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Flight Assignment:	NOTE: End date changed to 11/17/2020 per N	SSC information (Ed., 11/7/19)	
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	NOTE this is a successor agreement to "Electr Science per D. Stocker, NASA Glenn Research This project at the University of California, Irv the performance of energy conversion systems formation, while, as a sensing device, the elect to preparing for the proposed Advanced Comb aboard the International Space Station (ISS), we methods and the dynamic interaction between the downstream electrode in order to character computational models to predict chemi-ion con	h Center. vine continues to explore using electri . As an actuator, electric fields can in rical response at saturation is an inher ustion via Microgravity Experiments we have continued to enhance our und the flame and chemi-ions. We have rize the likely body forces resulting, and	c fields in combustion for improving approve flame stability and soot rent flame characteristic. In addition (ACME) E-FIELD experiments erstanding of the experimental neasured the distribution of ions at and we have begun to develop

Task Description:

forces from electric fields and those from enhanced gravity. This report summarizes recent findings in 2 main areas:

- 1.) Experimental There are two elements in the experimental progress: (a) the unreported first phase of E-FIELD Flames microgravity combustion experiments aboard the ISS. These experiments are with the co-flow burner, with positive and negative polarities, methane and ethylene as fuels, different fuel dilutions, different flow velocities, and cases with and without a small coflow of air. These are the first electric field experiments completed in the combustion integrated rack (CIR). And (b) the second phase of E-FIELD Flames microgravity combustion experiments aboard the ISS. These experiments are with a simple jet burner, with positive and negative polarities, methane and ethylene as fuels, different fuel dilutions, and different flow velocities. These are the first jet diffusion flame experiments under the influence of an electric field in zero gravity.
- 2.) Developing a computational model to predict ion concentrations in flames and the effects of ion driven winds in coflow and jet flames. A focus has been on a full Computational Fluid Dynamics (CFD) simulation with appropriate reduced chemistry using the Open Foam Optics And Mechanics (FOAM) platform of computation. This past year has concentrated on the appropriate reduced chemical mechanism that provides accurate chemi-ion concentrations with a sufficiently small number of reactions to allow a comprehensive CFD model that includes electrical forces. The configuration is for the coflow geometry but without coflowing gas.

Summaries of these findings appear in this report with the details of all the work appearing in the publications and conference proceedings identified at the end of this document. In the past year we have produced: 2 peer-reviewed journal articles; 2 invited technical presentations and a public presentation at a high school in Spain, and 7 conference papers

Rationale for HRP Directed Research:

Research Impact/Earth Benefits:

The control of combustion has the potential to improve efficiency and reduce emissions from burning fuels. Since high power density often requires combustion, these improvements will be important no matter what the fuel source. Electric fields acting on flames have the potential to aid in combustion control both for sensing and actuation. For example, electrical properties of flames can identify poor performing boiler flames that release poisonous carbon monoxide. Our studies show that a flame's electric signature can capture incipient quenching before dangerous emissions result. Electrically driven ions can produce local convection that changes combustion behavior. Understanding the links between electrical character and flame behavior may allow improved sensing of poor performing combustion systems.

ISS Experiments: The major accomplishment of the prior year was the completion of the first and second phase set of tests from the ACME E-FIELD Flames experiment. The first phase employed the same co-flow burner aboard the ISS as was used for the CLD Flames experiments, but an electrode mesh was installed downstream of the burner. The second phase set of tests used a simple jet flame configuration with the electrode mesh downstream of the jet tip. The experimental details for the coflow burner have been described in prior reports. The ISS experiments covered a wide range of conditions and outcomes, with 131 different tests run, and more than 120 of them successful in phase I with the coflow burner and 104 different tests run in phase II with the single-jet burner for a total of 235 testpoints. Color camera images, intensified camera images, total flame luminosity, and ion current, along with all test parameters and flow monitoring, were recorded in all cases.

