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## Effect of jet composition in hot jet ignition of premixed mixture in a constant volume combustor

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A jet of hot gas can serve as an ignition source in combustion devices, such as automotive engines, pulsed detonation engines and wave rotor combustors. Hot-jet ignition involves complex flow phenomena such as vortex evolution, fluid mixing, and turbulence generation. Further, the penetrating and distributed nature of ignition can be affected by mixture non-uniformity and can be advantageous for ignition success, thermal management, and emissions control. The jet itself may be inert or chemically reactive. In a hot jet produced by partial or recent combustion of an adjacent mixture, active radicals present may significantly affect the ignition process of the premixed mixture to be ignited, usually in a constant volume combustor (CVC). In a wave rotor constant volume combustor, rapid ignition and combustion also involves complex interactions of pressure waves with flames in the transient jet. In the present work, detailed numerical simulations are carried out to understand the effect of jet composition present in a turbulent hot jet on the ignition in an experimental constant-volume combustor. A transient but physically immobile hot jet is modeled in two ways: as an inert jet (nitrogen and argon) and as a chemically active hot jet. The composition of the chemically active jet is determined from chemical equilibrium for rich ethylene mixture in a pre-chamber supplying the jet. Combustion is modeled in the main constant-volume chamber for stoichiometric methane mixture. A hybrid eddy-break-up combustion model is applied, including finite-rate chemistry, modeled using detailed reaction mechanisms. Turbulence is modeled using a two-equation  $k-\omega$  model. Chemically active hot jet is seen to ignite the CVC chamber mixtures significantly faster than an inert nitrogen jet. The temperature rise and final products in the CVC chamber are higher in case of the chemically active hot jet indicating more complete combustion.

### 1. Introduction

Intentional hot jet ignition of premixed combustible mixture finds application in internal combustion engines (Toulsan et al. 2010, Attard et al. 2012), pulsed detonation engines (Lieberman et al. 2002) and wave rotor combustors (Matsutomi et al. 2010, Akbari and Nalim, 2009). Such ignition is of particular interest for wave rotor combustors (Zauner et al. 1993, Keller, 1990, Perera et al. 2011, Perera, 2010, Wijeyakulasuriya, 2011). Chemically active radicals and fast turbulent mixing in the jets create an explosion that is more energetic than a spark (Lieberman et al. 2002), allowing rapid ignition of lean mixtures. Further, the penetrating and distributed nature of ignition can overcome mixture non-uniformity. By enabling lean stratified mixtures, heat losses to the walls and pollutant emissions can be mitigated.

Hot jet ignition involves complex flow phenomena such as vortex evolution, fluid mixing, and turbulence generation. The presence of reactive species in the jet complicates the chemical kinetics of fuel combustion. A high-speed compressible transient jet is usually accompanied by shock formation in a confined volume, leading to subsequent deformation of flame fronts due to shock-flame interaction. The ignition delay time for a jet-ignited constant-volume combustor (CVC) may be defined as the time from jet initiation to the occurrence of rapid, visible, and pressure-generating heat release in the CVC chamber (Perera et al. 2011). There are many definitions of ignition delay time used in the literature. Auto-ignition delay in shock-tube and rapid compression experiments reflect purely chemical processes, while jet ignition and spark ignition also include physical processes. Ignition delay in hot jet ignition includes time for transient jet vortex development, jet mixing with the gas in the CVC chamber, and chemical evolution. In addition, in the present study of hot jet ignition, reflecting shock and expansion waves generated due to confined geometry also affect the ignition.

A combustible mixture can be ignited by an inert gas jet or reactive gas from another combustion source. Prior experiments mainly addressed mine safety using a steady non-reactive hot gas jet injecting into unconfined well-mixed stationary or quiescent combustible mixture. Toulson et al. (2010) made a review of turbulent jet ignition systems for

pre-chamber spark ignition engines. The pre-chamber mixture is more controlled and reliably spark-ignited and produces a hot jet that acts as a distributed ignition source, allowing reliable combustion of the main CVC charge over a broader range of air-fuel ratios, shorter flame travel distances, and more rapid combustion in traditionally slow-burning lean mixtures. Chemically reactive radicals (e.g. H and OH) and jet-induced turbulence is reported as providing the equivalent to two orders of magnitude higher energy than spark ignition (Attard et al. 2012). Wolfhard (1958) observed that jets of nitrogen and carbon dioxide achieved ignition with similar jet temperatures, while argon and helium jets needed higher temperatures for incipient ignition. Fink and Vanpée (1975) developed an overall rate expression for ignition of methane and ethane fuel-air mixtures by low-velocity hot inert gas jets. Cato and Kuchta (1966) experimented with laminar hot air jets and concluded that ignition depend on jet base temperature, jet dimensions, composition of the combustible mixture, and jet velocity. In contrast to the hot jet ignition reported here for confined constant-volume combustion, mine-safety experiments were typically without turbulence and at low velocities.

Tarzhanov et al. (2006) experimentally investigated using hot detonation products to detonate stagnant propane-air mixtures and found that detonation initiation depends on the initial volume concentrations of the mixture, mass fraction of hot detonation products, and the energy deposited from the detonation products. Mayinger et al. (1999) derived correlations between the induction time (ignition delay time), the mixing time of the jet, and the adiabatic auto-ignition time for the fuel-air mixtures. The experimental facilities in their work consist of two chambers separated by a partition with a single circular orifice.

Bilgin (1998) developed a constant-volume combustor with long aspect ratio and square cross-section, representing a wave rotor channel (Bilgin et al., 1998). The CVC is ignited by a jet of hot combustion products from a separately fueled pre-chamber that could be spun to cause the jet to traverse one end of the CVC. The relative motion reproduces the action of a wave rotor channel, and pre-chamber may be representative of a previously combusted channel supplying hot gas. Bilgin proposed a correlation between the Damköhler number and ignition of a fuel-air mixture in the CVC. For the geometry of this CVC, Baronia et al. (2007) performed numerical simulations for the stationary (non-traversing) torch jet case using global reaction mechanisms (one-step and four-step) for propane-air mixture. Bilgin's measurements were not well matched by Baronia's simulations, possibly due to lack of detailed chemistry and not accounting for active chemical species in the jet. Perera (2010) carried out experiments on the same CVC test rig for three fuels: methane, ethylene, and propane – under varying equivalence ratios in the pre-chamber and the CVC chamber. The ignition delay time variation for each fuel under constant experimental conditions and the ignitability limits, both lean and rich, for all three fuels in the CVC chamber were investigated. The variation of ignition delay time for fuels with different pre-chamber equivalence ratios and nozzle geometry were also observed.

