

# Effects of CO<sub>2</sub>, H<sub>2</sub>O and N<sub>2</sub> Dilutions on Emission Characteristics and Partially Premixed Combustion of Shale Gas



Suat Ozturk

**Abstract:** Environmental constraints of countries on hazardous emissions promote the usage of gas fuels in combustion systems for energy production. The shale gas recently shines out as one of the promising gas fuels of the future owing to its wide reserves discovered in the different gas fields of countries. This study numerically focuses on the emission characteristics and turbulent adiabatic combustion of partially premixed shale gas and humid air with dilution effects of CO<sub>2</sub>, H<sub>2</sub>O, and N<sub>2</sub> under different pressures. Ansys codes are used for the numerical computations of computational fluid dynamics on 2D model of a co-axial type combustor to find out the emissions and flame speeds during the combustion of shale gas and air. Based on the results, the maximum NO mass fractions are obtained at 1.42, 1.44, and 1.4 equivalence ratios for Barnette, New Albany, and Haynesville. The increasing equivalence ratio raises the mass fractions of CO and turbulent flame speeds. The rising CO<sub>2</sub> dilution into the additional air diminish the flame speeds, NO and CO fractions. The growing H<sub>2</sub>O addition decreases NO and CO mass fractions. On the contrary, it augments the flame speeds. The enhancing N<sub>2</sub> dope decreases NO and rears CO mass fractions. The rising pressure with 15% CO<sub>2</sub> dilution fades up the turbulent flame speeds, NO and CO fractions. The pressure increment with 15% H<sub>2</sub>O dope reduces CO and the flame speeds. But, it lightly relieves NO fractions. The growing pressure with 15% N<sub>2</sub> addition abates the mass fractions of CO and turbulent flame speeds.

**Keywords:** Shale gas, Partially premixed combustion, Turbulent, Emissions.

## I. INTRODUCTION

The requirement of high output, low pollution emissions and fuel consumption at hydro-carbon based energy production obliges to be developed the new technologies for the combustion systems using different types of fuels and operating under the various conditions as temperature, pressure, fuel mixtures. Among the new technologies, partially premixed combustion comes forward as a promising process at specially the elevated pressures under the environmental limitations [1].

Partially premixed means the case in that the additional

oxidizer and the molecularly premixed oxidizer/fuel at some equivalence ratio separately enter to the reaction zone of burner to establish the complete combustion. Partially premixed combustion exhibits superior emission characteristics because of its multiple reaction zones with respect to premixed and non-premixed. The interactions of reaction zones adjusted by transport and stoichiometry are able to optimize the emissions in flames of combustion [2].

The gas fuels as natural, shale, and synthesis gases compared to other fuels have especially become crucial to generate the lower main pollutant emissions as NO<sub>x</sub>, CO, and etc. being hazardous for the atmosphere and human health in the industrial and civil combustion systems. The most effective methods to prevent NO<sub>x</sub> and CO at the end of combustion for shale gas and the others seem as oxygen concentration adjustment, diluent usage in fuel, or bringing under control the reaction temperature [3].

Shale gas consists of methane, ethane, propane, carbon dioxide, nitrogen, hydrogen sulfide, and water similar to natural gas. Shale gas proceeds in the way of being one of the outstanding gas fuel of the future. USA is the first commercial producer and vendor of shale gas by extracting it from among shale rocks with horizontal drilling and hydraulic fracture methods. Indiana, China, South Africa, UK, and Poland also strain at shale gas production and China has the biggest shale gas reserves in the world [4, 5].

There are mostly studies related with the extraction procedures and its unfavorable environmental effects of shale gases in the literature. But, the investigations about combustion characteristic and hazardous emissions of shale gas have recently attracted the cares of researchers. Tian et al. studied oxygen diluted partially premixed combustion of CH<sub>4</sub>/air and the lower oxygen reduced NO<sub>x</sub>, but increases CO [3]. Vargas et al. concluded the shale gas 3 of 58% CH<sub>4</sub>-20% C<sub>2</sub>H<sub>6</sub>-12% C<sub>3</sub>H<sub>8</sub>-10% CO<sub>2</sub> has a higher laminar burning velocity than the shale gas 1 and 2 using GRI-Mech 3.0 mechanism [5]. Ozturk determined the inlet temperature increment raises NO<sub>x</sub> and reduces CO emissions, the rising humidity ratio decreases NO<sub>x</sub>, and the ascending inlet pressure uplifts NO<sub>x</sub> by Ansys software [6]. Chapiro and Bruining presented the parameters to reach the optimal temperature for providing the permeability at the shale gas combustion [7]. Cohen and Winkler detected the intensity of greenhouse gas emissions of shale gas fired electricity between 0.3 and 0.6 tCO<sub>2</sub>/MWh in South Africa [8].

