oxygen atoms at the incomplete combustion of hydro carbon fuels in the medium of low oxygen.

3. Methods

Combustion is a complex processes including thermo-dynamics, buoyancy, chemical kinetics, radiation, mass and heat transfers and fluid mechanics. Computer modeling and numerical solution of combustion are cheaper and easier to handle with respect to experimental way and consumes less time. It can be determined the flame composition, products, variation of temperature in the combustor for entered fuel compositions by Computational Fluid Dynamics (CFD) to study and analyze the combustion case [24].

Table 1: The shale gas compositions used in the numerical calculations [25]

Regions	CH_4	C_2H_6	C_3H_8	CO_2	N_2
Marcellus	85.2	11.275	2.875	0.35	0.3
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

Fluent used for the calculations in this study is the computational fluid dynamic (CFD) software with finite volume method. It is also utilized for the solution of problems including fluid mechanics, heat transfer, combustion phenomenon, etc.

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

The dimensions and wall temperature of the gas combustor and the inlet flow rates and temperatures of shale gas and air are depicted in Figure 1.

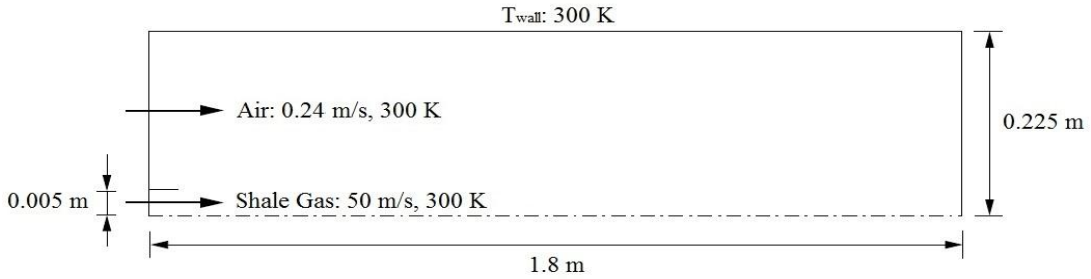

Figure 1: The cylindrical combustor and the inlet flow rates and temperatures [26]

The calculations of mass fraction of NO_x and CO emissions in shale gas/air combustions are performed in Fluid Flow (Fluent) from Analysis Systems of Ansys Workbench software. Fluent analysis the meshed geometry of a system and solves the equations of problem defined by mathematical models as laminar, turbulent, adiabatic, premixed, high-speed etc. with selected materials, boundary conditions, and solution controls. The mesh of the combustion field in two-dimension (2D) consists of 12261 nodes and 12000 elements. The following models and properties are chosen in the setup: Energy – On, Viscous Model – k-epsilon (2 eqn), k-epsilon model – standard, Near-Wall Treatment – Standart 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 N_2O Intermediate are selected).Low nitrogen of fuel is addedfrom underOxid at Boundary tab of PDF Table by changing Fuel (shale gas) and Oxid(air) ratios and flow rates for the complete combustions and others.

4. Results

The highest mass fraction of NO_x belongs to New Albany and Haynesville, Marcellus, and Fayetteville follow it in the decreasing order. Figure 2 shows NO_x mass fractions for all the shale gas combustion ascends with increasing inlet temperature of reactants. The temperature increment ascends thermal NO_x in the combustion chamber because increasing inlet temperatures raise the maximum reaction temperatures of all the shale gases. Thermal NO_x becomes dominant with regard to the prompt and fuel NO_x in high reaction temperatures. The NO_x increment between the emissions of combustions of New Albany and Haynesville at 255 and 315 K is around 39%. The percentage difference between these temperatures is about 36% for Marcellus and New Albany.