The ignition of combustible mixture using hot inert jet or combusted products has been rarely studied numerically using global reaction mechanisms and no studies are known that use detailed or skeletal reaction mechanisms. The present work seeks to use detailed numerical simulations to investigate the ignition by a hot jet and ensuing combustion of methane mixture. Chemical kinetics is modeled using the DRM-19 detailed reaction mechanism for methane. The hot jet is modeled as the equilibrium products of rich ethylene combustion in the pre-chamber as well as inert nitrogen and argon jets. The effect of jet composition on the combustion in the main chamber is the focus of this study.

## 2. Problem Description and Methodology

The constant-volume combustor (Fig. 1) designed by Bilgin (1998) was further experimentally investigated for ignition delay by Perera et al. (2011). The main CVC chamber has a square cross-section of side 39.878 mm (1.57 inches) and is 406.4 mm (16.0 inches) long. The pre-chamber internal cavity is of cylindrical design, 165.61 mm (6.52 inches) in diameter and width 39.1 mm (1.54 inches), forming an internal volume of approximately  $8.3574 \times 10^{-4} \text{ m}^3$  (51 cubic inches). The exit diameter of the converging nozzle that connects the pre-chamber with the CVC chamber is 5.99 mm (0.236 inches). The small gap between the pre-chamber and CVC chamber is not modeled, as it is assumed that the gas outflow is negligible at low pressure before ignition occurs in the CVC chamber.

A two-dimensional (2D) model (Fig. 2) of the combustor and jet are used to simulate the transient, turbulent, reacting and compressible flow at reasonable computational cost. For the 2D simulation, the height and length of the channel and nozzle are the same as those in the test rig. The varying vertical width of the nozzle is taken equal to the corresponding diameter. While this does not preserve the area ratio, it does retain the relative height ratio of the confined jet. However, the volume ratio of the pre-chamber to the test channel is preserved, neglecting the small volume of the

nozzle. This allows the same volume flow rate between the experiment and 2D numerical calculations, preserving mass and energy realism and the nominal pressure history. The simulation uses the velocity-pressure coupled, second-order implicit scheme available in the computational code used for this work (User Guide, 2010). The computational domain is discretized using polyhedral meshes with varying mesh density in the pre-chamber, converging nozzle, and CVC chamber (Fig. 2).

Turbulence is modeled using the shear-stress-transport (SST) two-equation  $k-\omega$  model (Menter, 1994). Combustion is modeled using a hybrid eddy-break-up model that considers finite-rate chemistry. The classic eddy-break-up (EBU) turbulent reaction model was presented by Spalding (1971) and later developed by Magnussen and Hjertager (1976). The present work uses a hybrid EBU model, with the reaction rate modeled as the minimum of the EBU rate and the kinetic reaction rate from detailed chemistry reported below. A good review of turbulent combustion models including hybrid EBU models is made by Hilbert et al. (2004). There are several studies that fruitfully employ hybrid EBU models (Hilbert et al. 2004, Magel et al. 1996).

The reaction mechanism used involves 21 species in 84 reversible elementary reactions (Kazakov and Frenklach) and is derived from GRI Mech 1.2 (Smith et al.). The initial pressure in the pre-chamber is specified as the pressure at diaphragm rupture measured from experiments (Perera, 2010). The initial temperature and composition of the pre-chamber is obtained by chemical equilibrium calculation for combustion of ethylene-air with the equivalence ratio of 1.1 using the program developed by Depcik (2000), which correlates well with the NASA equilibrium code (Gordon and McBride, 1996). The initial conditions for the pre-chamber and CVC chamber are listed in Table 1 and are the same for all the simulations in the present work.

A grid-sensitivity study was completed considering methane-air mixture in the CVC chamber and combustion products jet using a detailed reaction mechanism (DRM19). Two different grid sizes were used for the CVC chamber with minimum cell sizes of 1.0 mm (20,834 total cells), and 0.5 mm (63,728 total cells). The solutions for the two finer grids were found to differ very little (Fig. 3), until ignition is well under way with rapid combustion and shock-flame interaction. Therefore, the grid with minimum cell size 1.0 mm in the CVC chamber is used for the detailed simulations. It should be noted that the present study is not intended to resolve the flame thickness after ignition, nor estimating flame speed after ignition. The mesh used here is intended to predict the ignition delay time, but may not be adequate for predicting subsequent flame propagation.

Table 1 Initial conditions considered for the simulations

Thermodynamic Properties and Mass Fractions	Pre-chamber			CVC Chamber
	Argon	Nitrogen	Reactive Species	
Pressure (kPa)	649.0	649.0	649.0	101.325
Temperature (K)	2770	2770	2770	298
O <sub>2</sub>	0	0	0.0069176	0.219231
N <sub>2</sub>	0	0	0.719410	0.725824
CO <sub>2</sub>	0	0	0.142050	0
CO	0	0	0.050400	0
H <sub>2</sub>	0	0	0.000739	0
H <sub>2</sub> O	0	0	0.080490	0
CH <sub>4</sub>	0	0	0	0.054945