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Chang et al. compared the greenhouse gas emissions and water consumption for both coal and shale gas fired power plant in China [9]. Min et al. indicated the effects of CO<sub>2</sub>, N<sub>2</sub>, and Ar dilutions over the flame length and stability of laminar flame [10]. Lee et al. found the nitrogen addition in fuel suppressed NO<sub>x</sub> formation [11]. Liu and Most reported CO<sub>2</sub> addition reduces OH intensity, flame temperature, and reaction zone thickness better than N<sub>2</sub> addition [12]. Wang et al. presented CO<sub>2</sub> addition to hydrogen-enriched gasoline engine reduced NO<sub>x</sub> and HC emissions [13]. Persis et al. concluded CO<sub>2</sub> dilution decreases NO and increases CO emissions in methane combustion [14].

In this study, the combustion characteristic and emissions of turbulent, adiabatic, partially-premixed shale gas/air combustion is computationally investigated and the turbulent flame speeds, NO and CO emissions at the end of combustion at different equivalence ratio and pressures are determined under the dilution effects of CO<sub>2</sub>, H<sub>2</sub>O, and N<sub>2</sub> additions.

## II. MATERIALS AND METHODS

The combustion phenomenon can both numerically and experimentally be investigated. Researchers prefer more numeric solutions that are very close to the experimental findings because the experiments are too expensive and consume time much. Besides, the combustion reactions occurring in a narrow space are complicated and too fast to be observed. Computational fluid dynamics (CFD) is a numerical finite volume method that solves and analyzes the problems of combustion including fluid flow, heat transfer, chemical reactions, and etc. at defined boundary conditions. ANSYS software is used to make the calculations of computational fluid dynamics in this study. The solutions of partially premixed combustion of shale gas and air are expedited and simplified with a two dimension model of the co-axial type combustor. The two dimension model of the combustion field includes 12076 nodes and 11800 elements as shown in Fig. 1.

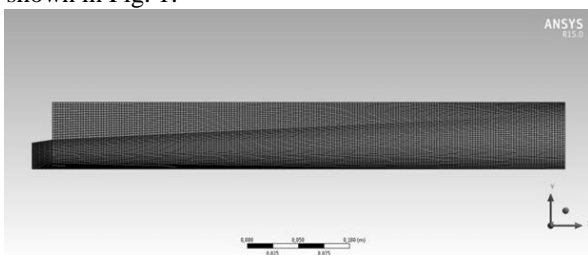


Fig. 1. The meshed field of 2D model.

The following model and property options for the solutions are selected in Fluent Setup: Viscous Model – k-epsilon (2 eqn), k-epsilon model – standard, Near-Wall Treatment – Standart Wall Functions; Species Model – Partially Premixed Combustion (Premixed Model – C Equation, Chemical Equilibrium, Adiabatic, and Flame Speed Model – Zimont are selected); NO<sub>x</sub> Model – On (Thermal, Prompt, and N<sub>2</sub>O Intermediate are selected). The inlet flow rates and temperatures, equivalence ratios, and etc. are entered form Zone of Boundary Conditions, Prompt Tab of NO<sub>x</sub> Model and Boundary tab of PDF Table by changing Fuel (shale gas-air mixture) and Oxid (air) ratios for the complete

combustions and others.

Barnette, New Albany, and Haynesville shale gases extracted from different field sources of USA are used for the combustion calculations in this investigation. The average values of the gas compositions are given in Table-I.

Table-I: The shale gas compositions [15]

Regions	CH <sub>4</sub>	C <sub>2</sub> H <sub>6</sub>	C <sub>3</sub> H <sub>8</sub>	CO <sub>2</sub>	N <sub>2</sub>
Barnette	86.75	6.725	1.975	1.675	2.875
New Albany	89.875	1.125	1.125	7.875	0
Haynesville	95	0.1	0	4.8	0.1

The inlet flow rates and temperatures of shale gas-air mixture (fuel) and air are depicted with the dimensions of the burner in Fig. 2. If any different condition is not mentioned, the premixed fuel consisted of shale gas and air enters by 30 m/s rate at 300 K as the additional air enters into the combustor chamber by 10 m/s rate at 600 K. Moreover, the air includes humidity at the rate of 1.5%. The diluents of CO<sub>2</sub>, H<sub>2</sub>O, and N<sub>2</sub> to examine the dilution effects on the combustions are added to the additional air at various ratios from 0 to 30%.

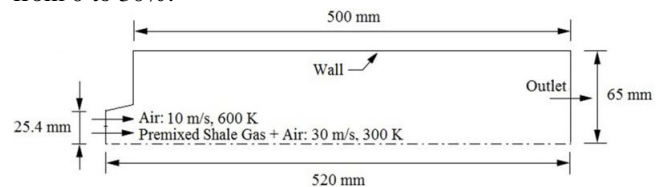


Fig. 2. The dimensions of the combustor and the inlet temperatures and rates of reactants [16].

