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Project Title: **Reduction of Laminar Burning Velocities of Liquefied Petroleum Gas Components by blending with CO_2**

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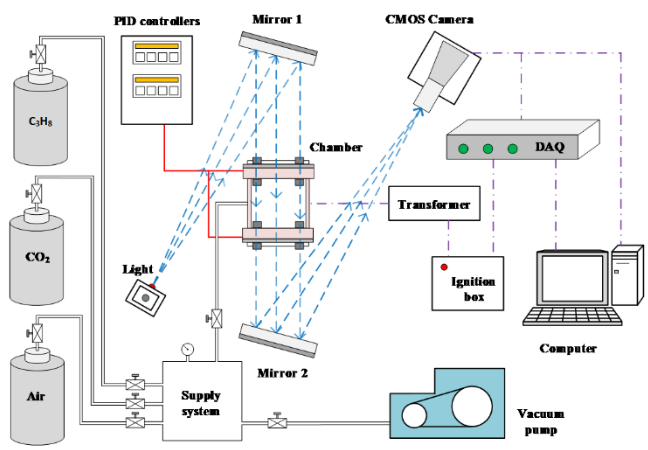
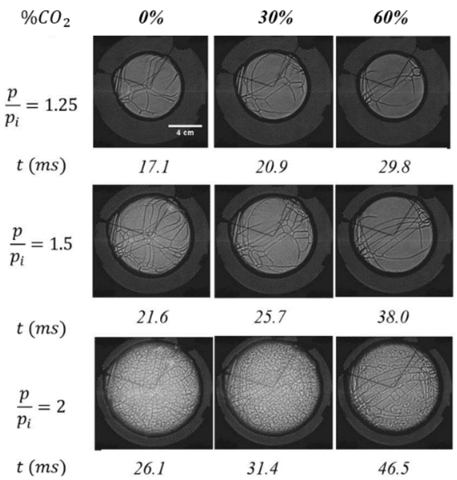
First Year Report (September 1 2018 - August 31 2019)

Liquefied petroleum gas (LPG) components (such as propane and butane) are of technological interest to a variety of applications. For instance, propane is an alternative fuel in spark-ignited engines and dual-fuel compression-ignition engines. In engine applications, propane is a viable alternative fuel as it has a lower carbon content compared to conventional gasoline and diesel fuel, and emits 13% less of the greenhouse carbon dioxide gas. LPG components are also considered as alternative refrigerants in refrigeration and air conditioning (RAC) applications. Manmade refrigerants, currently used as working fluids in RAC, are potent greenhouse gases with high global warming potential (GWP) and often high ozone-layer depletion potential (ODP). Therefore, a global phase-down of these refrigerants has been mandated and replacement fluids with appropriate thermodynamic, chemical, environmental and safety properties are needed. This research examines the combustion behavior of LPG components blended with carbon dioxide (CO_2). In the engine applications, the addition of diluent gases to the fuel, such as carbon dioxide which a component of exhaust gases (EGR) is beneficial because it lowers combustion temperatures and, thus it lowers thermal NOx emissions but increases the CO emissions This work targets blends of natural refrigerants, such as propane and butane with CO_2. These have already been considered as refrigerants and are code-named R-290, R-600 and R744, respectively. However, the former two are highly flammable and the latter needs to operate at elevated pressures on a trans-critical cycle. Nevertheless, all are non-toxic, have good chemical properties, low GWP, low ODP and low-cost. The hydrocarbons can be derived from Liquefied Petroleum Gas, and CO_2 may be captured from the refinery's emissions, thus, further reducing release of greenhouse gases. We proposed to assess the flammability of the mixtures by measuring fundamental parameters (ignitability, flame speeds, etc.) and to determine the levels of CO_2 needed to either reduce the flame speed below the mild flammability level (S_{flame}<10 cm/s) or eliminate flammability altogether (S_{flame}=0 cm/s).