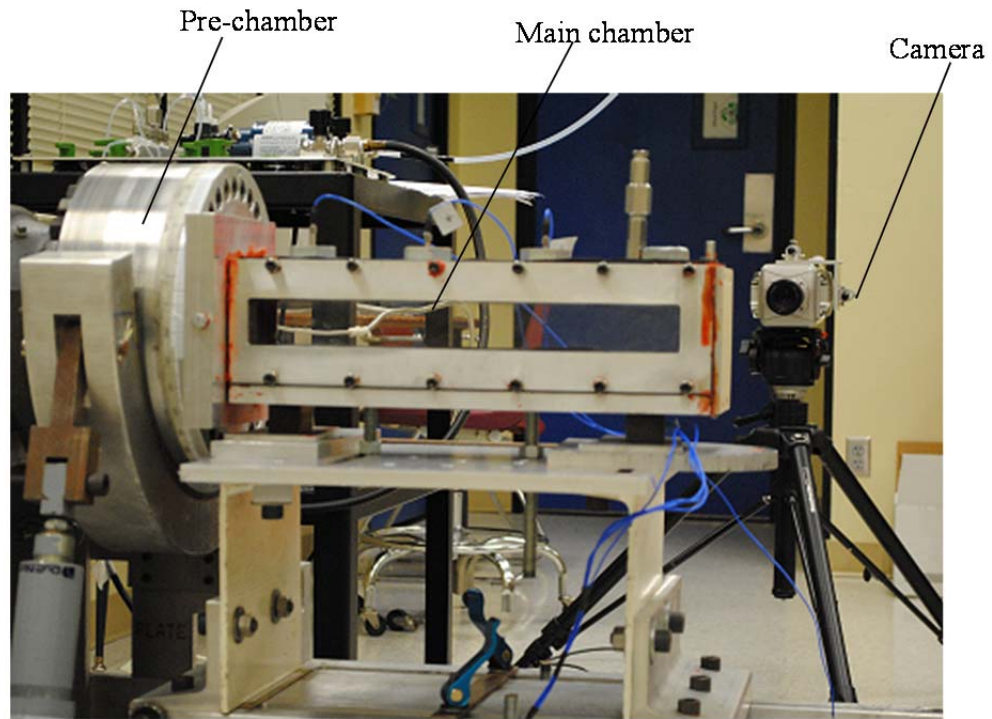
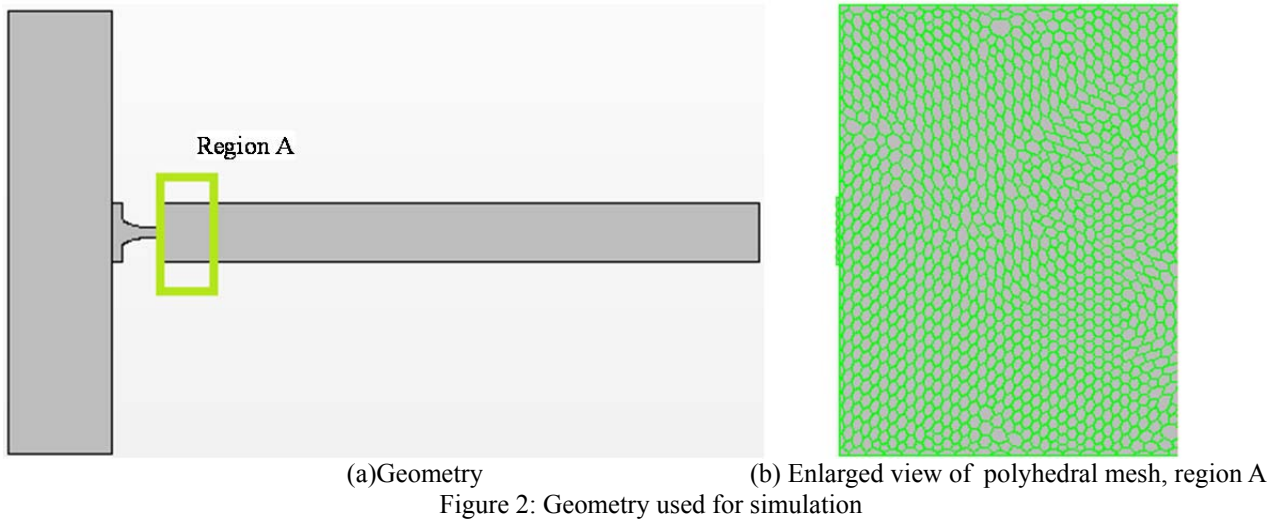


Figure 1: Constant volume combustor rig



(a) Geometry

(b) Enlarged view of polyhedral mesh, region A

Figure 2: Geometry used for simulation

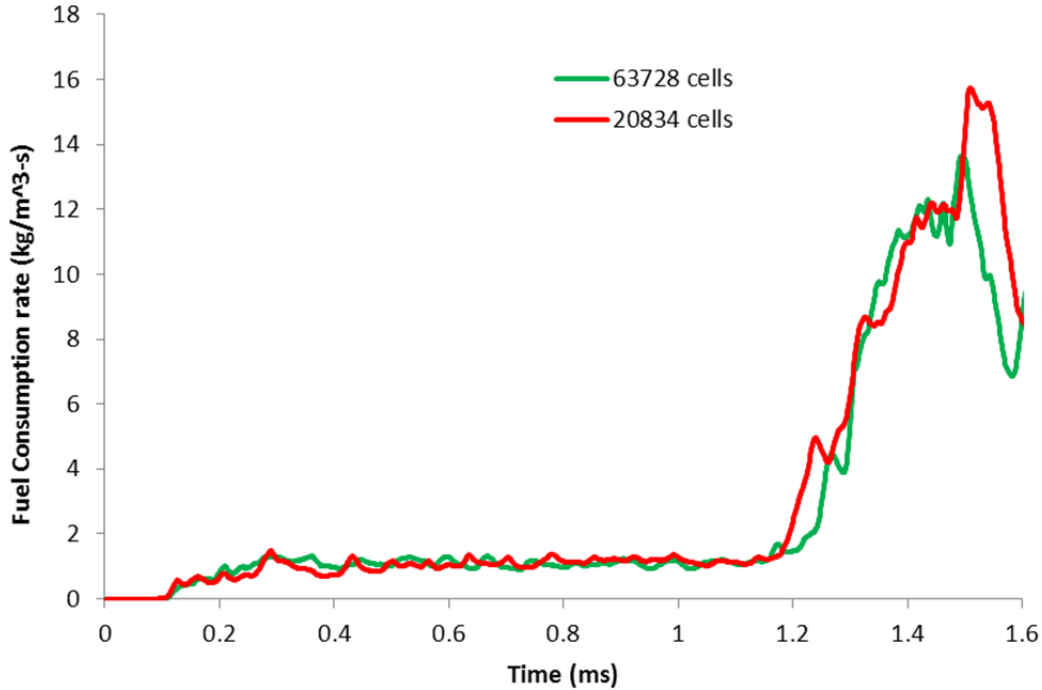


Figure 3: Fuel consumption rate in the CVC chamber for two grid sizes for methane mixture using the DRM19 reaction mechanism