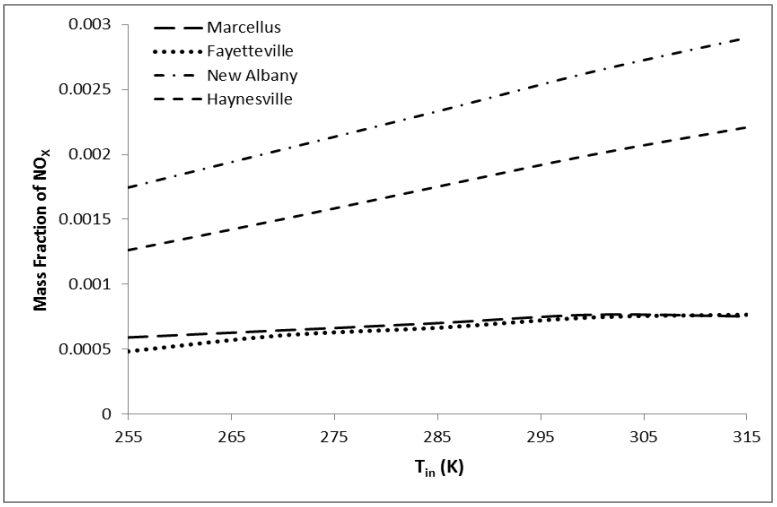

Figure 2: Variation of mass fraction of NO_x at different inlet temperature at ER=1, P=1 Bar, HR=0

It can be seen in Figure 3that the mass fractions of CO reduce with ascending inlet reactant temperature. The rank of mass fractions of CO from the highest to the lowest is Marcellus, Fayetteville, Haynesville, and New Albany. Increasing inlet temperature causes hydro-carbons to burn better in the burner with rising temperature and it descends CO mass fraction in the total. Variation of CO mass fraction is illustrated in Figure 4.The CO variation between the emissions of combustions of all the gases at 255 and 315 K is around 13%.

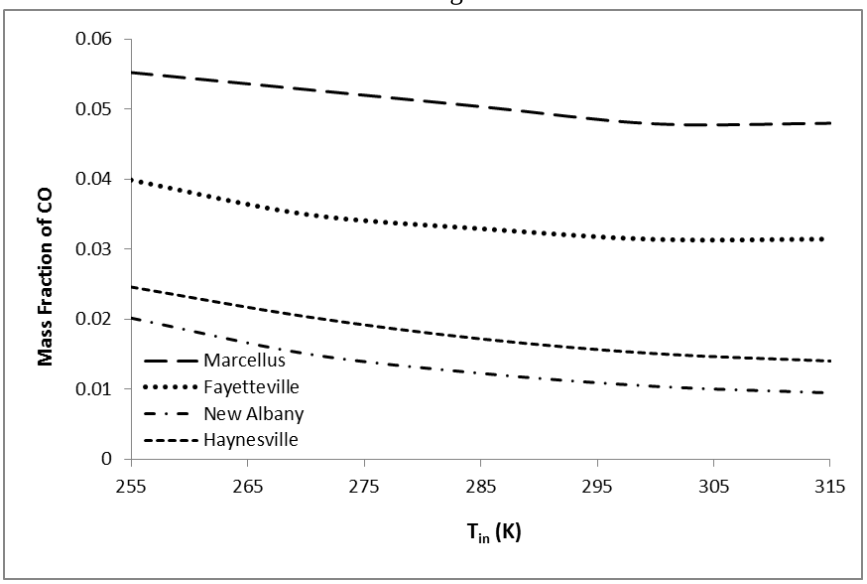

Figure 3: Variation of mass fraction of CO at different inlet temperature at ER=1, P=1 Bar, HR=0

Variation of mass fraction of nitrogen oxides with respect to equivalence ratio is presented in Figure 4. The maximum NO_x for the combustions of Fayetteville, Marcellus, Haynesville, and New Albany occurs at the equivalence ratios of 0.98, 0.915, 1.03, and 1.03 respectively. NO_x emission of New Albany is the highest and 0.0027.

