Fiscal Year:	FY 2024	Task Last Updated:	FY 03/14/2024
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Project Title:	PeleLM CFD of Ion Driven Winds from Dif	fusion Flames	
Division Name:	Physical Sciences		
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Program/Discipline Element/Subdiscipline:	COMBUSTION SCIENCECombustion sci	ience	
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Space Biology Element:	None		
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Space Biology Special Category:	None		
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Comments:			
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No. of Bachelor's Candidates:		Monitoring Center:	NASA GRC
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Key Personnel Changes/Previous PI:			
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	The ultimate objective of this project is to comprehensively simulate the behavior of a small diffusion flame under the influence of an externally applied electric field in zero-gravity and to use PSI data to confirm the accuracy of that modeling. A detailed model will be used that includes the chemistry of charged ions and chemiluminescent flame intermediates to capture any feedback between ion-driven convection and combustion behavior, and to allow quantitative comparisons with experimental measurements. To date, the capability of accurately simulating electric field flames has eluded researchers because the system exhibits dramatic ranges of coupled temporal and spatial scales. Moreover, in earth gravity the hot combustion products are subject to buoyancy effects that are difficult to isolate from those generated by the electric field. We propose implementations to an existing powerful simulation framework (PeleLM) for this problem, and to use the PSI data set from E-FIELD Flames for validation of the model and		

Task Description:	PeleLM is a state-of-the-art reacting flow code tailored with a unique integration scheme that efficiently couples high-speed processes with he slower evolution of the flow structures using the adaptive mesh refinement (AMR) structs. This project is to improve the ion chemistry (particularly employing reduced chemical mechanisms available in the published literature) to generalize the electric field configurations in PeleLM, and to then simulate zero-g collow flames in the E-FIELD Flames dataset. Comparisons include V-1 (voltage-ion current) curves and flame shapes (deduced from CH ^a images), varing with fluel types, compositions and flow rates. The data includes step function changes in voltage that can be used to evaluate the time response of the flame. It is important to also consider the impact of image and ion current collection timescales, which will be critical for model validation. The work takes advantage of the unique E-FIELD Flames data, measured in microgravity, to validate the proposed PeleLM model augmentations, to permit a detailed investigation of the ion dynamics under the influence of electric field forcing to affect thermal transport and sooting in diffusion flames. Once the simulation is validated against the zero-g data, it will be possible to further extend the simulations to flames in earth gravity, where potential applications for improved heat release and emission reduction can be explored. This utilization of zero gravity data from the E-FIELD Flames experiment was conceived and directed to create a data set that would permit the detailed assessment of the effects of ion-driven winds and charged species chemistry on non-premised flames. A microgravity environment is required because the forces of ion driven winds and of gravity driven buoyancy winds are too close in magnitude to effectivel segmante their effects with any carth-gravity experiments where analyal convection is a significant contributor to the combustion process. This rationale has been provoe of yetartions over sin month
Rationale for HRP Directed Research	:
Research Impact/Earth Benefits:	Once the simulation is validated against the zero-g data, it will be possible to further extend the simulations to flames in Earth gravity, where potential applications for improved heat release and emission reduction can be explored. This utilization of zero gravity data from the E-FIELD Flames experiment for beneficial purposes on Earth and for a better understanding combustion control is compatible with the NASA objectives.
	As in the above objectives listing, this year has major aspects of establishing the 1-g laboratory microgravity image data that resemble the International Space Station (ISS) conditions, testing the previous reduced mechanism in 1-g condition (which was tested in microgravity condition), and modifying the new reduced mechanism (with charged and excited species) with implementing the PeleLM computational fluid dynamics (CFD) code for simulating flames under the influence of an electric field. This year, progress has been made on all the items (1-5) with 3 & 5 nearly completed. Specifically, the progress includes: Computational Modeling Verification (with and without electric fields) — This task continues from the previous computational modeling effort in 0g ISS condition of E-FIELD Flames using a reduced mechanism to predict ion concentrations in flames and the effects of ion driven winds in coflow. The focus is to simulate in gravity condition, and observe how the CFD simulation captures the difference between microgravity, using the E-FIELD Flames Physical Sciences Informatics (PSI) dataset for effective validation of the computational models and 1g experiments. Experiment in 1g using ISS condition — This test is to establish the in-laboratory experiments similar to the conditions on the ISS, and validating the results of the computational models described above.

include in the computation is essential and the most challenging. This task is to find the best scientific method to include more charged species and excited species implementation into the CFD simulation with appropriate reduced chemistry to ensure robust simulation capability.