### 3. Results and Discussion

#### *Ignition and Combustion Characteristics*

There are several definitions of ignition delay time used in the literature, most of which refer to auto-ignition by rapid or shock compression of a fuel-oxidant mixture with no trace of other highly reactive species initially present. Hot jet ignition and auto-ignition have both common and different challenges in defining the ignition delay time. Ignition could reasonably be defined as occurring either at the time of maximum rate of change or at the time when the peak value of some species or variable such as [OH], [CH], or peak pressure is reached, or could be based on an extrapolation of the maximum slope to the zero signal level. Davidson and Hanson (2004) reported that, in general, pressure rise is a good indicator of ignition at high fuel concentrations. They also found that the  $\text{CH}^*$  (formed by the reaction,  $\text{C}_2\text{H} + \text{O} \rightarrow \text{CH}^* + \text{CO}$ ) and OH (and intermediate species  $\text{C}_3\text{H}_6$ ) mole fraction histories show clear evidence of a change owing to ignition for the cases investigated. The complexity of defining ignition delay time is further increased in hot jet ignition case, where the chemically active hot jet mixes with the cold combustible mixture. The active radical species introduced will likely influence reaction initiation of the fresh fuel. The rate of quenching by rapid entrainment of cold mixture will depend on the entrainment ratio and mixing rate. Examination of fuel consumption rate or production rates of some of the intermediate species may not adequately define ignition delay. The ignition in the present work is determined based on several parameters, including maximum fuel consumption rate and different intermediate species concentrations.

#### *Effect of Hot Jet Composition*

The objective of this work is to investigate the effect of the hot jet composition on the ignition in the CVC chamber. The hot jet chemical composition would significantly vary with the fuel mixture and the equivalence ratio used in the pre-chamber. The present work is primary attempt at gaining insight on the effect of jet composition on the CVC chamber ignition, and to understand the role of some of the species present in the jet. Three different compositions are considered: a) products of combustion of rich combustion of ethylene and air, at equivalence ratio of 1.1, considering the major stable species as listed in Table 1; b) pure nitrogen, which is the major component of a typical jet, but is inert with respect to the major species considered; and c) pure argon.

The simulations with argon are intended to provide a sense of the variability of ignition processes when no active radicals are present in the jet. The argon and nitrogen jets differ due to thermal rather than chemical properties of the jet, and the jet behavior is affected by different gas density and different energy content due to variation in specific heats. The difference between argon and nitrogen jets at the same temperature then provides a point of reference to compare the difference between inert nitrogen and combustion-product jet composition due to chemical rather than thermal differences. The combustion products jet contains  $H_2$  and  $O_2$  which react to form small amounts of intermediate species H and OH. The presence of OH in the jet can significantly affect the combustion process as many of the reactions are started by OH attack (Turns, 2000). For more detailed investigation of the effect of the small intermediate species present in the hot jet on the CVC chamber ignition, the small intermediate species need to be considered in the future works.

In Fig. 4 the mass fraction levels for different hot jet composition for stoichiometric methane mixture in the CVC is presented for the three different jet compositions. Significant fuel consumption is seen only after 2.8 ms in case of inert argon jet while inert nitrogen jet shows this as early as 1.6 ms. It should also be noted that while shock-flame interaction causing the sudden compression plays decisive role in the ignition of the methane mixture as observed in earlier works (Karimi et al. 2013), this shock compression is not sufficient to cause ignition in the case of argon jet. Careful examination of the frames in Fig. 4 at 1.2 ms and 1.6 ms reveals backward movement and large distortion of the flame front, indicating a shock wave interaction with the flame. More detailed insight is possible from the fuel consumption rate averaged in the CVC chamber as presented in Fig. 5 for three different jets. For the sake of standardized presentation, the fuel consumption rate is averaged over the entire CVC chamber, although it is recognized that the fuel consumption activity is spatially localized. The fuel consumption trends for nitrogen jet and combustion products jet are similar with a relative delay of about 0.2 ms for the nitrogen jet. The low heat capacity of argon compared to nitrogen is attributed to lower ignition delay time in shock tube studies with argon as diluent (Shen, 2008). The chemistry heat release rate averaged in the main chamber presented in Fig. 6 indicates that the combustion is much faster in case of nitrogen inert jet.

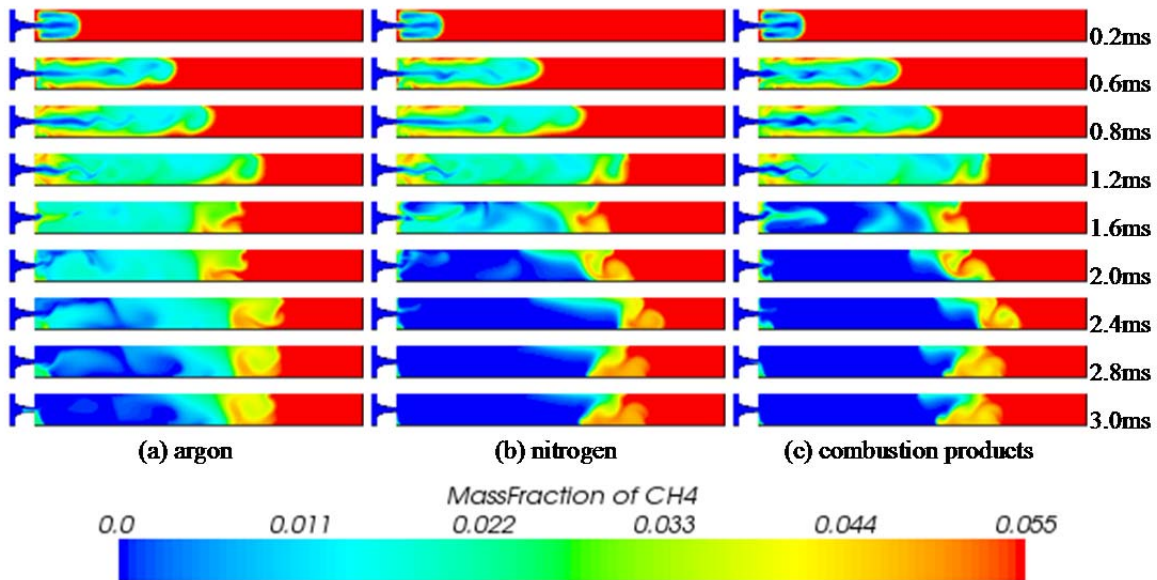


Figure 4: Fuel mass fraction levels for stoichiometric mixture of methane for different hot jet composition