Results and Discussion

The key measurement for the E-FIELD Flames experiments is the ion current as a function of applied voltage (the V-I curve). This curve provides information on the flames ability to produce chemi-ions based on its saturation ion current, and it provides a measure of combustion performance in that ion production is a function of carbon influx into the flame and the vigorousness of the combustion process. As was reported last year, more compact, higher temperature flames produce more chemi-ions than do larger more diffuse reaction zones of lower overall temperature for the same fuel flow. Another interesting feature of these microgravity V-I curves is the peak value. Traditional electrical aspects of flames studies look for a saturation ion current plateau, where the ion current remains fixed despite an increase in applied electric field. For these zero gravity flames, there is a pronounced peak in the ion current at saturation and then a gradual decrease to a global saturation plateau. This is a strikingly different behavior than is seen in 1-g, and the behavior is even more pronounced for the case where there is zero coflow.

The first data from the ISS experiments used 100% methane as fuel, while later experiments varied the methane concentration with the balance nitrogen. The flame images of methane diluted with nitrogen at positive field strength and negative field strength are taken with different shutter speed based on the flame luminosity and subtracted with several background images in average. There is no coflow in the outer concentric region to help enhance the air/fuel mixing, and hence the flame is relatively less stable and less bright as compared to the equivalent coflow flames, in general. For both positive and negative field strength, the ion current peaks when the flame is the most compact. For the positive field, the voltage-current (V-I) curve in microgravity shows a very similar trend as is observed from the very first sets of results with the 100% methane fuel condition but with some additional information over a larger range of voltage. The ion current increases parabolically with the nominal field strength and then reaches a peak. With the enhancement of voltage, the current undergoes another parabolic like decrease and slowly increases back up again. The second increase of the ion current is not complete and clear due to the very low fuel concentration with the limitation of the capability of the power supply and the constrained fixed distance of the mesh electrode. The flame images also relate to the ion current to field strength curve, showing that the flame reduces in size as the ion current increases and, as the current drops, the flame size increases. The flame size reduces again as the ion current climbs back up close to the end of voltage-current curve.

With the negative field, the overall ion current remains low (below 0.3 microamps) for both the 70% and 40% methane conditions in comparison to the positive field condition. In contrast to tests with the positive electric field, the ion current also reaches its peak sooner, at around 0.4 kV/cm, and then decays immediately with the increasing of electric field strength until the flame extinguishes. The ion current decay also corresponds to the flame appearance. For both of the fuel dilutions, the flame extends wider and the flame base is gradually lifted after the saturation peak. The flammability limit (i.e., just before flame blowout with the field) in the perspective of nominal electric field strength is 1.46 kV/cm and 1.30 kV/cm for 70% and 40% methane, respectively.

Single Jet Burner: In a positive field, the jet flames are relatively more stable initially and less stable under high voltage

than the previously reported flames using a coflow burner with no coflow. As the positive field is applied to the jet, the flame becomes compact along the width and height. The immediate change observed is the bright soot aggregating around the flame tip. With an increase of electric field strength, the soot distributes less at the tip as the flame shrinks. The ion current corresponds to the flame appearance in that the current increases and reaches a peak at the most compact flame. With further electric field increase, the flame starts fluctuating and a distinct dancing phenomenon can be seen from the V-I curve where the ion current oscillates widely at the same field strength. These very high peak values may represent an incipient corona or discharge event.

Unlike in the positive field, the methane jet encounters the downward ion wind around the flame and does not sustain after 1.76 kV/cm for 24 cm/s, being blown out by electric field. The 19 cm/s flame lasts until 1.93 kV/cm. When the flame experiences a negative field, its height decreases and the full flame is moved onto the tube, similar to a downward pointing jet flame in 1g. The change of the flame width is not as clear and obvious as with a positive field but still changes. The ion current also increases with the field strength but differently than with the positive field without a clear curved slope. Instead, it decreases parabolically after reaching the current peak. The current peak corresponds to the most compact flame at 0.32 kV/cm for 19 cm/s and 0.41 kV/cm for 24 cm/s. Soot also appears at the flame tip but with a wider distribution along the reaction sheet. The soot reduces with increasing negative field strength, and it disappears at 0.80 kV/cm along the parabolic decay line after passing the ion current peak. The flame width and height also expand after the most compact flame. There are several sparkler-like soot particles at 1.18 and 1.93 kV/cm. Further evaluation of this soot sparking is underway.