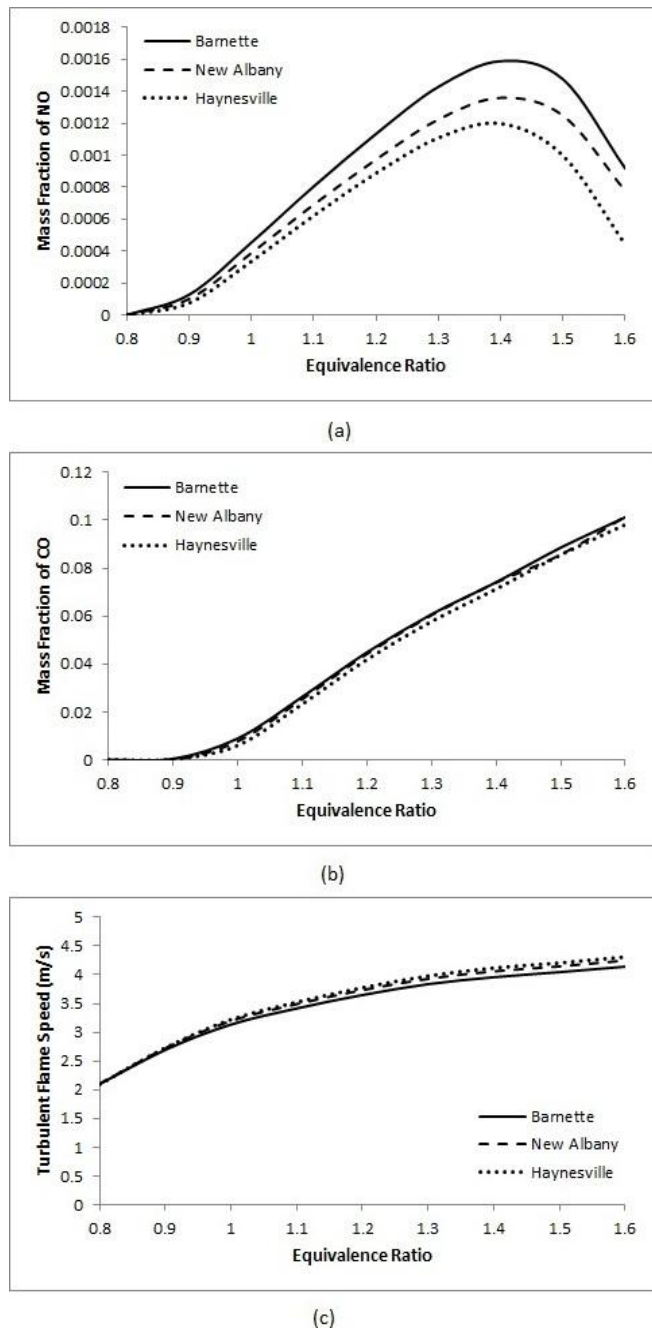
NO<sub>x</sub> emissions are evaluated in terms of NO concentration at the outlet. Furthermore, NO mass fraction can be used in the place of the mass fraction of NO<sub>x</sub> being the sum of NO and NO<sub>2</sub> because there is approximately a difference of 10<sup>-3</sup> between mass fractions of NO and NO<sub>2</sub>.

## III. RESULTS AND DISCUSSION

The mass fractions of NO at different equivalence ratios (ER) are illustrated in Fig. 3a. The equivalence ratio in Figs stands for the equivalence rate of shale gas and air in the premixed mixture. The values of NO mass fractions of Barnette, New Albany, and Haynesville reach to the maximum at 1.42, 1.44, and 1.4 of equivalence ratio. The highest NO belongs to the combustion of Barnette shale gas as 0.00159 kg NO/kg followed by New Albany and Haynesville. There is a difference of 15.5% and 35% between Haynesville and the others for NO mass fractions at ER=1. The rising equivalence ratio means rich fuel in the premixed and causes the temperature drop and the incomplete combustion after a certain point because of low air in the combustion chamber. Thermal NO especially reduces with decreasing reaction temperature. Fig 3b depicts CO mass fractions. CO raises with increasing equivalence ratio as expected because of excessive carbon and hydrocarbon compounds in the combustor. That is also one of the outcomes of incomplete combustion. The ranks for CO mass fractions are same as NO.