#### Combustion Progress and Pathways

For the analysis of combustion characteristics after ignition, the temperature levels for three different jet composition cases are presented in Fig. 7. There appear to be large differences in the flame temperatures of combusting gases, between the case of the nitrogen jet and combusted gas jet, even though the ignition-delay difference (defined by rapid increase in fuel consumption) was relatively small. At some locations the difference between the two cases is as much as 700 K. The intermediate species production/consumption as well as reaction pathways for the combustion are thus important to analyze for this understanding this difference. As expected for the lower energy content of the argon jet, the temperatures are relatively lower.

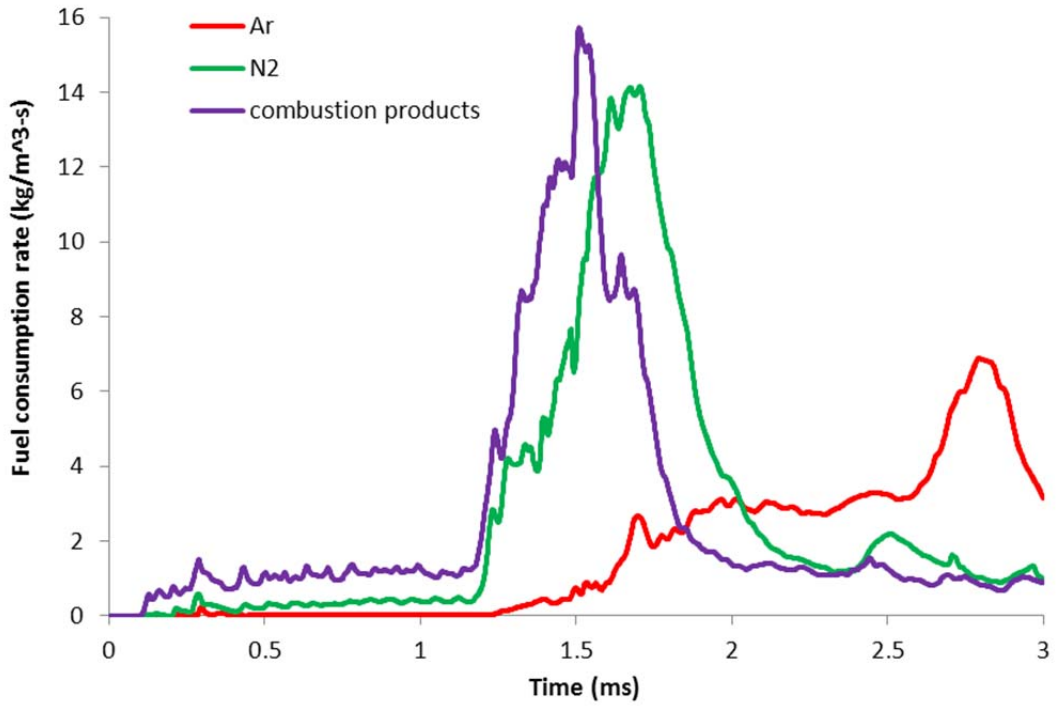


Figure 5: Fuel consumption rate averaged in CVC chamber for hot jets of different composition

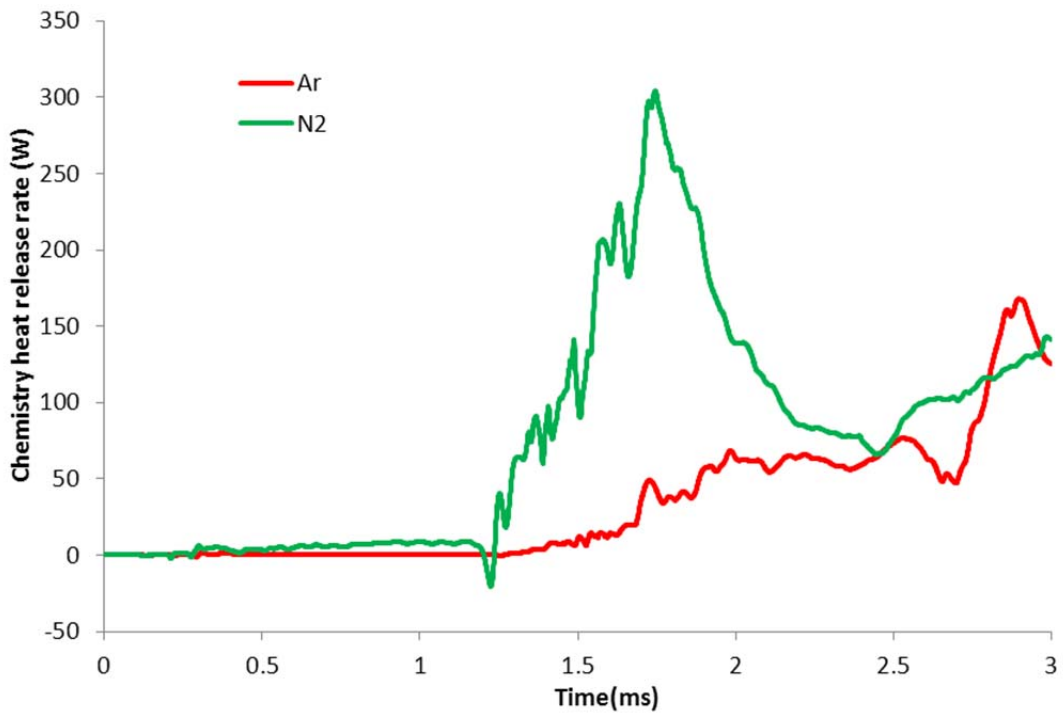


Figure 6: Chemistry heat release rate averaged in CVC chamber for argon and nitrogen jets