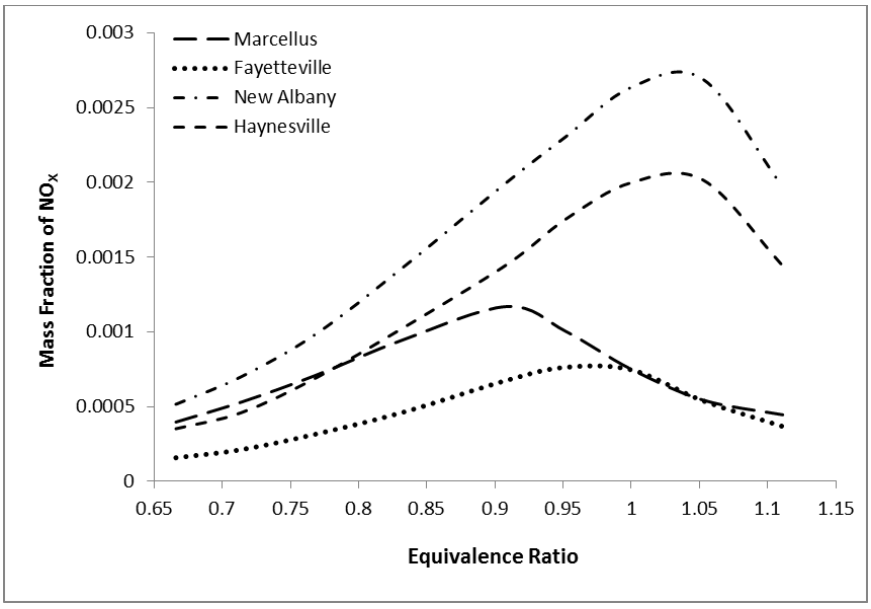

Figure 4: Variation of mass fraction of NO_x at different ERs at T_{in}=300 K, P=1 Bar, HR=0

In Figure 5, increasing equivalent ratio enhances mass fraction of CO as expected. Ascending equivalence ratio means low burning air in the burner. This case causes the incomplete combustion of fuel stream and grows up CO emissions. The variation of CO emission between 0.666 and 1.111 of equivalence ratiois roughly 59.5% for Marcellus combustion.

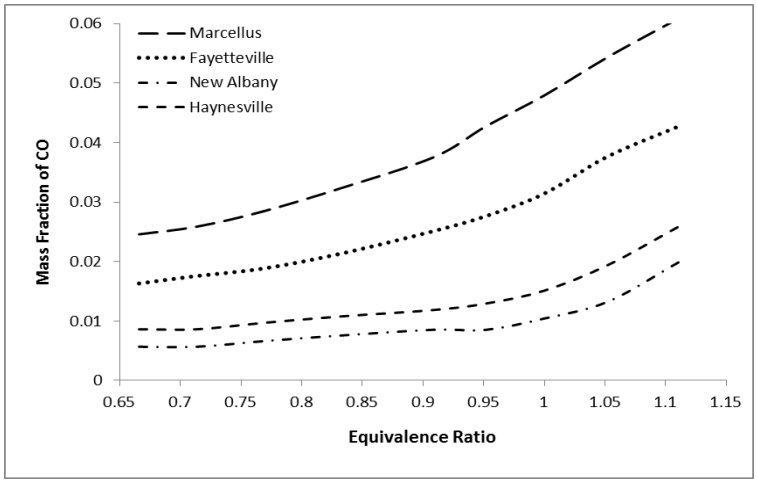

Figure 5: Variation of mass fraction of CO at different ER T_{in}=300 K, P=1 Bar, HR=0

Figure 6 shows the augmentation of humidity in the burning air causes the temperature of reaction to decrease and the decreasing temperature leads to the reduction of NO_x.It is the one of ways to descend NO_x emissions. NO_x variation between 0 and 0.025 of humidity ratio is 46.6%, 48% and 61.8%in the descending tendency for New Albany, Haynesville, and the others respectively.

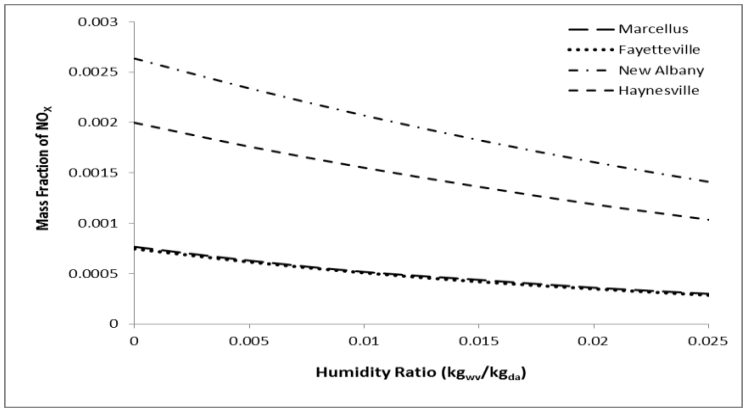

Figure 6: Variation of mass fraction of NO_x at different humidity ratio at ER= 1, T_{in}=300 K, P=1 Bar