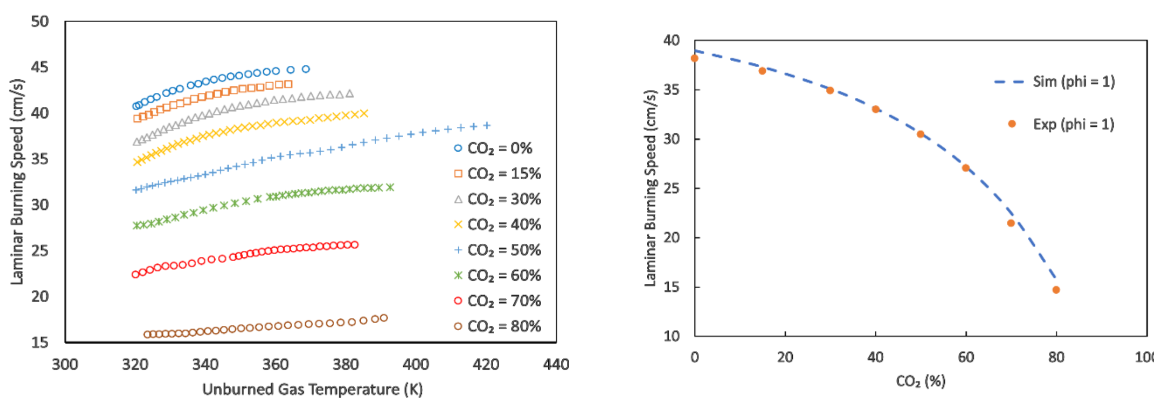


During the first year of this grand experimental and theoretical research was undertaken. Experiments were conducted to examine the effect of CO_2 as a diluent on the laminar burning speed of propane-air mixtures. Combustion took place at various CO_2 concentrations, different equivalence ratios and over a range of temperatures and pressures. The experiments were performed in a cylindrical constant volume chamber with a Z shaped Schlieren system, coupled with a high-speed CMOS camera to capture the propagation of the flames. A schematic of the experimental facility is shown in the adjacent figure. The experimental pressure rise data as a function of time during the flame propagation in the cylindrical vessel was the primary input of the multi-shell thermodynamic model, which was used to measure the laminar burning speed of smooth flames. This model was developed by Metghalchi, Keck, and co-workers, and it has been modified to include several correction factors. Which include the effects of radiative and conductive energy losses to the chamber walls, effects of temperature gradients in the burned gas, effects of preheat zone, wall and electrode boundary layers and as well as the effect of conductive energy loss to spark electrodes.

It was experimentally observed that the laminar burning speed increases with unburned gas temperature and the increase in pressure has an inverse effect on the laminar burning speed. It was also seen that with the rise in CO_2 concentration, the laminar burning speed decreases. A change in CO_2 concentration from 0% to 80% decreases the laminar burning speed non-linearly, consequently, a change in CO_2 concentration from 0% - 10% reduces the laminar burning speed by 2%, and a change in CO_2 concentration from 70% to 80% reduces the laminar burning speed by 33%. Representative images of propane/air/CO_2 mixture flames at different pressures and different CO_2 concentrations at a P_i=2 atm, T_i=298 K and equivalence ratio φ=1.2 are shown in the adjacent photographs. Laminar burning speeds as functions of the CO_2 concentrations at Ti = 298 K, φ = 1, pi = 1 atm are shown in the two plots below. In the plot on the left side the temperature of the unburned gas temperature is also depicted. The unburned gas temperature along the isentrope was obtained by the experimental pressure rise coupled with the isentropic compression assumption. Flame ceases to exist at CO_2 concentrations above 82.5%. It is known that the maximum amount of EGR used for an IC engine is ~20%. By an addition of up 20% CO_2 from 0% the laminar burning speed of the mixture decreases by 10%, which may be tolerated in engine performance for the sake of reduced NOx emissions. Similarly, for a refrigeration system, a mixture with a high percentage of CO_2 is needed to reduce the flammability risk of any accidental leaks. The laminar burning speed was found to be maximum near an equivalence ratio of 1.1 at the tested operating conditions.



Theoretical studies were also conducted to compare the collected data with numerical simulations from a one-dimensional laminar premixed flame code from *Cantera*, using a detailed $H_2/CO/C_1$-C_4 kinetics model including 111 species and 784 reactions. Experimental laminar burning speed results are in good agreement with simulation results, using Wang's Mechanism for stoichiometric conditions, but the simulation results deviate a little from the experimental results for non-stoichiometric conditions. The comparison is shown on the right side of the figure below.



Publication resulting from this ACS funding: Yelishala, S. C., Wang, Z., Metghalchi, H., Levendis, Y. A., Kannaiyan, K., & Sadr, R. "Effect of Carbon Dioxide on the Laminar Burning Speed of Propane–Air Mixtures." *Journal of Energy Resources Technology,* **141**(8), 082205-082209, 2019. doi:10.1115/1.4042411,

This research has an impact on the career of the PI (YAL) since it is exposing him to research concerning the combustion of Liquefied Petroleum Gas (LPG) components (such as propane). More specifically, with the help of the co-PI (HM), the PI is involved in the techniques for measuring the laminar flame speed (LFS) of these hydrocarbons. LFS is a fundamental property of these species, and it enables the assessment of their combustion rates. This knowledge is important for engine operation when such gases are used as fuels, and it is equally important for safety when such gases are used as alternative natural refrigerants. Furthermore, this research is also impacting the careers of both the PI and the co-PI, as they are now exposed to refrigeration-related research, a new research field for both of them. This has enabled them to attract industrial interest to conduct a preliminary study on the selection of hydrocarbons as refrigerants based on their thermodynamic behavior. Finally, this research is also impacting the education of more than two graduate students and one undergraduate student on the utilization LPG components in the applications of power generation and refrigeration.