Fiscal Year:	FY 2018	**Task Last Updated:**	FY 09/24/2017
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Project Title:	ACME: EFIELD – Electric Field Effects On Laminar Diffusion Flames		
Division Name:	Physical Sciences		
Program/Discipline:			
Program/Discipline--Element/Subdiscipline:	COMBUSTION SCIENCE--Combustion science		
Joint Agency Name:		**TechPort:**	No
Human Research Program Elements:	None		
Human Research Program Risks:	None		
Space Biology Element:	None		
Space Biology Cross-Element Discipline:	None		
Space Biology Special Category:	None		
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Zip Code:	92697-3975	**Congressional District:**	48
Comments:			
Project Type:	Flight	**Solicitation / Funding Source:**	NOT AVAILABLE
Start Date:	11/18/2016	**End Date:**	11/17/2019
No. of Post Docs:	1	**No. of PhD Degrees:**	1
No. of PhD Candidates:	2	**No. of Master' Degrees:**	
No. of Master's Candidates:	1	**No. of Bachelor's Degrees:**	
No. of Bachelor's Candidates:	2	**Monitoring Center:**	NASA GRC
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Flight Program:			
Flight Assignment:			
Key Personnel Changes/Previous PI:	September 2017 report: Dr. Alice Chien is joining the project.		
COI Name (Institution):	Karnani, Sunny Ph.D. (Army Research Labs)		
Grant/Contract No.:	NNX17AC51A		
Performance Goal No.:			
Performance Goal Text:			

NOTE this is a successor agreement to “Electric Field Control of Flames (NNX11AP42A),” in Microgravity Combustion Science per D. Stocker, NASA Glenn Research Center.
This project at the University of California, Irvine continues to explore the use of large electric fields in combustion for improving the performance of energy conversion systems. As an actuator, electric fields can improve flame stability and soot formation, while, as a sensing device, the electrical response at saturation is an inherent flame characteristic. In addition to preparing for the proposed ACME E-FIELD experiments aboard the International Space Station (ISS), we have continued to enhance our understanding of the experimental methods and the dynamic interaction between the flame and chemi-ions. We have measured the distribution of ions at the downstream electrode in order to characterize the likely body forces resulting, and we have begun to develop computational models to predict chemi-ion concentrations in flames, including a comparison between enhanced body forces from electric fields and those from enhanced gravity. This report summarizes recent findings in 4 areas:

Task Description:	1.) A study on the effect of burner geometry on the flame response to electric fields, such as flame shape changes and ion current differences. 2.) Research and developing computational models to predict ion concentrations in flames, specifically on the effects of ion driven winds. In particular, different ion chemistry models are surveyed and reviewed in detail in order to provide in-depth understanding of how ions are produced in hydrocarbon flames. In this case, the simulation study is carried out at multiple gravity levels to observe the variation of physical properties such as species concentration in the active regions under different body forces in flames. 3.) Examining the linkage between experimental flame geometries under the influence of various electric fields on Earth (at 1-g condition) and computational results under various enhanced gravity conditions. This study is focused on investigating the distribution and location of CH chemiluminescence species. 4.) Exploring alternative numerical approaches that will potentially lead to high efficiency computation of flames under the influence of electric fields. 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; 3 invited technical presentations, 3 conference papers, and 1 Ph.D. dissertation. Understanding electric field interactions with flames is central to combustion control, particularly in situations near limit operation of the flame where small effects are amplified dramatically. Electric fields have been shown to modify burning rates as well as to enhance and reduce flame propagation even to the point of flame extinguishment. Our experiments provide a unique ability to make simultaneous measurements of both physical and electrical properties of flames.
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. In addition, 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. Understanding the links between electrical character and flame behavior may allow improved sensing of poor performing combustion systems.
	Both experiments and computations are part of the project. The experiments employ a coflow burner that is dimensionally equivalent to the ISS coflow burner but with a fuel jet matching the dimension of the ISS jet burner. The burner consists of two stainless steel plenums threaded together. Fuel, introduced in the bottom plenum, is passed through a stainless-steel tube (2.13 mm ID) and exits the top surface fully developed. Air entering the top chamber passes through flow straightening beads and a honeycomb mesh. The air exits the top surface with a top hat flow profile at the exit. In many experiments, the center fuel jet was slighting extruded above the top surface of the coflow burner to more closely approximate a jet burner. A variable high-tension power supply connected between the burner and 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, 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 the building ground. An acrylic chamber shields the flame from room air currents. (1) Electric Field Effects On Flame Geometry External electric fields have long been known to modify the geometry of the flame. It has been demonstrated that flames may deflect in the direction of an electrode with a negative electrical bias. This study shows how an electric field affects the behavior of a non-premixed, conical shaped flame that is stabilized on a coflow burner when the central tube is extruded 3mm above the coflow surface. The burner acts as the ground electrode in the electrical circuit. Chemiluminescence images for this study were captured with a Nikon D90 digital camera and a 430 nm (10 nm full width at half max) filter. Details on the procedure of imaging and quantifying of flame chemiluminescence can be found in the literature, e.g., Walsh et al. [1998], Giassi et al. [2016], and Tinajero [2017]. After the external field was initiated, the flames re-stabilized before the images for this study were taken. These images were deconvolved with an onion-peeling Abel inversion to reveal the two-dimensional flame contour. Details of the Abel inversion algorithm can be found, e.g., in Dasch [1992]. What can be extracted from this study is that the geometry of the flame subtly responds to the external electric field with a slight decrease in flame height and a slight decrease in flame width. The more significant change observed is the lifting of the flame's base and increased CH* light emission at high field strengths. These two flame characteristics were quantified as a function of field strength. Previous simulations have predicted that the enhancement to saturated ion currents may be caused by enhanced mixing of fresh oxidizer with fuel in this flame base region, which results in a partially premixed flame as described by Yamashita et al. [2009]. The mixing is explained by entrainment of ambient air into the gas ow forced by the ion wind. The lifting of the flame seen during this study may be the result of this mixing. A summary of the analysis for all experimental configurations shows that for the burner with the protruding fuel tube, a clear trend can be seen between the height of the flame's base, the intensity of light emitted from the flame by CH*, and the chemi-ion production (identified by the ion current above 1 kV/cm). For a flush fuel tube, on the other hand, the height of the flame's base is uncoupled from the CH* chemiluminescence and chemi-ion production. Regardless of the unchanged height of the flame, the CH* chemiluminescence and the chemi-ion production both demonstrate enhanced levels when the electric field strength rises above 3 kV/cm. (2) OpenFOAM Simulations - I As discussed earlier, 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.

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. Excited species are important as an indicator for many flame properties including reaction zone position. 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 new combination of models that contains both, excited species and chemi-ions, is part of this study.

Moreover, a study of the behavior of the flame under different gravity conditions is performed to better understand how buoyancy affects flame behavior. This study could provide interesting insights should we choose to use combustion processes in current and future missions to Mars and other environments where gravity conditions differ from those on Earth, as well as helping elucidate the contribution of the buoyancy forces to the flame.

Chemical Kinetics and Reaction Mechanism

The chemical kinetic mechanism used is a new combination chemical kinetic model (i.e., a selected collection of reactions from published models) for the prediction of major species and minor species such as ions and excited species. It contains 299 reactions, which reactions 1 to 280 come from the model proposed by Prager et al. [2007] except that the parameters have been reviewed and checked with the references proposed in the original document. A submodel proposed by K.T. Walsh [1998] that predicts excited species (OH* and CH*) has been added to the combined chemical kinetic model proposed. Species transport coefficients were predicted by using Cantera® software. The excited species transport coefficients were presumed to be the same as their respective ground state specie. The ionic species transport was presumed to be the same as for air, as a first approximation. Refinements to the model will include using transport coefficients for ions that match their neutral counterpart but for the current work this was not necessary because the concentration of these species is so small.