It is given in Figure 7 that the augmentation of humidity in the burning air slightly raises mass fraction of CO.It points out the incomplete combustion of gases. The CO variations between 0 and 0.025 of humidity ratio are approximately 2%, 7.3%, 15%, and 13% for the combustions of Marcellus, Fayetteville, Haynesville, and New Albany.

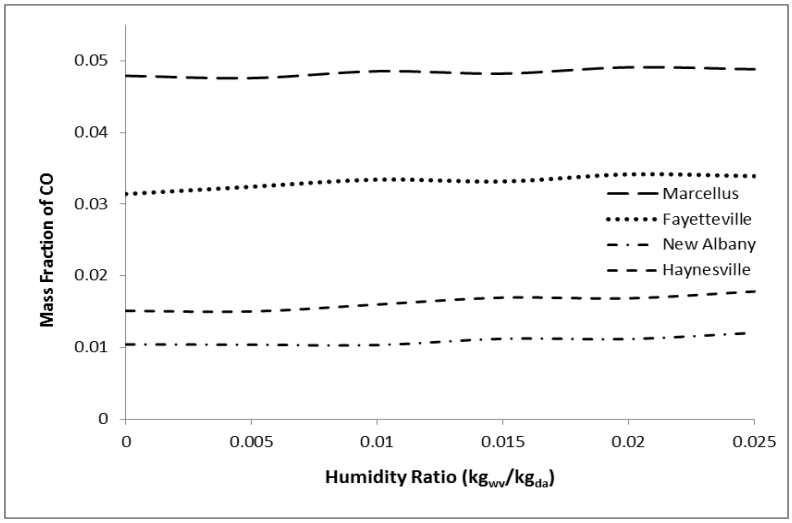

Figure 7: Variation of mass fraction of CO at different humidity ratio at ER= 1, T_{in}=300 K, P=1 Bar

The pressure measured by the gauge is relative to the atmospheric pressure as the zero point in the gas combustions. Rising inlet pressure raises mass fraction of NO_x for all the combustion, as given in Figure 8. The increment tendency is lower after the pressure of 2 bars. NO_x variations for 10 bars are around 50%, 56%, 75%, and 68.5% in the ascending tendency for New Albany, Haynesville, Marcellus and New Albany combustions.

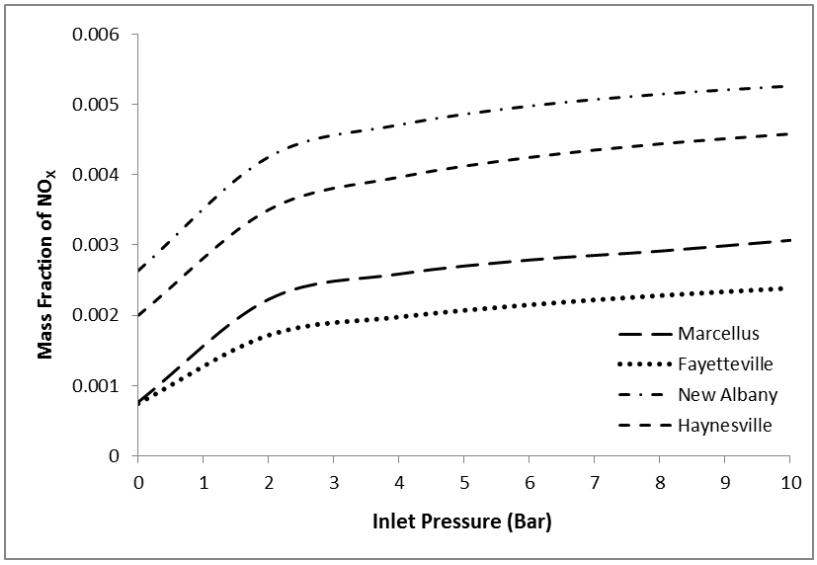

Figure 8: Variation of mass fraction of NO_x at different inlet pressure at ER= 1, T_{in}=300 K, HR=0

Figure 9 shows the mass fraction of CO reduces till 2 bars, after that, it stays constant at the certain value. The CO variation for 10 Bar is about 7-9% for all the shale gas combustions. The highest value of CO belongs to Marcellus by0.047.

