



Combustion characteristics of several typical shale gas mixtures



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ABSTRACT

In this study, we numerically and experimentally determined several combustion properties of three different shale gas mixtures. The gas compositions that were studied include 86% CH₄ – 14% C₂H₆ (shale gas 1), 81% CH₄ – 10% C₂H₆ – 9% N₂ (shale gas 2) and 58% CH₄ – 20% C₂H₆ – 12% C₃H₈ – 10% CO₂ (shale gas 3). Laminar burning velocities were determined numerically and experimentally, while the other properties, such as the thickness of flame fronts, lower and higher heat values, Wobbe indices, flammability limits, dew points, and adiabatic flame temperatures, were determined analytically and numerically. The environmental conditions were a temperature of 295 ± 1 K and atmospheric pressure of 849 mbar, which correspond to the local environmental conditions of the city of Medellín, Colombia. We used several mechanisms for the numerical simulations, including GRI-Mech 3.0, C1–C3, and USC-Mech II. Experimental laminar burning velocities were determined using the burner method and the spontaneous chemiluminescence technique. Numerical calculations were also conducted using 3 detailed reaction mechanisms, which reproduced the experimentally obtained behavior under the same conditions and demonstrated that the results of the laminar burning velocity for shale gas 3 was higher than that of shale gas 1 and 2. Finally, sensitivity analyses of the laminar burning velocities of the shale gases were performed using the GRI-Mech 3.0 mechanism, which showed that the reaction H + O₂ = O + OH (R38) was the most sensible reaction.

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1. Introduction

Advances in drilling technologies and shale gas production strategies such as hydraulic fracturing and horizontal drilling have led to a growth in shale gas production (Cao et al., 2010; Lyu et al., 2015; Speight, 2013a; Tan et al., 2014; Vengosh et al., 2013; Wang et al., 2014; Zeng et al., 2016). In the United States, shale gas production has grown to account for nearly 25% of the country's gas production and is expected to keep rising (George and Bowles, 2011; Guarnone et al., 2012). The United States Energy Information Administration (EIA) projects an increase in shale gas production of 340 billion cubic meters per year by 2035, which will account for approximately 50% of the total gas production projected in the United States (Vengosh et al., 2013). Furthermore, this topic is of special interest for developing regions where there are significant shale gas reserves (Nexen Inc, 2012).

Generally, shale gas has a high methane content, similar to

conventional natural gas, but it also includes heavy hydrocarbons, especially ethane (Etiopie et al., 2013; Speight, 2013b). For adequate fuel handling and high efficiency combustion processes, it is necessary to know the fuel properties, flue gas composition, and flame stability properties. The most commonly used properties in the literature are the lower heating value (LHV), higher heating value (HHV), Wobbe index (Wo), adiabatic flame temperatures (Law, 2006), flammability limits, ignition delay times (Hernandez et al., 2005; Huang and Bushe, 2006), stoichiometric air quantity, maximum percentage of carbon dioxide, amounts of wet and dry exhaust gas and laminar burning velocities (Burbano et al., 2011a, 2011b; Serrano et al., 2008).

The laminar burning velocity, S_L is one of the most important parameters of a fuel or fuel mixture. Information about S_L is fundamental for the analysis of combustion phenomena, such as the structure and stability of premixed flames, flashback, blowoff and extinction, turbulent premixed combustion, and validation of reaction mechanisms in the presence of diffusive transport at high temperatures. Additionally, it provides information on the diffusional and chemical coupling effects (Bourque et al., 2009; Burbano et al., 2011b; Hernandez et al., 2005; Serrano et al., 2008).

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There are few references and studies on the laminar burning velocity of shale gas. Most of the work found in the literature refers to gaseous mixtures of hydrocarbons, especially methane (CH₄), ethane (C₂H₆) and propane (C₃H₈). Lowry et al. (Lowry et al., 2011) conducted measurements and numerical predictions of laminar burning velocities on blends containing 60% CH₄ – 40% C₂H₆ and 80% CH₄ – 20% C₂H₆ (by volume). They found that an increase in ethane concentration raised the fuel's laminar burning velocity. For example, the laminar burning velocity of methane is 33.83 cm/s at an equivalence ratio of 1 and 1 atm of pressure. While the laminar burning velocity of a 60% CH₄ – 40% C₂H₆ mixture was 36.2 cm/s and corresponded to a 7% increase with respect to methane, an 80% CH₄ – 20% C₂H₆ mixture had only a 2% increase in the laminar burning velocity.