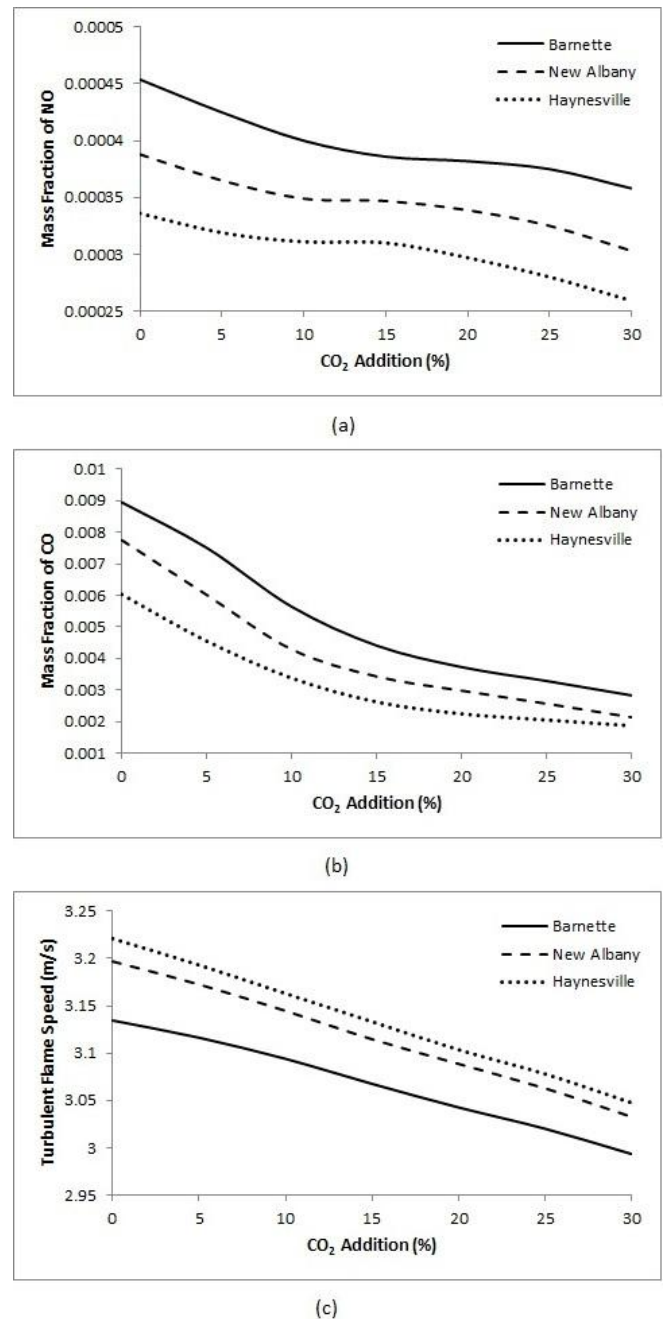
The difference between Haynesville and the others is 28.5% and 48.5% at ER=1. The turbulent flame speeds are illustrated in Fig 3c. The rising equivalence ratio enhances the turbulent flame speeds for all the shale gases. The order from the highest to the lowest is Haynesville, New Albany, and Barnette. The flame speeds approximately indicates an increment of 100% for equivalence ratio of 0.8 to 1.6 and are 3.221, 3.196, and 3.134 m/s for Haynesville, New Albany, and Barnette respectively.



**Fig. 3. The flame speeds and mass fractions of NO and CO at different equivalence ratios.**

NO mass fractions under the dilution effect of CO<sub>2</sub> in the additional air are given for ER=1 in Fig 4a. The growing CO<sub>2</sub> addition from 0 to 30% reduces the mass fractions of NO by 21.1, 21.9, and 22.9 % for Barnette, New Albany, and Haynesville because CO<sub>2</sub> addition decreases flame temperature and the waning flame temperature reduces NO

production. It also causes a reduction in reactive species concentrations, reaction rates, and flame velocities that fades flame stability [17]. The addition of CO<sub>2</sub> abates the mass fractions of CO by 68.3, 72.4, 69% as given in Fig 4b. Fig 4c represents the turbulent flame speeds of all the shale gas combustions. The dilution of CO<sub>2</sub> between 0 and 30% lowers the flame speeds by 5.3, 5.13, and 4.5% for Haynesville, New Albany, and Barnette respectively.



**Fig. 4. The flame speeds and mass fractions of NO and CO at different CO<sub>2</sub> addition rates.**

The rising H<sub>2</sub>O dilution diminish NO and CO mass fractions as depicted in Fig 5a and 5b. It relieves NO by 26.8, 26.2, and 25.2% for Barnette, New Albany, and Haynesville at ER=1 from 0 to 30%. H<sub>2</sub>O causes a higher NO drop according to CO<sub>2</sub> by decreasing the reaction temperature because of its high heat hold capacity.



Meanwhile, H<sub>2</sub>O addition has a minor reducing effect on CO mass fractions by 1% roundly. On the contrary, the addition of H<sub>2</sub>O into the additional air slightly uplifts the turbulent flame speeds as presented in Fig. 5c. The increment ratio is averagely 0.9% for all the shale gases. If compared with respect to NO and CO emissions together, CO<sub>2</sub> dilution can be preferred because it displays a better performance than H<sub>2</sub>O to reduce CO mass fractions.