Numerical Model

OpenFOAM was chosen as the numerical solver to analyze the effects of chemi-ionization and electric fields on coflow flames. 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.

Implementing Maxwell’s equations into the model is still work in progress. The coflow burner has been modeled as two concentric cylinders, whose upper bases correspond to the exit area of the nozzle; the origin of the reference frame has been set here. Pure (fuel) and pure air (oxidizer) are ejected respectively from the internal nozzle and the external annulus. In OpenFOAM it is easy to deal with axially symmetric geometries; for cylinders it is sufficient to solve the problem in a wedge of small aperture. To do that, a cylindrical plate has been considered; in this way, properties vary only along the radial coordinate and the axial coordinate. A large external domain must also be included to make sure that the boundaries do not affect the core combustion processes and behaviors.

Simulations

The simulations of this study predict flames behavior under microgravity (0G), partial gravity (0.5G), gravity (1G), and supergravity (1.5G, 2G, and 3G). Hence, the gravity conditions used in the simulations are in all the range of the gravity values for the Earth-Solar System.

Results and discussion.

The profiles computed are the temperature in the flame as well as the CH* (which acts as the visible flame marker) profile and the profile of the two main ions produced in the flame, H3O+ and HCO+ (which highlights the source of electric body forces if a field were to be applied).

1. Temperature profile. Due to the co-flow air that is surrounding the inside fuel jet, the completely spherical shape expected from a 0G flame is slightly modified in the wings since air is coming from the sides. As gravity increases, buoyancy forces pull the flame upward and make it narrow. The effects observed in the temperature profiles were not unexpected in response to changing gravitational acceleration. New experimental data is expected to be available from the ACME project to validate the 0G profile.

2. CH* profile. Chemiluminescence associated with the relaxation of CH* to CH is directly correlated with the luminosity of the flame and how the flame looks to the eye. In the 1G flame, the flame height correlates with previous experimental results and the location of the CH* is well predicted.

3. HCO+ and H3O+ profiles. The main ions naturally produced by the flame, H3O+ and HCO+, are shown to be in similar or higher concentration than the CH*. This fact strengthens the hypothesis of modification of flame behaviors by using electric fields and interacting with these species, since it has been observed that electric fields change the luminosity and flame shape of laminar diffusion flames (Lawton and Weinberg [1970], Karnani [2011], and Tinajero [2017]).

On the other hand, as previously mentioned for CH* profiles, the height of the flame does not seem to be affected by the change in buoyancy forces but the flame width does shrink to create a thinner flame. This might be the explanation of the higher production of H3O+ species at super-gravity, since the flame shrinking more tightly packs the species.

Conclusions and Future Work

Simulations including excited species and ionic species reproduced successfully many of the main characteristics of the flame, such as flame height, flame temperature, as well as major and minor species naturally produced by the flame. Flame height was shown to not be affected by a change in gravity field while flame width was affected by producing a thinner plume, as was expected. However, detachment from the burner tip was observed numerically though it was not seen experimentally, and this detachment seems to result from the numerical challenge related to the prediction of these boundary conditions.

More work must be done to accurately predict the bottom of the flame and the interaction of the flame with electric fields. Nevertheless, the combination chemical kinetic model proposed containing excited species and ions has shown an ability to predict important characteristics of the non-premixed methane laminar jet flame. To better understand the

Task Progress:

reasons why the observed concentration profiles using the simulations differ from the experimental results, the combination of chemical kinetic models used was previously tested for 1D simulations by using CHEMKIN software.

(3) OpenFOAM Simulations - II

This study case tested the effect of boundary conditions and compared multiple important flame parameters, e.g., flame geometry via CH* chemiluminescence and predicted Schlieren profiles, alongside experimental results without external electric fields. The experiments are available for the electric field case but not yet the simulation. This work examines the use of simulated experiments, rather than simulated flames, as the key comparator with experimental results.