Experimental Conclusions: This experimental work reports the initial flame appearance and voltage-current (V-I) plots for the unique condition of a nonpremixed flame under the influence of an electric field in microgravity conditions using coflow burner (without turning on coflow). The flame images in microgravity with no coflow are distinct in the change of size and reaction zone location while there are relatively small differences observed in normal-gravity laboratory experiments. The ion current results at low gravity do not exhibit the typical sub-saturation, saturation, and supersaturation trend as recorded in terrestrial tests, suggesting that buoyancy driven flows play an important role in this characteristic ion current behavior. This work will continue and further compare with similar carbon content at different fuel flow rates in 0g as a marker to research how the soot, ion current, and flame luminosity vary with each other.

The positive field allows the soot to concentrate and compresses the flame into a high current density thermal source and leading to an unpredicted oscillation before extinguishing with the increasing field strength. The negative field allows the flame to maintain its spherical characteristic in microgravity. The yellow soot appears for both of the electric field directions within the flame around the tip and disappears with increasing field strength after the reaching the current peak. The role of soot in the V-I behavior of these flames requires further investigation.

OpenFOAM Simulations: Electric fields can affect flame shape, burning velocity, temperature profile, speed of propagation, lift-off distance, species diffusion, stabilization, and extinction. The primary reason is that combustion of hydrocarbon fuels involves chemi-ionization, which generates ions and electrons that can be manipulated by the field producing a body force also referred to as an ion wind.

Chemiluminescence of the flame is considered in these simulations. Chemiluminescence is an important feature in flame diagnostics and is an electronically excited species present in flames. The reactions involved in chemiluminescence were not included in the original GRI-Mech 3.0 because excited species are in low concentration and are not significant contributors to the major chemical pathways. Recent work has suggested, however, that there is a strong link between excited species and chemi-ion production. Excited species are also important as an indicator for many flame properties including reaction zone position. It is valuable, therefore, to add reactions involved with important excited species, such as excited hydroxyl, OH*, and methylidyne, CH*. At the moment, there is no published model for non-premixed co-flow methane/air flames that contains both chemi-ions and excited species. Hence, a combination of chemical kinetic models that contains both, excited species and chemi-ions, is part of this study.

The final goal is to fully understand how flame behavior is altered by different electric fields. For that purpose, the effect of the electric field force to the 1g flame has been studied for a range of different applied electric fields.

The axisymmetric geometry models for the different jet methane flames studied are a burner with the inlet tube (from which fuel is flowing) extruded from the burner and a jet burner.

The chemical kinetic model used in this study contains neutral and charged species. H3O+ has been reported as the most long-lived ion in the flame and HCO+ is generated by the primary reaction creating ions and electrons. Similar boundary conditions have been applied to the jet case (which differs on the height of the burner to be 10 cm instead of 3 cm).

Results and discussion: For the flush and jet burner geometries, I-V curves are not matching with the ones in the literature. Further investigation must be performed, starting by revising the boundary conditions and the electric force and flow field mapping without flame. Calculations of the z-current densities for both burner geometries studied show physically plausible values, but deeper analysis has to be performed from the numerical simulation results in order to understand the physical meaning of these results.

Conclusions and Future Work: Promising work in electric field forces studies has been performed. The electric field simulations still need to be developed to acquire more reliable results that match after the saturation point (i.e., the saturation plateau) in order to assure and assume that the fluid dynamics, chemistry, and body forces phenomena that are happening in the flame and are changing its behavior are well captured by the simulation. However, the results obtained up to now align with the literature. Once 1g flame simulations show comprehensible results matching with the literature for all the burner geometries, these simulations will be re-run at a 0g environment in order to compare the obtained results with ISS experimental results.