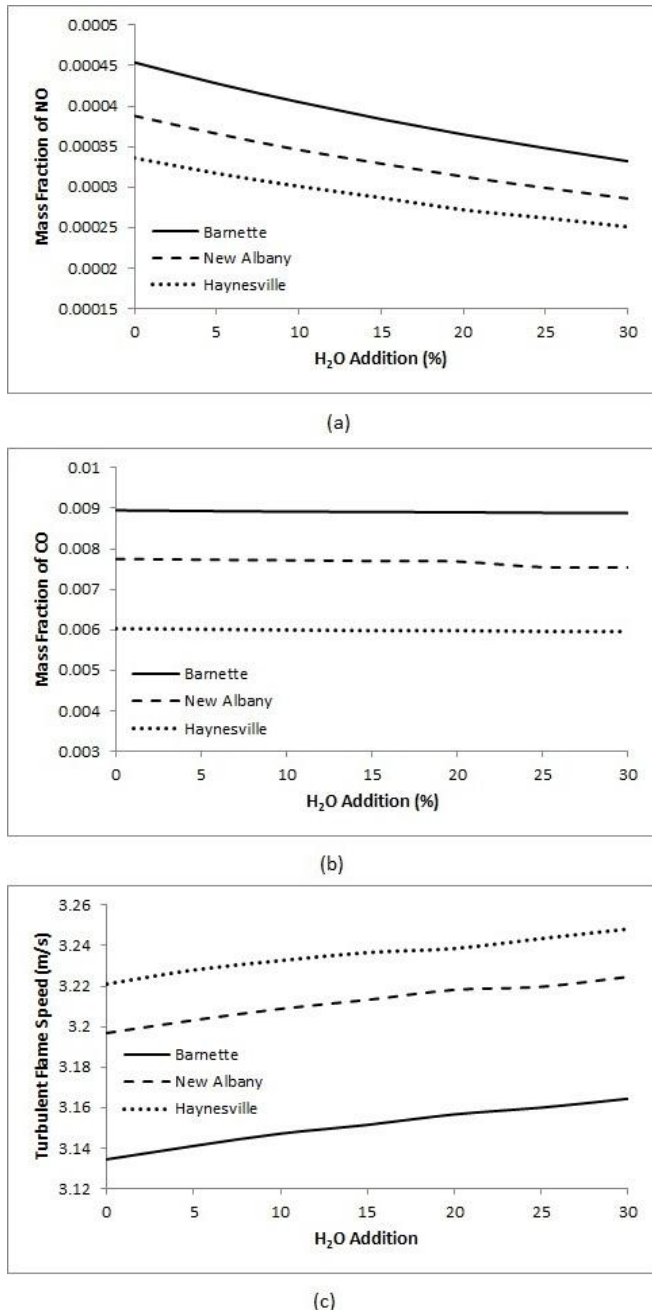


Fig. 5. The flame speeds and mass fractions of NO and CO at different H<sub>2</sub>O addition rates.

Fig 6a indicates the effects of the dilution of N<sub>2</sub> to the additional air. The increasing N<sub>2</sub> addition decreases NO mass fractions for all the shale gas. The degradation ratios from 0 to 30% of N<sub>2</sub> dilution are 7, 6.7, and 5.6% for Barnette, New Albany, and Haynesville. It can be expressed that N<sub>2</sub> induces NO drop because it reduces the adiabatic flame temperature by changing the kinetic pathways encouraged by the temperature [1]. The mass fractions of CO shows 0.5%

increment by the ascending N<sub>2</sub> addition for all as illustrated in Fig 6b. Moreover, it is seen in Fig 6c that N<sub>2</sub> dilution has almost no effect on the turbulent flame speeds.