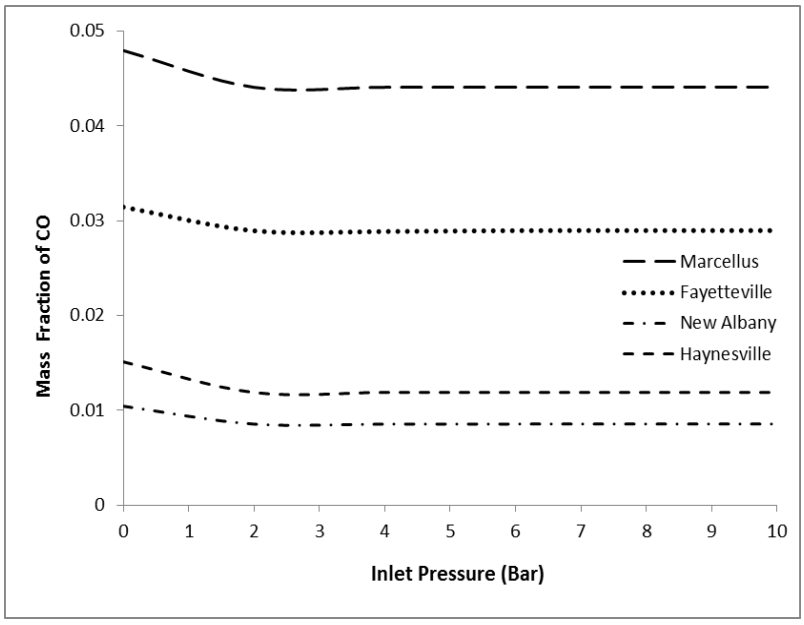

Figure 9: Variation of mass fraction of CO at different inlet pressure at ER= 1, T_{in}=300 K, HR=0

Figure 10 indicates the variation of NO_x at the folds of different inlet flow rates. Escalating flow rates reduces the mass fraction of NO_x. High rates cause incomplete combustion because of entering excessive mass in the burner. Figure 11 shows it leads to the slight ascent of mass fraction of CO after 1.5 folds of flow rates. NO_x variations1x and 3.5x folds of flow rates are 55.3%, 52.8%, 15.7%, and 39% in the decreasing tendency for New Albany, Haynesville, Marcellus, and New Albany combustions. The variations for CO mass fractions between 1x and 3.5x folds are 8-9% for all the combustions.

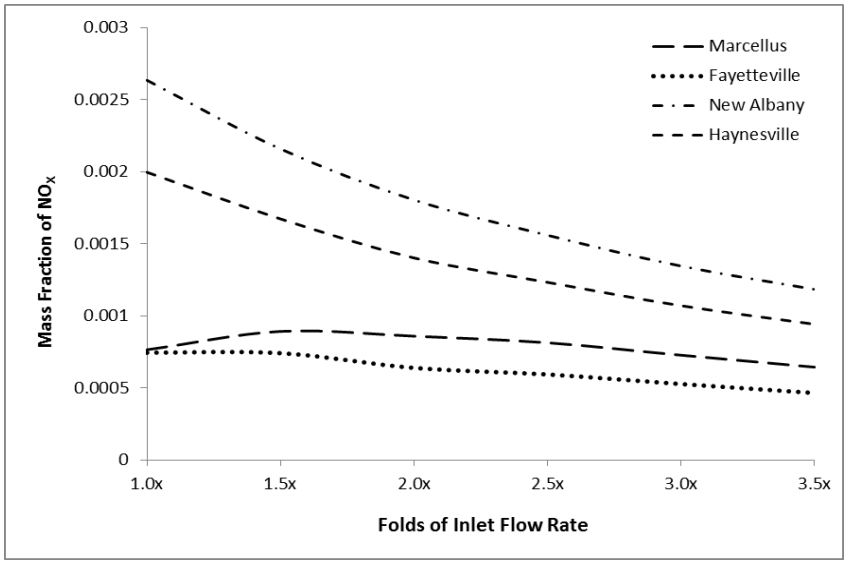

Figure 10: Variation of mass fraction of NO_x at folds of inlet flow rate at ER= 1, T_{in}=300 K, P= 1 Bar, HR=0