GRI-Mech 3.0 from Smith et al. [1999] was used as the base mechanism for all neutral molecules and their reactions. The files containing the reaction parameters, transport properties and thermodynamic properties can be found from http://combustion.berkeley.edu/ . Detailed studies were performed on the validation of various chemiluminescence mechanisms by Panoutsos et al. [2009] and Kathrotia [2011]. The reaction parameters for excited species CH* were borrowed from Walsh [2000] and Hall et al. [2005]. Separate simulations were performed with both chemiluminescence mechanisms for comparison; however, Walsh [2000] was used as the baseline mechanism.

Numerical Validation

1. Temperature. Temperature profiles were predicted by the simulations with two different inlet velocity profiles. The differences between the non-uniform and the uniform velocity profiles are very subtle. Perhaps the only real difference is that a non-uniform velocity profile produces a slightly higher profile near the burner tube wall.

2. CH*. The peak CH* mole fractions calculated from the simulations were on the order of 5e-12. This is about 1 order of magnitude lower than the peak mole fractions experimentally obtained and computed by Walsh et al. [1998] and Walsh [2000] but the current flame is much smaller. Therefore, the CH* mole fractions shown in this study are reasonable.

A qualitative comparison between the simulated prediction of CH* and the experimentally obtained results was made. In both cases, the numerically predicted CH* profiles match well with the experimentally obtained profile. However, the non-uniform velocity profile shows a better spatial match, qualitatively. Specifically, the flame heights match better between the non-uniform velocity simulation and the experimentally obtained flame compared to the uniform velocity simulation. Also, the shape of the flame base-edge produced by the non-uniform velocity profile simulation matches qualitatively better with the experimental flame base-edge. In both simulated cases, the calculated flames sheets are thinner than the experimentally obtained flame sheets. Walsh et al. [2000] studied the effects of optics geometry (particularly the effect of f-number) on the Abel inversion results. Giassi [2017] expanded on this study and showed the effect of other excited species that could potentially emit light within the range of the light filters. Both cases, optical geometry and unknown chemiluminescence, result in broader flame thicknesses. A reasonable f-number of 5.6 and a narrow band filter (10 nm full width at half max) centered at 431 nm were chosen to minimize these effects. However, their contribution in the uncertainty of the experimental flame thicknesses should be noted.

3. Stoichiometric mixture fraction. Here, Cst (stoichiometric proportion) is tested with the numerical model to examine how well it matches with the visual marking considered to be the flame. CH* is the most logical marker for the reaction zone since it is what can most easily be seen (in most flame applications) by the human eye. Therefore, it makes sense to compare Cst with the CH* mole fraction profile. The CH* profile is found to lie just outside of the Cst line (on the oxidizer side). The Cst line stands about 0.1 to 0.2 mm from the peak mole fraction along the CH* curve. This is true everywhere except at the upstream leading edge of the flame. The edge of the flame diverges from the Cst line because the Cst is a property of non-premixed flames. Even though conical co-flow flames are considered non-premixed, the flame's edge contains many premixed flame characteristics because of the higher level of mixing occurring in this region.

The stoichiometric mixture fraction may not be a perfect marker for the CH* profiles but the spatial off-set distance (1/10th mm) is small enough for the theoretical simplification to be justified with typical experimental spatial uncertainty. Another test for the Cst line is to also compare it to the region of substantial local heat-release of the flame. Like the CH* comparison, the local heat-release is on the oxidizer side of the Cst line. The offset distance between the line and the peak locations along the heat-release curve is again on the order of 1/10th of a millimeter.

Schlieren Prediction

Schlieren imagery is an age-old technique with applications in many scientific disciplines. However, the difficulty in using schlieren is determining how to make quantified measurements. For instance, a schlieren image can be used to determine the location of a shock-wave formed by an extremely fast moving object through a fluid but acquiring measurements of temperature or density from the schlieren image is much more difficult to achieve because it requires derivatives of potentially noisy signatures that then amplifies the noise. Here, simple schlieren and light theory was applied to the numerical prediction of an axially symmetric co-flow flame in order to provide another form of validation to the OpenFOAM simulation and to see what the experimental schlieren images tell us about chemi-ion driven flows.