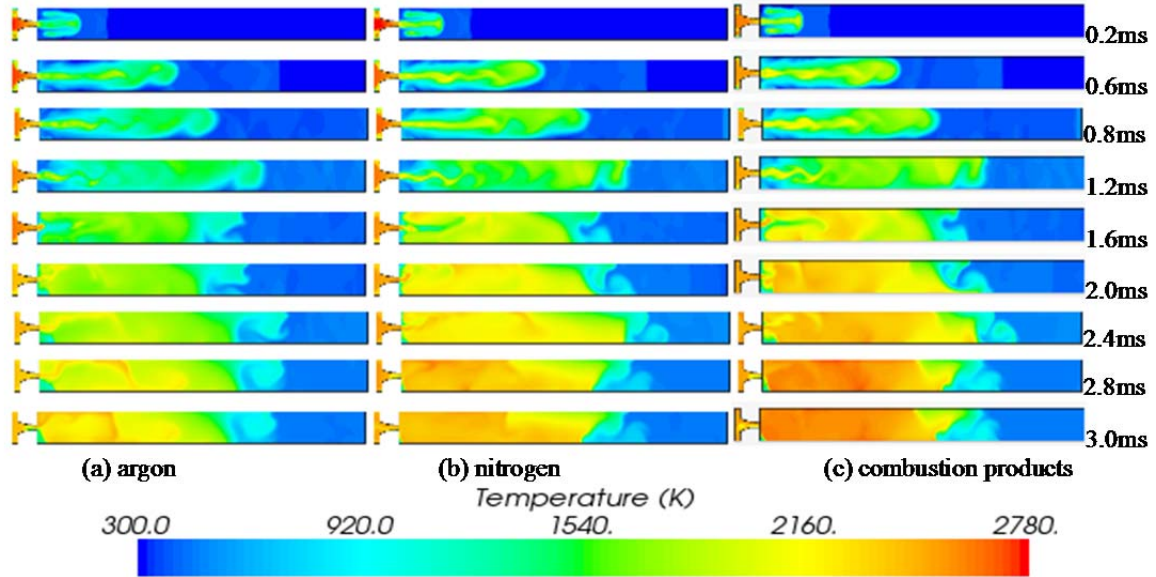


Figure 7: Temperature levels for stoichiometric mixture of methane for different hot jet composition

The molar concentration histories in the CVC chamber are presented for important single-carbon ( $C_1$ ) and two-carbon ( $C_2$ ) species (respectively,  $CH_3$  and  $C_2H_4$ ), in Figs. 8 and 9 respectively for different hot jets considered. Similar to previous line plots, the concentrations are averaged over the entire CVC chamber for standardization, but should be interpreted carefully, considering spatial localization. It is observed that there is higher but relatively slower production of  $C_1$  and  $C_2$  species after ignition in case of nitrogen jet compared to combustion products jet. The molar concentration histories for the more stable species like OH, CO and H are also analyzed in order to understand the combustion completion leading to final products. The molar concentration history of CO averaged in the CVC chamber is presented in Fig. 10. It is observed from the figure that a large amount of CO is supplied from the pre-chamber in case of the combustion products jet and therefore the total amount of CO in the CVC chamber is significantly higher for this case. However, the production trend of CO in the CVC chamber for nitrogen hot jet and combustion products hot jet is similar. The molar concentration histories of H and OH in the CVC chamber are presented in Figs. 11 and 12 respectively. Significantly larger amount of these two species are seen to be produced in case of combustion products hot jet as compared to the nitrogen inert hot jet case. This implies that while the fuel consumption is not significantly delayed in case of nitrogen hot jet compared to combustion products hot jet, but the combustion progress is still significantly delayed. The faster production of  $C_1$  and  $C_2$  species in when the hot jet contains even stable combustion products is apparently due to the ready disassociation of the jet species compared to the need for hot nitrogen to transfer enough thermal energy to break bonds in fuel and oxidant species before chemical reactions can begin. Thus temperature rise and the higher production of other reactive species, H and OH, are seen with the combustion products jet.

In future work, a more detailed study needs to be carried out using different compositions of the hot jet considering more intermediate species to accurately determine the best hot jet composition. In particular, it is necessary to explain the behavior of jets of combustion products of different temperature and equivalence ratio on the success and ignition delay in the CVC chamber.



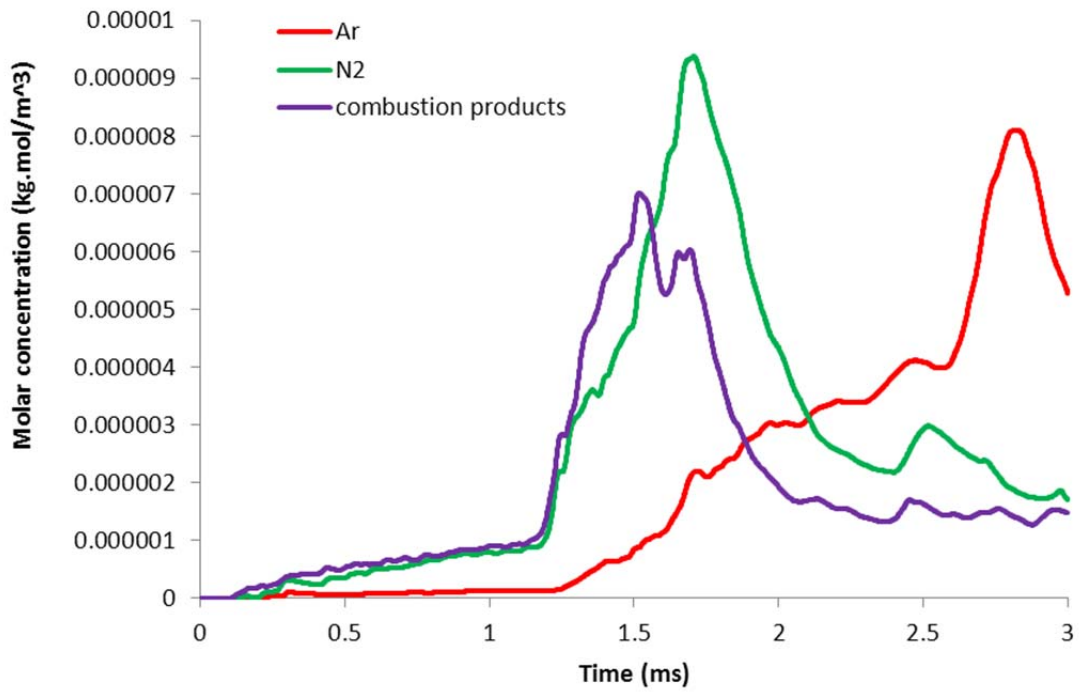


Figure 8: Molar concentration of  $\text{CH}_3$  averaged in CVC chamber for hot jets of different composition