The previous PeleLM simulation computation capability validation using pressurized conditions also continues. Further details of the project progress through the second year in both the experimental and computational aspects are described in the following.

PeleLMeX Computations - Computational Results and Discussion

The progress in the PeleLM computational aspects of the project are described in a series of conference papers provided in the publication section of this report and in a recent publication (Chien, et al., 2023). [Ed. Note: See References and Cumulative Bibliography.] Much of the work has so far concentrated on the cases without an electric field in order to assess the complications of the code implementation, its conversion to cylindrically symmetric geometry, to identify the choice of reduced models, and to ensure that the boundary conditions are appropriate to simulate an extruded fuel tube.

Using PeleLM with various pressures and fuel dilution with different species - no electric field

This part of the progress investigates high pressure methane diffusion flames with water addition, in comparison to CO2 addition using PeleLM simulation (see reference). The study used the same geometry coflow burner as for E-FIELD Flames but examined its behavior under the pressure conditions of previous tests of water addition simulation. This work is to study the behavior of a methane diffusion flame with various amounts of water vapor and CO2 added to the fuel and to compare the flame behavior with various percentages of water vapor and CO2 content (0% to 65%). It provides the detailed temperature, CO, and CO2 and other species concentration distribution using the PeleLM adaptive mesh refinement (AMR) code. This work uses a coflow burner in PeleLM for simulating of the flame jet by computing the combustion behavior. The flame was simulated to pressures of 1.0, 1.4, 5.7, and 11.1 atm. The results extracted and analyzed include temperature profiles and various species mole fractions compared with their equilibrium state.

Regarding physical properties, both water and carbon dioxide present similar behaviors. At atmospheric pressure and high water content, the flame lifts off from the burner tip, while as the pressure rises the flame anchors back near the burner tip. In contrast, CO2 addition does not lift the flame from the burner tip. As pressure rises, the flame width reduces. Both water and CO2 addition decrease the flame peak temperature. This artificial horizontal expansion highlights the narrowing of the flame with changes in pressure while much smaller change is visible with changes in diluent fraction. There is also relatively limited effect of diluent composition as the thermal images of flames diluted with water and carbon dioxide are very similar under similar pressure and dilution conditions.

In order to provide more structure details, the mole fraction of oxygen, water, carbon dioxide, and carbon monoxide in the different conditions of the flames along the radius of the burner is observed. In both cases, the temperature profile follows the same path as water and carbon dioxide respectively. The maximum mole concentration of CO2 and CO were also investigated for all conditions. For the water addition, the CO2 and CO have an increase of maximum concentration when pressure rises. From 1 to 1.4 atm, there is a decrease in the maximum concentration of CO. As for the CO2 addition, there is an increase of CO in all conditions. H2O and CO2 concentration profile was also compared for all the conditions along the centerline of the diffusion flame. The rise of pressure produces an increase of water concentration approximately 0.4-0.6 mm from the burner, and it is observed that the water concentration decays slower than at lower pressure conditions. The addition of water and carbon dioxide has similar results on the flame behavior. Future work will include an analysis of existing high-pressure experiment results and the superequilibrium prediction for the species (H and O) at different pressures.

These details show that the PeleLM framework is able to capture the proper boundary conditions even though the absolute geometry is slightly different because the experiment has a slightly extruded fuel tube and the simulation has a flat inlet. The flow inlet is varied to approximate the conditions expected for the extruded case. Further results appear in all of the conference presentations and publications listed in the publications section of this report.

Preliminary Results 1g Electric Fields using ISS conditions - PeleLMeX

The PeleLMeX computation of this research is implemented on the UCI High Performance Community Computing Cluster (HPC3) running on Linux 8.6. Its aim is to boost the effectiveness of simulations by utilizing a considerable number of cores. To handle user admission and resource allocation, the cluster employs entities like login nodes and the Slurm scheduler.

The goal of this project is to use the reduced mechanism Donzeau et al. (2023, see reference) tested for microgravity condition with a newer version of the PeleLMeX as well as newer HPC3 hardware. This work initiated with reproducing the behavior of the coflow burner used in the ISS. The primary distinction between the numerical and experimental setups lies in the extruded fuel pipe. As the PeleLMeX code has not integrated the extruded geometry, it is unable to replicate the impact of the fuel pipe on the inflow velocities or temperature. The effect of the extruded tube is simulated using a customized inlet velocity profile. The primary assumption is that the Low Mach number regime is in effect. It is acknowledged that the velocities will remain within this regime. This is a widely accepted hypothesis in the study of combustion and was validated at the conclusion of the simulations. The chosen hypothesis pertains to the chemistry model. The mechanism was selected, comprising 26 species and 134 reactions. The project's goal is to validate or invalidate this chemical mechanism's efficacy in describing the E-FIELD experiment.