The simulated schlieren profiles showed good qualitative agreement with the experimental profiles. This positive comparison between measurement and calculation is important because it confirms the reliable prediction of the thermal field around the flame (i.e., the broader convective transport) in addition to the appropriate location of the reaction zone.

Effect of body forces

Simulations were performed on testing the effect of enhanced gravity on various non-premixed coflow flame parameters, e.g., flame geometry, flame tip height, flame base-edge height, CH* chemiluminescence, and schlieren profiles. While it cannot be expected that enhanced gravity will produce exactly what would be produced if chemi-ion chemistry and Maxwell's equations were employed, parallels can be drawn where applicable to assess the performance of enhanced body forces as the source of the observed flame/flow dynamics seen previously. Qualitatively the effect of enhanced gravity produces what was found to happen when external electric fields are used in experiments. That is, the flame height decreases slightly, the radius of the flame decreases slightly, the base of the flame increases significantly, and the peak mole fraction increases with increasing gravity. The gravity level at which point the flame could not sustain itself (extinction limit) was not exactly determined in this study, but as a general guide the flame was not

sustainable (blow out) around and above 3G. In all cases, the spatial comparison of simulated flame location with experimental results shows very good agreement.

The comparison of the flame's base height shows that the enhanced gravity levels between 1-2 times that of normal gravity could increase the base height to the same levels as seen with external electric fields. This increase in flame base lifting would increase the local mixing in this region which would be the cause of the observed increase in CH* light emission from the flame. This is seen to happen in the simulations, however, the percent increase in peak CH* mole fraction is much less than the percent increase in pixel light intensity from the CH* chemiluminescence images taken from the experiments. The incompatibility between the two results could be due to multiple causes.

1. the similarities between ion wind body forces and buoyancy forces are enough to explain transport but are unable to capture CH* chemistry, 2. the simulation is unable to capture the proper CH* mole fractions at enhanced gravity, 3. the simulations are predicting CH* correctly and the CH* experiments need to be quantitatively calibrated to ensure linearity.

The results of the predicted schlieren radius under different gravity levels also shows good correspondence. The peak axial velocity predicted by the OpenFOAM simulations under increasing gravity fields shows, as would be expected, the axial velocity increases, but only by about 40%. The velocity measurements underpredict what was suggested by the experiments using external fields. This finding seems reasonable in that thermally driven buoyancy is likely to be a more diffuse body force as compared to the more narrowly focused ion wind body force effect. While the overall influence is similar, the local acceleration will be more sensitive to streamline compression from the tightly directed electric field driven forces.

Future Work

While it is possible that experimental effects are partly responsible, the very significant uncertainties in chemical kinetics and the extremely low concentrations of excited species suggest that a quantitative comparison with computations is a major challenge.

Conclusions

The results showed that enhancing gravity was enough to explain nearly all the experimental observations, especially spatial variations in flame shape. The CH* peak mole fraction and peak velocity were found to have disparities when compared to the experimental results by significantly underpredicting the experimental results. It is not yet clear what is the reason for the difference. Thus, further studies should be made to clarify if the issue is in the hypothesis, the experiment, or the simulation.

(4) High Performance Computing Approach – Collaboration with LBNL

Previous experiences suggest that it will be difficult to couple the small concentration ions with the overall flow field in a numerical simulation. To have a better chance at accomplishing this coupling, we are exploring a highly adaptive mesh refinement approach pioneered at Lawrence Berkeley National Laboratory (LBNL).

Overview

The code under development at the LBNL uses AMReX, a software library containing the functionalities (written either in C++ and Fortran90) required to perform adaptive mesh refinement (AMR); the basic idea of this technique is that the governing equations can be solved, at each timestep, on a multilevel grid. In a multilevel grid, the mesh is refined at each level but only where it is needed (typically where high gradients occur), and the solution is recomputed only in these zones. This allows to refine the solution without having to recompute it on the entire domain, which saves time and computational costs. AMReX can solve problems with simple geometry in 2D and 3D, and in either Cartesian and cylindrical coordinates. The applications range would go from combustion to astrophysics and cosmology, from porous media to fluctuating hydrodynamics.