Reduction of Chemical Kinetic Mechanisms: Currently, experiments alone cannot explain the phenomena contributing to the flame behavior when an electric field is applied since ion chemistry and the transport effects produced by the application of an electric field cannot be easily decoupled. As discussed before, simulations that accurately reproduce and interpret the experimental observations can provide insight into the key features of ion effects in combustion, especially when an electric field is applied. However, the appropriate ion chemistry to include in these simulations remains uncertain. Moreover, simulations of flames with applied electric field require a comprehensive small chemical kinetic model in order to be able to be performed in a cluster within a reasonable amount of computing resources and time

To tackle these issues, a chemical kinetic model that captures the interactions occurring during methane-air combustion

Task Progress:

processes is developed. Achieving a reduced-order model that is faithful to the ion production but also captures the appropriate flame chemistry for this fuel will help to decouple the effects of ion chemistry and applied electric fields for flames, providing a fundamental understanding for further development of devices that might actively control combustion.

Once the full chemical kinetic model for non-premixed methane-air flames is achieved, the next step is to reduce it until it is of a size appropriate for use in a 2D Computational Fluid Dynamics Simulation (CFD simulation) of a real burner. This reduction is needed because large chemical kinetic models (i.e., with more than 35 species) cannot be practically applied in a 2D CFD simulation due to the high computational cost related to data storage and simulation time.

The last step will be to validate the reduced chemical kinetic model. To do so, a 2D OpenFOAM CFD simulation is performed with reduced chemical kinetic model developed. The validation proceeds by comparing the results obtained with the experimental data available from Earth experiments gravity (1g) and International Space Station experiments (0g). This comparison will include flame shape as marked by the chemiluminescent species locations, the ion current as measured at the downstream electrode of the applied electric field, and the soot location and luminosity as recorded photographically. As for the validation at this step, the acceptable tolerances will be of a 1% difference in flame structure of major species and temperature and less than 20% difference in minor species of importance (ions and excited species) and soot precursors. The reduction has been made using the PSR module in Chemkin-Pro® and only for The San Diego Mechanism with the excited species submechanism has been added later as it is without further reductions (the number of reactions and species has increased from with the addition of the submechanism for charged species included). The target species in the reduction have been: C2H, H2O, O, CH, O2, and OH. The species to keep during the reduction have been: CH4, C2H, CH, CH*, CO, CO2, H2O, N2, O, O2, OH, OH*.

A reduced model containing excited species CH* and OH* and neutral species has been achieved. The detailed model (330 reactions/70 species) has been reduced to have 152 reactions and 31 species. Validation between the reduced and the detail models has been done by comparing the results gotten from using each of the models (detailed and reduced) using PSR and counterflow burner geometries in Chemkin-Pro® and at temperatures of 1500K, 2000K, and 2500K. After these comparisons, the submechanism for charged species was added to both detailed and reduced model. Further comparison between the reduced model and the detailed model has been made for validation purposes using the counterflow geometry in Chemkin-Pro®. Once the results using 0D and 1D burner geometries were showing differences within an acceptable tolerance for all cases, a 2D OpenFOAM axisymmetric simulation for the extruded geometry was run for 1g and no electric field applied in order to compare these results against experiments.

Numerical Conclusions: A new reduced chemical kinetic model for methane/air flames has been developed and promising results have been obtained when comparing this reduced model to the detailed mechanism. Further validations have to be made in order to assure that this reduced model for methane/air is capable to accurately predict the flame behavior, including the changes when an electric field is applied to the flame and the quantity of soot produced. Comparison with the ion current as measured at the downstream electrode of the applied electric field and the soot location and luminosity are planned to be carried out in the near future.

Bibliography Type:	Description: (Last Updated: 02/12/2024)	
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