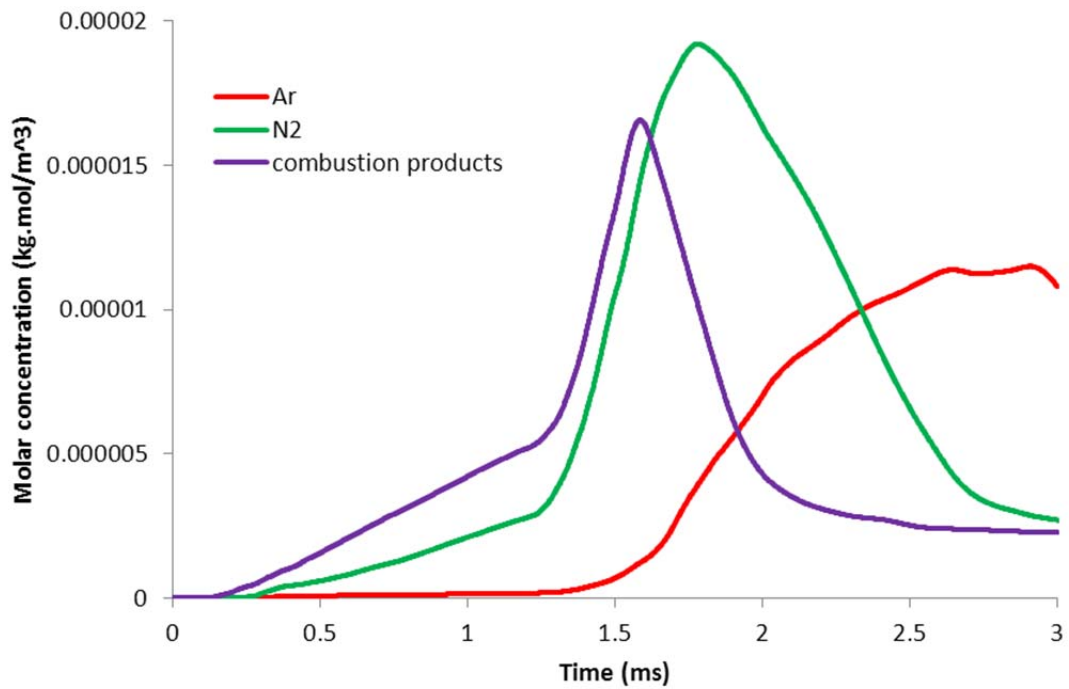


Figure 9: Molar concentration of  $\text{C}_2\text{H}_4$  averaged in CVC chamber for hot jets of different composition

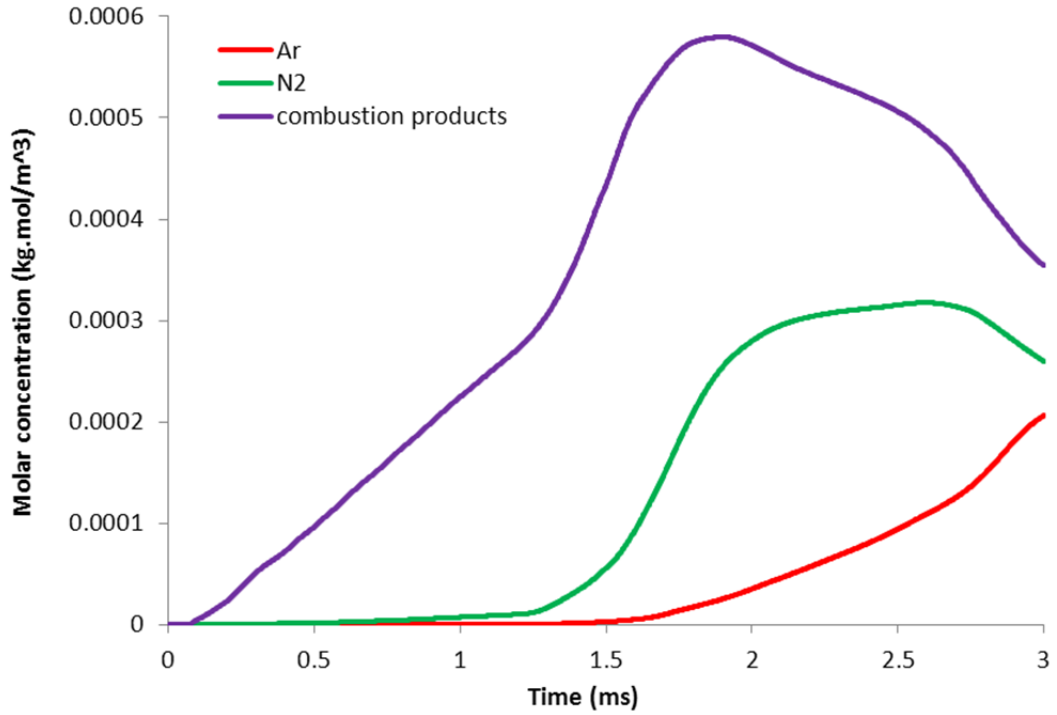


Figure 10: Molar concentration of CO averaged in CVC chamber for hot jets of different composition