In this case study, we are interested in laboratory-scale experiments involving time-dependent open systems running at atmospheric pressure, in which the characteristic velocity of the fluid is much smaller than the speed of sound. The low Mach number conservation equations used were the ones proposed in M.S. Day and J.B. Bell [2000], with the addition of the Poisson’s equation and the electric field contribution in the mass, momentum, species, and enthalpy equations. In this regime, conservation equations take the form of a system of differential algebraic equations representing coupled advection-diffusion-reaction-electrostatic processes. These equations evolve subject to a constraint which is represented by the Equation of State (EOS) written in the form of a divergence constraint on the velocity; this constraint equation can be derived by differentiating the EOS in the Lagrangian reference frame of the moving fluid, and enforcing that here the thermodynamic pressure pEOS remains constant. The model used allows a ~ 1/Mach # increase (typically, 10-100) in the admissible timestep with respect to a fully compressible method.

Numerical Model

In such a stiff regime, chemistry and diffusion occur at faster timescales than advection; that is what imposes the restriction on the timestep. Subsequently, reaction-diffusion can be modeled implicitly, while advection requires explicit treatment. Furthermore, an explicit treatment of the Poisson’s equation introduces a severe limitation on the timestep, which is represented by the dielectric relaxation time.

The presence of an electric field has been modeled through a modified version of the Poisson’s equation, whose implicit coupling with the species diffusion fluxes ensures that the predicted electric potential is numerically consistent with the iteratively-lagged diffusion-induced charge separations. This procedure is necessary to eliminate the physics induced by the dielectric relaxation of unphysical numerically-induced charge separations.

To the best of our knowledge, an entirely implicit treatment of the charged species has not been implemented yet. Here, a fully implicit treatment of the drift fluxes of both ions and electrons in the low Mach number regime is introduced. The drift fluxes are then coupled with the diffusion fluxes, which have also been modeled implicitly.

The low Mach number combustion code (PeleLM; previously known as LMC) developed at LBNL is a finite volume code that implements the variable density projection in the low Mach number regime.

In order to test the new algorithm, a simple well-known configuration is considered, for which a lot of experimental and numerical results are available in literature. This configuration and algorithm is determined for a 1D premixed

methane/air flame, using a reaction mechanism from J. Hu et al. [2000] that includes neutral and charged species H3O+, HCO+, e-. The thermal and transport properties are based on GRIMech-3.0 and on the CHEMKIN-III database

Numerical results show that a flame is generated around ~ 0.3cm from the base, with a peak temperature of about 2200K. However, the applied electric field does not affect the flame temperature too much, so changes were not reported for the temperature profile. The focus of this study was, then, on the effects of the electric field on the most important charged species.

The time evolution of the electric field and electric potential for 1000V shows that the code captures the generation of plasma sheaths in the flame zone and at the outflow electrode: charges move to the electrode of opposite charge so they mask the effects of the electric field inside the domain. In fact, there is a strong electric field in the flame zone, but as time passes and charges move to the opposite electrode (ions to the left, electrons to the right) the electric field becomes almost zero inside the domain. Hence, the flame is charge neutral in that region.

Summary and Future Work

In summary, these preliminary results show that the code:

• correctly couples the different processed involved (advection-diffusion-reaction-electrostatic) ; • reproduces the physics associated with the formation of plasma sheaths.

Additional work is required in order to: • better manage the timescales of charged species transport; • further increase the timestep (up to 1e-6); • make the code more robust and suitable for AMR; • extend the code to 2D and 3D, in both Cartesian and cylindrical coordinates; • optimize the code to run on CORI/EDISON (tiling); • implement more complex geometry.

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Dissertations and Theses	Tinajero J. "Flame Dynamics and Chemi-Ion Flows Driven by Applied Electric Fields." Dissertation, University of California, Irvine, September 2017. , Sep-2017