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PI Name:	Dunn-Rankin, Derek Ph.D.	r	
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PI Email:	ddunnran@uci.edu	Fax:	FY
PI Organization Type:	UNIVERSITY	Phone:	949-824-8745
Organization Name:	University of California - Irvine		
PI Address 1:	Department of Mechanical & Aerospace Engineering		
PI Address 2:	4200 Engineering Gateway Bldg, EG3224		
PI Web Page:			
City:	Irvine	State:	CA
Zip Code:	92697-3975	Congressional District:	48
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Contact Monitor:	Stocker, Dennis P	Contact Phone:	216-433-2166
Contact Email:	dennis.p.stocker@nasa.gov		
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	NOTE this is a successor agreement to "Electr Science per D. Stocker, NASA Glenn Researc 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 experiments aboard the International Space State experimental methods and the dynamic interact distribution of ions at the downstream electrod begun to develop computational models to pre enhanced body forces from electric fields and	h Center. vine continues to explore using electric. As an actuator, electric fields can imprical response at saturation is an inher sustion via Microgravity Experiments ation (ISS), we have continued to enhaltion between the flame and chemi-ion ie in order to characterize the likely be dict chemi-ion concentrations in flame	c fields in combustion for improving approve flame stability and soot rent flame characteristic. In addition (ACME) ACME E-FIELD ance our understanding of the as. We have measured the ody forces resulting, and we have es, including a comparison between

main areas:

Task Description:

- 1.) The first phase of E-FIELD 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).
- 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 CFD simulation with appropriate chemistry using the Open FOAM platform of computation. This past year has concentrated on the coflow geometry.

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: 1 peer-reviewed journal article, 5 invited technical presentations, and 7 conference papers.

The project includes both experimental and computational parts. The experiments employ a coflow burner that is aboard the ISS.

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 - First Phase

The major accomplishment of the prior year was the completion of the first 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 Coflow Laminar Diffusion Flame (CLD Flames) experiments, but an electrode mesh was installed downstream of the burner. The experimental details have been described in prior reports. The burner consists of two stainless steel plenums threaded together. Fuel, introduced in the bottom plenum, passes through a stainless-steel tube (2.13 mm ID) and exits the top surface as a fully developed parabolic flow. Air entering the top chamber flows through straightening beads and a honeycomb mesh. Ground-based characterization studies show that the air exits the top surface with an approximately top hat flow profile at the exit. The center fuel jet was slighting extruded above the top surface of the coflow burner to more closely approximate a jet burner and to offset the flame ignition region from the coflow surface. A variable high-voltage power supply connected between the burner and the downstream mesh electrode produces an applied electric field. Although the electric field distribution is deformed locally by the flame's space charge, defining an applied field strength, E = V/H (where V is the voltage applied and H is the distance from the burner to the electrode) is useful when describing experimental results. Ion current is calculated using Ohm's law and the potential drop across a shunt resistor between the electrically isolated burner and ground.

The hardware on the ISS comprises the ACME insert and the combustion integrated rack (CIR), and the complexity of this system is far greater than the burner component identified above. The detailed description of operations and hardware provides the context under which the ACME experiments are conducted, and their complexity makes the flame conditions trivial in comparison. In short, however, we have a simple coflow flame, with just a small jet of fuel surrounded by a weak (or sometimes non-existent) coflow of 'air' which also fills the chamber. A test includes starting the gas flows to prime the system, energizing the igniter to initiate a flame, retracting the igniter, and allowing the flame to steady slightly before energizing the electric field to its initial value. We found that in some cases the electric field assisted in the stabilization and so this first stabilization time was often kept short. The flame is again allowed to steady before beginning a voltage sweep over a specified range with steps or smooth ramps of specified voltage changes and durations. The sweep can be in one direction or can include cycles of sweeps. After each test, a duplicate field sweep is made to ensure that there are no current leaks, i.e., other than the ion current through the flame.