The simulation initiated with 15 and 19 cm/s fuel flow velocity with 3.1 cm/s coflow air with 300K initial temperature with CFL 0.1. This case without the electric field can help explain the operation of PeleLMeX. Moreover, the cases without electric field are distinctive for its shorter compilation time due to the reduced number of equations/species to be solved resulting from the deactivation of the electric field. The results depict the OH concentration in flames at different velocities. A comparison between these findings and the Abel inverse transform of the experimental flames is also conducted. A distinctive shape is observed for both flames with a reasonably uniform distribution of OH. The normalized colorbar facilitates comparison of concentrations. A greater concentration of OH is found in the 19 cm/s flame, which is expected due to the increased velocity leading to higher OH emission Into the flame. This effect is also apparent in the experiment in the following paragraphs. For an inlet velocity of 19 cm/s, velocity increases exponentially with respect to Y position. The velocity at y=0 is 19 cm/s and the maximum velocity of the mixture exceeds 86 cm/s, which is well above the flame. Velocity within the flame ranges between 19 and 35 cm/s.

For these simulations, the electric field implementation is in operation, requiring the use of HPC3, a supercomputer, due

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	to its substantially longer computational time. Multiple convergence difficulties emerged during these simulations. The resolution is no longer straightforward, and there are residual values that struggle to converge during the solution of the Newton's equations. To resolve these issues, the input includes a constant time step of 10E-6 seconds. Boundary condition issues on the cathode and anode are resolved by utilizing a Dirichlet condition in the X direction and a Neumann condition in the Y direction. To clarify, the Neumann condition is a flux condition, while the Dirichlet condition enforces a specific temperature at the boundary. After resolving these matters, we determined the necessary computation time to achieve a stable state. With the use of the electric field method, it takes 1 hour and 10 minutes to reach 1000 steps, in contrast to 3 minutes without it. Additionally, the preceding section illustrates that a stable state is achieved in the simulation within 60 milliseconds in simulation time. With the electric field, 1,000 steps correspond to a maximum of 10E-4 seconds. This requires over 30 days of consecutive simulations on the supercomputer to attain a steady state. Due to time constraints, the initiated simulations did not reach a steady state but are still being computed. Nonetheless, it is still possible to observe the variation in temperature profile between, with and without the electric field.
	1g in-laboratory experiments
	The 1g in-laboratory experiments include a coflow burner, rotameters for fuel and air, and a high voltage power supply (Trek 609A) with shunt current resistance for measuring ion current. The details of the experiment setups are described in Chien et al. (2018) Energies 11(5), 1235 and Chien et al. (2019) Combust. Flame 204(250-259). The mesh is set at 27 mm height above the burner. The data collected includes ion current to applied voltages, natural flame images using a Nikon D90 camera, and also OH* imaging from a PI-MAX 4 (Princeton Instruments).
Task Progress:	The measurements are made with two fuel flow speeds, 15 cm/s and 19 cm/s, performed with $d = 37$ mm and airflow of 3.1 cm/s. Positive and negative electric fields are tested and analyzed. These results indicate that a positive E-FIELD leads to the appearance of three regions. In the sub-saturation region, ion current increases with applied voltage until it reaches a plateau, known as the saturation region, which is reached at around 1.65 kV/cm for each flame speed. Finally, there is a final increase in ion current at around 2.2 kV/cm in the supersaturation region. For the negative electric field, a plateau is reach around 0.6 kV/cm. However, it's important to note that the presence and magnitude of the ion current in these flames may not provide a direct or straightforward indication of combustion efficiency.
	Several factors can influence the ion current, making its interpretation more complex. Ionization processes are heavily influenced by temperature. The degree of ionization tends to rise with hotter temperatures. In a non-premixed flame, temperatures can fluctuate significantly within the combustion zone, resulting in regions with varying ionization levels. Regions with higher temperatures in the flame may display greater ionization and subsequently a higher ion current. This fluctuation in temperature poses a challenge to using ion current as a direct measure of combustion efficiency.
	The flame visualization is captured by camera of each data point presented and related to the current–voltage curve (IV curve). There are four cases, two pertaining to speed and two to electric field.