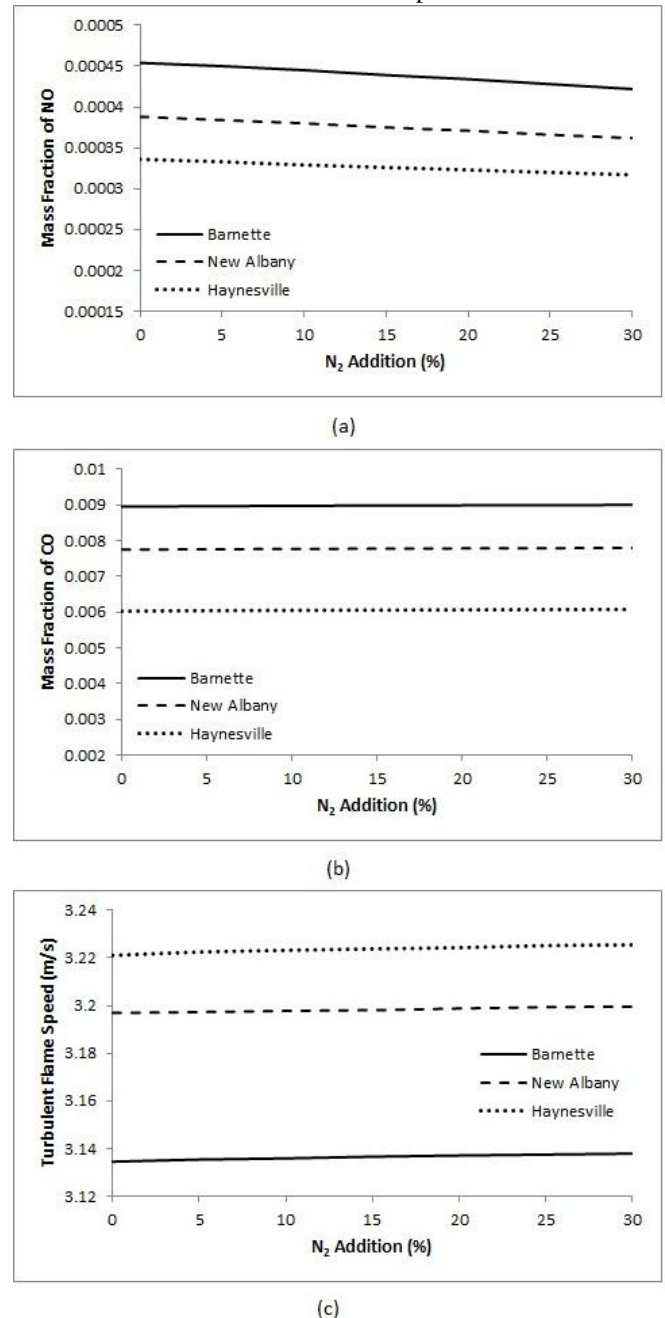
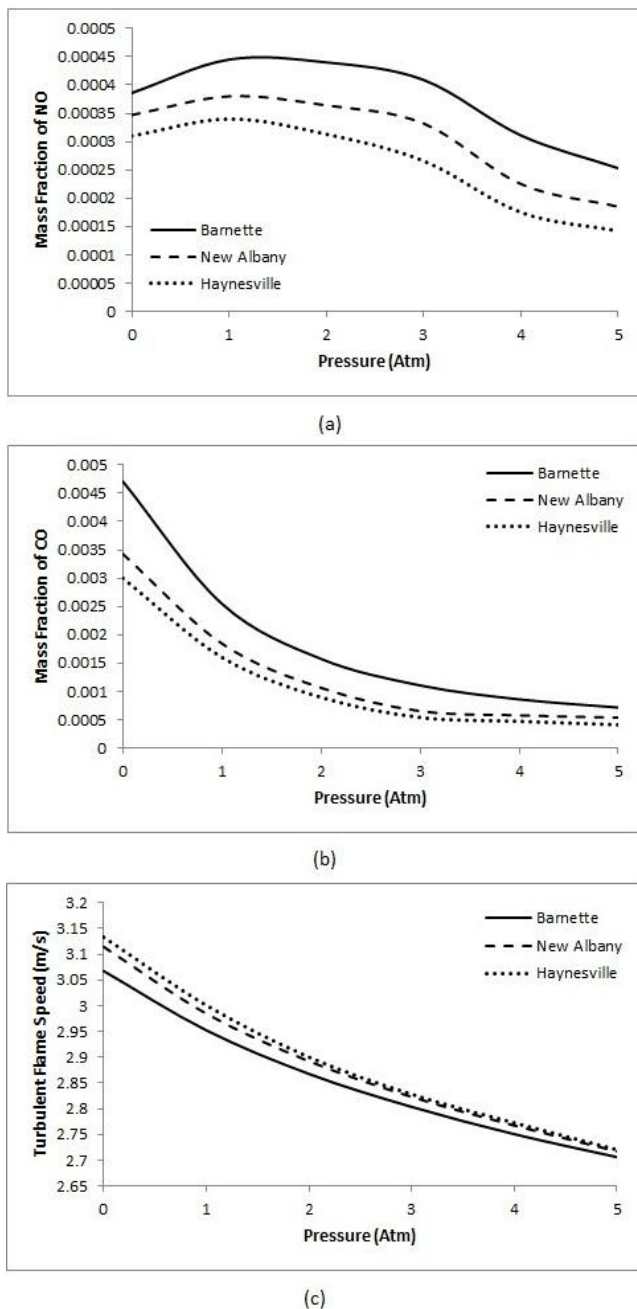


Fig. 6. The flame speeds and mass fractions of NO and CO at different N<sub>2</sub> addition rates.