The first phase tests in E-FIELD Flames employ the coflow burner geometry, with the fuel tube extending slightly above the burner surface. The results in this reporting period are for tests conducted with 100% methane in a chamber atmosphere and coflow (when used) of synthetic 'air' (i.e., 21/79 oxygen/nitrogen by volume) at a nominal pressure of 100 kPa. The mesh is held at a negative potential relative to the burner in these tests. The sweeps shown generally span the full range to -10 kV, where the voltage is increased in small steps (e.g., of 100 V), with each step lasting 1-2 seconds.

The ISS experiments covered a wide range of conditions and outcomes, with 131 different tests run, and more than 120 of them successful. 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.

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. 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. The first effect (i.e., the relationship between carbon influx and peak ion current) can be seen as the flow of 15 cm/s methane produces slightly above 2 microamps of ion current at the peak (1.5 kV/cm) and the flow of 19 cm/s methane has a peak of 2.75 microamps. The peak ion current is nearly proportional to the flow velocity. 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 the 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.

As is apparent from the flame images, the flame is most compact at the voltage consistent with the peak ion current.

With increasing voltage, the flame becomes less compact and the ion current decreases. We presume that the flame remains at saturation throughout this period (that is, the flame is producing as many ions as it can, and those ions are being removed from the reaction zone as soon as they are created) so the decrease in ion current results from a change in combustion intensity. We can explore this hypothesis further using the PMT data collected in the experiments.

In all of the curves, the jagged features are spikes following a voltage step change that are mostly associated with the transient capacitance of the system when rapid steps are requested. These overshoots notwithstanding, the V-I curves follow smooth and reproducible trajectories. The results are too recent to allow a detailed analysis and discussion of the differences, but some significant observations from these results and the comparison with 1-g experiments follow.

- 1. The ion current reaches a peak at approximately the same field strength for both velocities in 1-g while in microgravity the ion current peak for a lower fuel velocity occurs at a lower field strength. The field strength at the peak current seems to scale linearly with the fuel velocity.
- 2. In microgravity, the ion current does not smoothly increase to saturation nor does it show a gentle peak with a mild decrease as is seen in the normal gravity results. Instead, in microgravity there is a distinct peak in the ion current with a severe decrease throughout the saturation condition, with a final saturation plateau observed at voltages substantially above the voltage at peak ion current. That is, the microgravity final saturation is not the maximum ion current observed. This difference is more dramatic when there is no coflow, which suggests that entrainment plays an important role whether caused by buoyancy or a forced coflow.
- 3. The peak ion current is higher for microgravity than comparison 1-g flames. The reason is not obvious at this point but may result from a more focused upward flow from the electric body force and ion-driven wind as compared to the combined effects of the ion wind and buoyancy.
- 4. The peak ion current is approximately proportional to fuel flow velocity, which, as described in prior studies, reflects the relationship between ion production and the carbon flux into the system. The peak ion current also increases with the coflow which suggests that healthier oxidizer transport helps increase the ion production.

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 a chemi-ionization process, which generates ions and electrons that can be manipulated by the field producing some alteration of the chemical kinetics and generation of a body force. The former arises because the chemistry of the system is affected by the redistribution of charges under the applied electric field; the latter generates an ion wind. The predominance of the literature indicates that changes in chemistry are minor, though the effects on soot formation and transport remain somewhat uncertain.

The simulations in this project also consider chemiluminescence of the flame. 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, like charged species, are in low concentration and are not significant contributors to the major chemical pathways. Recent work has suggested, however, that there is a link between excited species and chemi-ion production. Excited species are also important as an indicator for many flame properties including reaction zone position, and chemiluminescence is one of the measurements being obtained on the ISS in ACME. 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, combining chemical kinetic models that contains both excited species and chemi-ions is part of this study.

The final goal of the numerical simulation component of the research is to understand how flame behavior is altered by different buoyancy force environments and external electric fields. For that purpose, two separate studies have been performed using three different burner geometries. The first study focuses on the effect of the buoyancy force on the flame, observing the flame behavior in different gravity environments. The second focuses on the effect of the electric field force, studying the 1g flame behavior for a range of different applied electric fields.

The axisymmetric geometry models for the different jet flames studied are the burner with the inlet tube (from which fuel is flowing) extruded from the burner, the burner with a flush inlet tube, and the jet burner (i.e., no surrounding coflow). The geometries are based on the geometry of burners on the International Space Station (ISS), as part of the Advanced Combustion via Microgravity Experiments (ACME) project equipment which will eventually provide experimental data against which the described simulations can be compared.