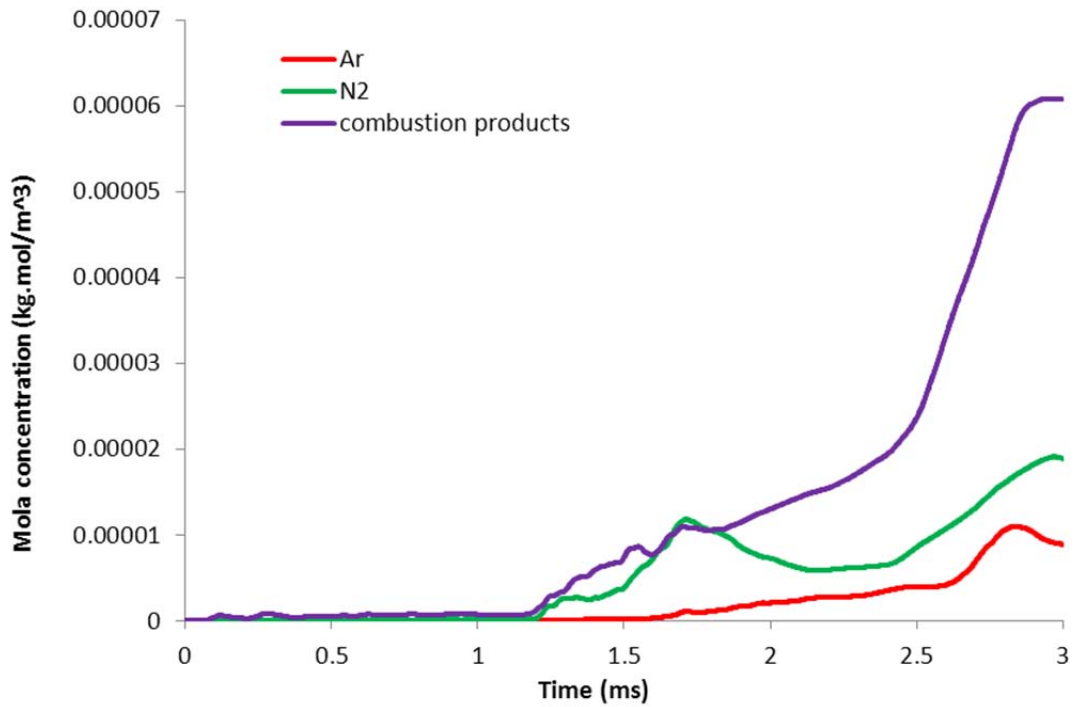


Figure 11: Molar concentration of H averaged in CVC chamber for hot jets of different composition

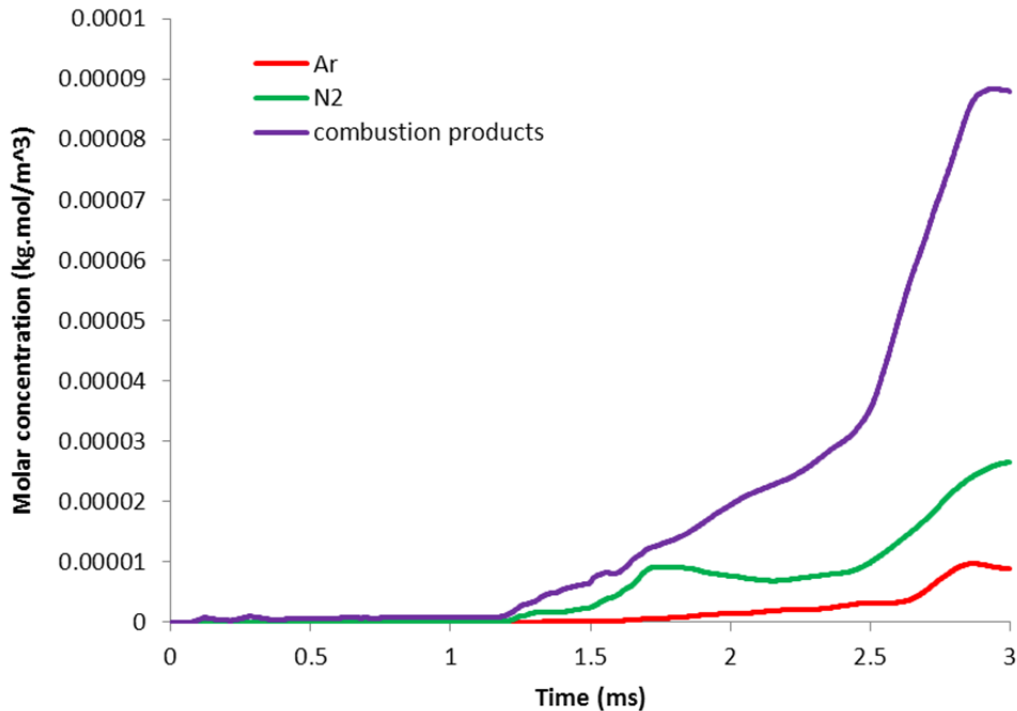


Figure 12: Molar concentration of OH averaged in CVC chamber for hot jets of different composition

#### 4. Conclusions

Hot jet ignition of combustible methane mixture in a constant-volume combustor is investigated numerically. The effect of the hot jet composition on ignition in the CVC chamber is analyzed by comparing an inert nitrogen jet with the chemically more reactive hot jet from the combustion products. The ignition delay time and reaction pathways of the combustion of methane in air are studied. The ignition delay of the mixture in the CVC chamber is significantly affected by the composition of the hot jet. The chemically reactive hot jet is able to ignite the mixture much faster compared to inert hot jets. Expectedly, a nitrogen hot jet causes faster combustion than an argon hot jet at the same temperature, due to the much smaller specific heat, and therefore heat content of the argon jet, which simply served as an additional reference case to provide a sense of the variability due to thermal rather than chemical properties of the jet. Reaction pathways for the combustion are also affected by the hot jet composition. More  $C_1$  and  $C_2$  species production is seen in case of inert nitrogen jet compared to chemically active jet. The stable species, H and OH, are produced faster in larger amount in case of the chemically active hot jet than the inert nitrogen hot jet. A more detailed study including other intermediate species in the hot jet should be carried out in future to accurately determine the best composition of the hot jet for faster and more efficient combustion in the CVC chamber.

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