Fig 7a represents the mass fractions of NO under the effect of 15% CO<sub>2</sub> dilution at the rising pressure. The pressure values used in Figures refer to the absolute pressure. The ascending pressure up to 1 Atm raises NO mass fractions. However, NO production begins to reduce after 1 Atm for all the shale gas combustions. The total reduction in the mass fractions of NO from 0 to 5 Atm is 34.4, 46.6, and 54.1% for Barnette, New Albany, and Haynesville. The mass fractions of CO diminish by 84.8, 84.2, and 64.7% under the growing pressure as presented in Fig 7b.

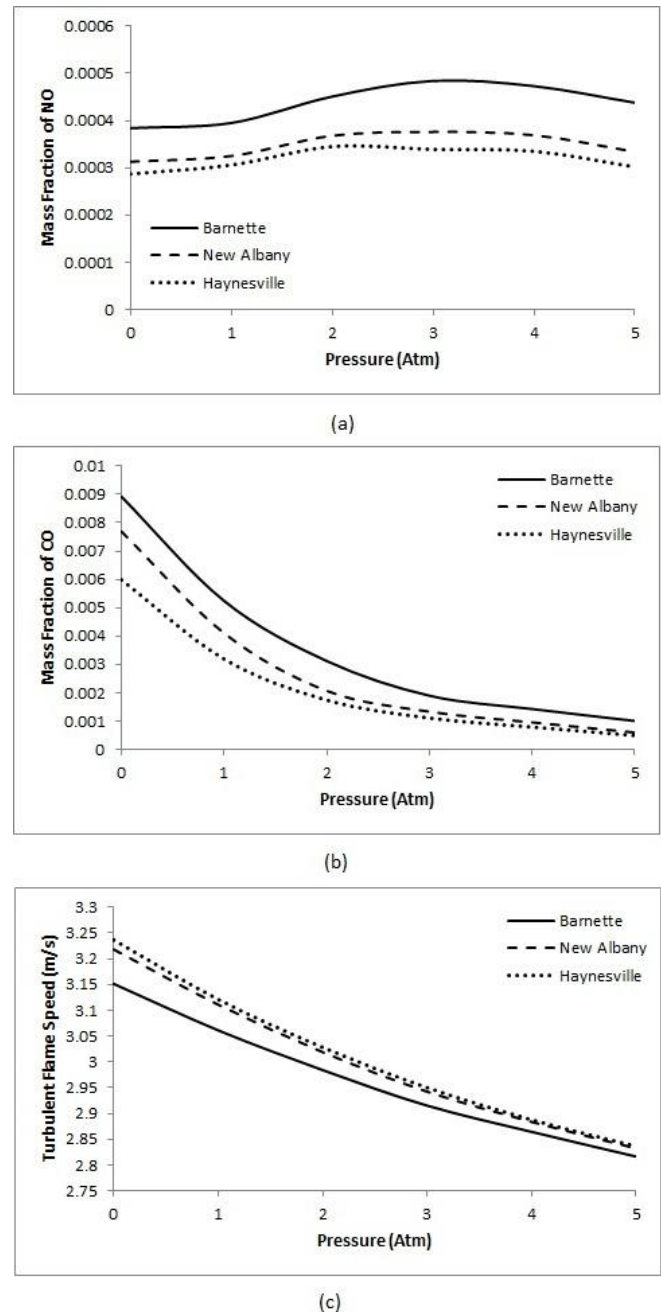


The reducing effect of the increasing pressure with 15% CO<sub>2</sub> dilution on the turbulent flame speeds is given in Fig 7c. The shortening rate is roughly 13% on the average for all.



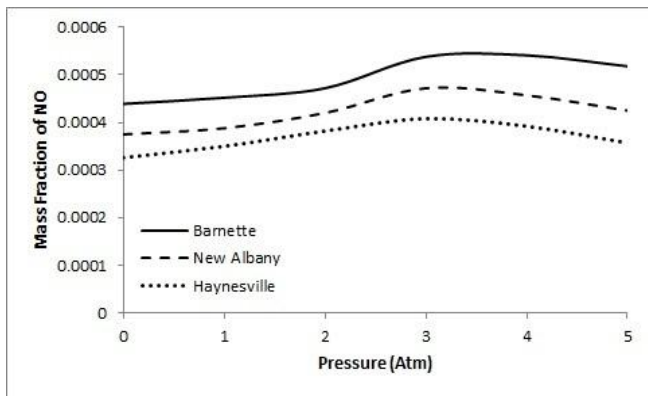
**Fig. 7. The flame speeds and mass fractions of NO and CO at different pressures with 15% CO<sub>2</sub> addition.**

The effect of pressure with 15% H<sub>2</sub>O addition on NO mass fractions is depicted in Fig 8a. There is no change for NO until 1 Atm. It is seen a minor lift between 1 and 3 Atm. After 3 Atm, it begins to fall lightly. The mass fractions of CO decreases by 88.7, 92.2, and 91.7% rates for Barnette, New Albany, and Haynesville under the rising pressure as illustrated in Fig 8b. The higher pressure causes CO to get lowered because there is no enough time for CO to react with oxygen [18]. Fig 8c demonstrates that the turbulent flame speed is also lessened by the enhancing pressure. The degradation ratio is averagely 12% for all the shale gas. It is seen in literature that the pressure increment reduces the flame speed [19].