Notice that the extruded and the flush tube burner geometries would accept an inlet of air from the burner outer ring, creating then a co-flow flame. However, the jet flame without the co-flow air (i.e., natural convective/diffusive flow only) was considered for this study. Further work will include co-flow air coming out from the outer ring.

For the buoyancy study, CH* is taken as a marker for the luminosity of the flame; 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 (CHO -> CHO+ + e-), well-known as the principal chemi-ionization reaction. Hence, these three species are the minor species that have been taken into consideration for the buoyancy study and will be discussed later in this report. For the electric field study, the methodology followed to achieve comparable results with the literature has been developed along with our informal collaborators at KAUST, which models the ion production without the chemi-ionization reaction included formally in the chemical kinetics mechanism.

OpenFOAM was chosen as the numerical solver. The solver used was a modified version of the reactingFoam solver in OpenFOAM. The mass transport equation was modified by imposing a Schmidt number equal to 0.7 condition. Previous studies showed that this approximation was suitable for combustion processes. Maxwell's equations have been implemented in the solver by Professor H.G. Im's research group at the Clean Combustion Research Center (KAUST), as part of this project's informal collaboration.

In OpenFOAM it is easy to deal with axially symmetric geometries; for cylinders it is sufficient to solve the problem in a 5 degree wedge. To do that, a cylindrical control volume has been considered; in this way, properties vary only along the radial coordinate x and the axial coordinate z. A large external domain must also be included to make sure that the boundaries do not affect the core combustion processes and behaviors.

Task Progress:

The boundary conditions were the same for all geometries studied. The horizontal top wall (35 mm higher than the base of the mesh) has a zero-gradient condition. A non-uniform parabolic velocity profile of the inlet methane was imposed following previous literature procedures. The gravity force considered has been applied in the Z-direction, in contra-direction with the fuel jet exit flow.

For the temperature, a condition of zero gradient --i.e., normal gradient of temperature is zero-- has been set on all boundary walls. Since only steady state is examined for all cases, the simulations were run from ignited simplified cases in which air and fuel were entering the system at 800K. Once the simplified computation reached steady state, the temperatures were changed to 300K and the simulation cases were continued until they reached steady state again. The air was considered as molar fractions of 0.76, 0.2395, and 0.0005 for nitrogen (N2), oxygen (O2), and carbon dioxide (CO2), respectively. The initial pressure is atmospheric for all cases.

The burner acts as positive electrode for the all cases studied and the metallic upper mesh acts as negative electrode, since only negative voltages have been considered so far for this study. Positive voltages will be considered in future simulations, having to modify the Poisson and charged species boundary conditions accordingly.

The buoyancy environment conditions that have been considered so far are microgravity (0g), partial gravity (0.5g), gravity (1g), and supergravity (range from 1.125g to 3g).

The geometry of the burner plays an important role when buoyancy forces are applied. This might have been expected since other body forces (such as those produced by the electric field) have been shown experimentally to also be strongly conditioned by the burner geometry used.

Also, simulations for a jet burner geometry of different tube heights have been performed in order to check if there is a height where the flame at the jet burner geometry acts similarly to the extruded tube burner geometry. No clear correlation has been found between the concentrations observed (CH*, OH*, H3O+, and HCO+) and the height of the jet burner tube extrusion.

The electric field conditions that have been considered in this study vary depending on the burner geometry used. However, in all cases, the maximum electric field applied in the simulation was the one found experimentally at saturation.

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

Promising work with both buoyancy and electric field forces studies has been performed. The study of the buoyancy effects shows that different burner geometries will affect the flame when gravity changes. Deeper understanding on the fundamental reasons that cause these differences is still to be achieved. Electric field simulations still need to be completed for the geometries matching the experimental conditions to acquire more reliable results that match with the literature 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. Once 1g flame simulations show reliable results matching with the literature for all the burner geometries, these simulations will be run for the 0g environment in order to compare the obtained results with ISS experimental results.

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