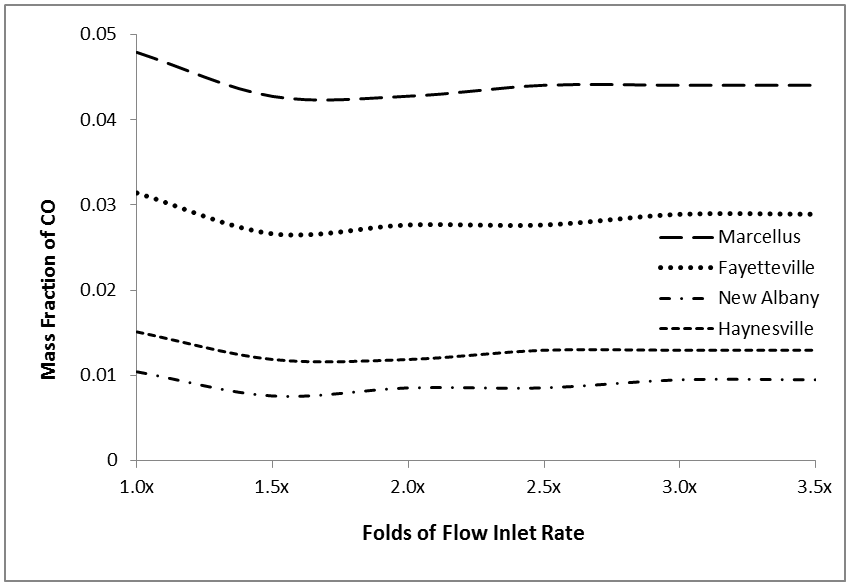

Figure 11: Variation of mass fraction of CO at folds of inlet flow rate at ER= 1, T_{in}=300 K, P= 1 Bar, HR=0

The emissions of NO_x, CO, SO_x, and the other pollutants in engines, power plants and heating systems including the gas combustion process are able to reduce to the acceptable levels by using the methods of water injection, compressed air, catalytic reduction, humid combustion air, exhaust gas re-circulation, low sulphur gas, liquid shower, etc.

5. Conclusion

The hazardous emissions of turbulent, non-premixed, and non-adiabatic combustions of four different shale gases extracted from various regions of USA are computationally investigated and the variations of mass fractions of NO_x and CO with disparate reactant inlet temperature, equivalence ratio, humidity ratio, inlet flow rate, and pressure are determined in this study. The following results are obtained:

- The mass fraction of NO_x increases with ascending reactant inlet temperatures for all the gases. The order of NO_x from the highest to the lowest is New Albany, Haynesville, Marcellus, and Fayetteville. The mass fraction of CO decreases with rising inlet temperatures. The rank of mass fractions of CO from the highest to the lowest is Marcellus, Fayetteville, Haynesville, and New Albany.

- The maximum NO_x mass fractions for the combustions of Fayetteville, Marcellus, Haynesville, and New Albany arise at the equivalence ratios of 0.98, 0.915, 1.03, and 1.03. Ascending equivalent ratio raises the mass fraction of CO because of low burning air.
- Increasing humidity ratio causes the mass fractions of NO_x to reduce. On the contrary, it lightly grows CO mass fractions.
- Ascending reactant inlet pressure raises NO_xmass fractions. But, it reduces CO mass fractions until 2 bar. CO mass fractions stay constant after 2 bar.
- Rising reactant inlet flow rates diminish the mass fractions of NO_x and slightly increases CO mass fractions.

The high emissions of nitrogen oxides and carbon monoxide emerging under the given combustion conditions could be brought under control at an acceptable level by using some methods as water injection, catalytic reduction, exhaust gas re-circulation, etc. in the gas combustion systems.

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