Bourque et al. (Bourque et al., 2009) performed experiments to determine the laminar burning velocities of a typical natural gas (98.125% CH₄ – 1% C₂H₆ – 0.5% C₃H₈ – 0.25% nC₄H₁₀ – 0.125% nC₅H₁₂) and two gaseous blends containing relatively large levels of heavy hydrocarbons (62.5% CH₄ – 20% C₂H₆ – 10% C₃H₈ – 5% nC₄H₁₀ – 2.5% nC₅H₁₂ and 81.25% CH₄ – 10% C₂H₆ – 5% C₃H₈ – 2.5% nC₄H₁₀ – 1.25% nC₅H₁₂). The experiments were carried out at different equivalence ratios ranging from 0.7 to 1.3. In general, the laminar burning velocities for mixtures with heavy hydrocarbons were higher than for the natural gas results, ranging from approximately 10% at lean conditions to as much as 40–50% for rich mixtures.

Vagelopoulos and Egolfopoulos (Vagelopoulos and Egolfopoulos, 1998) and Davis and Law (Davis and Law, 1998) performed laminar burning velocity calculations under atmospheric conditions for CH₄, C₂H₆ and C₃H₈ with different equivalence ratios. The authors found that adding ethane and/or propane to methane increased the laminar burning velocities.

As described above, most of the work found in the literature refers to gaseous mixtures of hydrocarbons. However, in practice, shale gas compositions can contain inert gases such as CO₂ and N₂. For this reason, the present work is intended to analyze more realistic shale gas compositions following data previously reported in the literature, as shown in Table 1. The purpose of this study is to provide theoretical, experimental and numerical data for these shale gases and compare their properties with high-demand fuels such as methane. The analysis includes laminar burning velocities (both numerically and experimentally) and other combustion properties including lower and upper flammability limits, lower and higher heating values, Wobbe indices, adiabatic flame temperatures, and the thicknesses of the flame fronts.

2. Methodology

2.1. Chemical compositions of the studied shale gases

Three shale gas compositions were selected following those previously reported in the literature. Table 1 shows the mixtures used to emulate the shale gas compositions reported by Speight (Speight, 2013b) and Etiope et al. (Etiope et al., 2013). High purity certified gases and rotameters specifically calibrated for each

component gas were used to generate the required mixtures. Pure methane, ethane, propane, carbon dioxide and nitrogen gases delivered by the supplier were used to emulate the shale gas compositions, and their purities are shown in Table 2.

2.2. Experimental methodology

The burner method was implemented to determine the laminar burning velocities of the shale gases listed in Table 1. Flames were generated using burners with contoured rectangular ports to maintain laminar Reynolds numbers for the equivalence ratios under study and to reduce the effects of stretch and curvature in the direction of the burner's axis (Burbano et al., 2011b). This burner design allowed for a uniform velocity profile output, which generated a triangular flame with acceptably defined straight edges as shown in Fig. 1.

Only average values of S_L could be obtained using this technique because local burning velocities vary along the flame front due to effects of stretch, curvature at the flame tip, and heat loss near the burner walls. The experimental methodology described by Pareja et al. (Pareja et al., 2010) was implemented to reduce these effects.

An ICCD camera (PI-MAX; Princeton Instrument) was used to measure chemiluminescence. To capture the light emission of CH radicals (CH*), the lens was equipped with an interference filter with a center wavelength of 430 nm. The full-width-half-maximum (FWHM) was 11.02 nm, and the minimum transmissivity was 45%. In chemiluminescence measurements, the CH* images were taken 25 times under each condition, and the signal-to-noise ratios were less than 10% of the maximum intensity. The full assembly used to obtain the images is shown in Fig. 2. More details on the experimental setup can be found in previous studies (Amell et al., 2014; Burbano et al., 2011a; Londoño et al., 2011; Oh and Noh, 2012).

The experiments were carried out at an environmental temperature of 295 ± 1 K, average relative humidity of 68 ± 3% and atmospheric pressure of 849 mbar, which corresponds to the environmental conditions of the city of Medellin, Colombia. The equivalence ratios varied from lean conditions $\phi = 0.7$ to rich conditions $\phi = 1.3$. The air was supplied by an air compressor and dried using two inline water traps. The equivalence ratios were fixed using rotameters that were specifically calibrated for each component gas. The errors in the final composition were estimated to be lower than 2%.

The mean velocity at the exit of the burner nozzle was calculated from the nozzle area and the flow of the fuel-air mixtures, while the flame angle was measured using chemiluminescence (CH*) photographs. First, the digital photographs obtained by the ICCD camera were stored as a pixel array of 1024 × 1024. Then, a background image previously taken before the experiments was subtracted using Matlab code, and the flame was located where the maximum intensity was registered. The code detected the edges of the flame fronts; thus, the corresponding flame angles were calculated.

Error analysis was used to determine the errors in the laminar burning velocity measurements and was based on the measurement errors of the average velocity of the unburned gases to the

Table 1
Shale gas composition in percent volume (Etiope et al., 2013; Speight, 2013b).

Component (% by volume)		Methane	Shale gas 1	Shale gas 2	Shale gas 3
Methane	CH ₄	100	86	81	58
Ethane	C ₂ H ₆	0	14	10	20
Propane	C ₃ H ₈	0	0	0	12
Carbon Dioxide	CO ₂	0	0	0	10
Nitrogen	N ₂	0	0	9	0

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