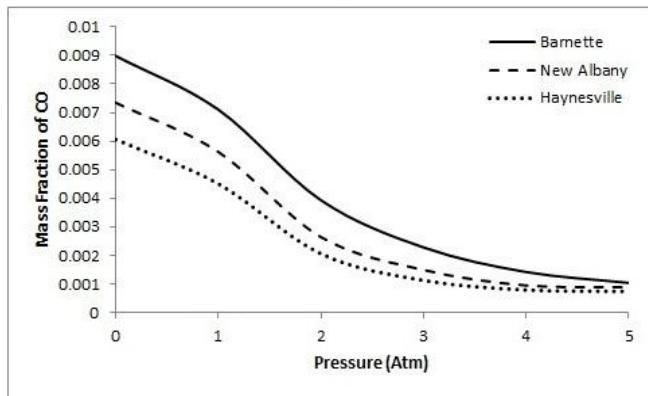


**Fig. 8. The flame speeds and mass fractions of NO and CO at different pressures with 15% H<sub>2</sub>O addition.**

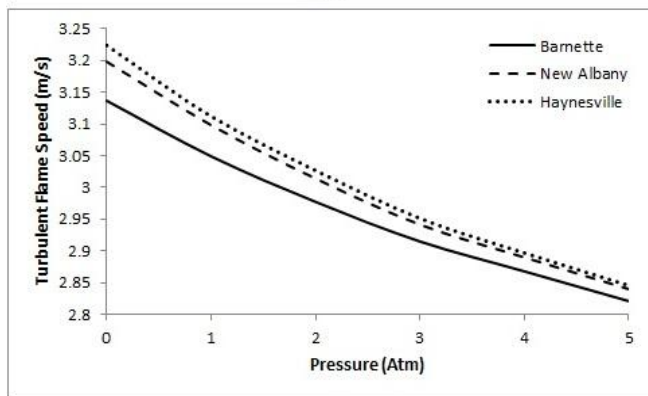
Fig 9a displays the effect of the rising pressure on NO with 15% N<sub>2</sub> dilution. It is seen an increment up to 3 Atm and a degradation of NO after that. CO mass fractions fall away at the ratio of 88% on average as revealed in Fig 9b. Fig 9c screens that the turbulent flame speeds for all get lowered by the increasing pressure. The degradation ratios are 11.6, 11.2, and 10% for the combustions of Haynesville, New Albany, and Barnette shale gases in turn.



(a)



(b)



(c)

Fig. 9. The flame speeds and mass fractions of NO and CO at different pressures with 15% N<sub>2</sub> addition.

#### IV. CONCLUSION

The combustion characteristics and undesirable emissions of turbulent and adiabatic partially premixed combustions of humid air and shale gases extracted from Barnette, New Albany, and Haynesville fields of US are computationally examined. Moreover, the turbulent flame speeds and mass fractions of NO and CO are determined for different equivalence ratios and pressures under the effects of various diluents. The following results are obtained:

- The mass fractions of NO for the combustions of Barnette, New Albany, and Haynesville shale gases reach to the maximum value at 1.42, 1.44, and 1.4 of equivalence ratio respectively. The highest NO belongs to the combustion of Barnette followed by New Albany and Haynesville. CO and the turbulent flame speeds increase with the rising equivalence ratios.

- The enhancing CO<sub>2</sub> dilution into the additional air decreases the turbulent flame speeds and mass fractions of NO and CO for all. The rising H<sub>2</sub>O dose fades NO and CO mass fractions. But, it raises the turbulent flame speeds. The growing N<sub>2</sub> addition abates NO mass fractions for all the shale gas. It slightly increases CO and doesn't affect the turbulent flame speeds.

- The increasing pressure with 15% CO<sub>2</sub> dilution decreases the turbulent flame speeds, NO and CO mass fractions. The increment in pressure with 15% H<sub>2</sub>O addition has a slight detractive effect on NO mass fractions. It decreases CO fractions and reduces the flame speed by 12% averagely. The raising pressure with 15% N<sub>2</sub> dope uplifts NO mass fractions up to 3 Atm and reduces it after that value. The increasing pressure lowers both CO mass fractions and the turbulent flame speeds.

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