	When an electric field is positive, the flame tends to increase in width and appear bluer, indicating there is more air entrainment into the diffusion flame reacting with the fuel. Therefore, electric field can control the efficiency of the flame. Electric fields can indirectly accelerate the movement of ions and charged particles within the flame. This increases the ionization rate of the flame, promoting the formation of more ions. The increased ionization tends to enhance combustion by improving the mixing of fuel and oxidizer, which can result in a broader, more stable flame. The flame appears bluer, which is often associated with a higher combustion temperature and a more complete combustion process. Flames have an optimal or stoichiometric fuel-to-air ratio at which they burn most efficiently. This is the ideal balance of fuel and oxidizer that results in complete combustion.
	Next, we observe how the introduction of electricity affects the formation of soot in the diffusion flame generated by the coflow burner. To increase the amount of soot particles in the flame, a high flow rate of methane up to 65 mL/min was utilized. Specifically, the fuel employed was CH4; using ethylene, for example, could result in even greater soot emission, which is why the flow rate was increased. Due to their yellow color, it is easier to track the greater volume of soot that results from the higher flow rate. A Nikon D90 camera was employed with the following settings: ISO 100, f/4.5, and a shutter speed of 1/10s. A positive electric field increases the velocity of the flame, causing it to go from 15,20 cm/s to over 100 cm/s. As a result, the soot residence time decreases and the amount of soot in the flame decreases as well. When a negative electric field is applied, the prevailing airflow towards the burner surface lengthens the time that soot particles spend in the flow, thus promoting soot accumulation. Results of this case were not taken with a higher flow rate since the previous negative field images have shown an increase of the soot volume in the flame.
	The OH chemiluminescence images are captured and Abel inverted to reveal the local non-integrated chemiluminescence within the reaction sheet. While the quantitative value of the concentration of OH* cannot be determined, a qualitative comparison of the location of this excited species is possible after normalizing all the flame pictures. This information will be used for initial comparison with the computation results.
	To analyze the variation in width with changes of electric field strength, a simple imaging method is used. This analysis is comparing the flame width variation with no a flame with no electric field applied. Wb is the width of the flame and Wb,0 is the width without electric field. The results are analyzed for the positive field for the two fuel flow speed. The result shows 3 sections for the width of the flame, similar to the ion current. It follows the IV curve, showing the first sub-saturation, the saturation zone, and then supersaturation. For a flame of 19 cm/s the width increases compared to Wb,0 but for the 15 cm/s flame the flame width decreases compared to Wb,0 but increases with the electric field. The use of an electric field is connected to stoichiometry. In slower flames, it decreases the initial width and then broadens it later. Conversely, higher velocity flames tend to expand beyond their initial width. A further analysis for the increase in flame width is in the sub-saturation zone for the two flowrates are also plotted with their linear regression. This may provide a means of comparing the development of flame width in relation to the electric field between the experiment and the simulation, particularly for the sub-saturation region.
	Comparison between simulation and experiments
	An initial comparison of the OH chemiluminescence and the OH species from the computation specifically for flame widths for both flame velocities are conducted. While we understand that the amount chemiluminescence is small and yet to be simulated, we would like to observe based on what we can get from the experiments and results from PeleLMeX. An example of images can present the comparison of (a) a flame from the experiment and (b) a simulated OH, both with a velocity of 19 cm/s and an electric field of 0 kV /cm.

The discrepancy in flame appearance is due to the scale, which may be misleading. At a similar scale, the experimental

	flame measures 3.15 mm, while the simulation displays a flame of 2.8 mm, resulting in a 11% error to the experiments. Although this may appear significant, uncertainties in measuring the experimental flame width must be considered. Even a slight variation in air flow during image capture can affect the width of the flame. Furthermore, the camera calibration has a relative uncertainty of 0.5 mm. A summary Table 1 of flame widths between the simulation and the experiment is presented.
	OH* and OH are situated in the reaction sheets closed to each other (although the analysis is qualitative), while the flame width are closely within 10% difference. To fully authenticate the chemical mechanism, the next step is to compare the experiment and the simulation within the context of an electric field flame.
	The work is currently being carried out on a local high performance computing cluster, but there are limited hours available for that system so additional computational resources will be explored. Further results appear in the conference presentations and publications identified in that section of this report.
	Preliminary Outcome for 0g implementation with more species - PeleLMeX
	To bridge the gap between simulation outcomes and empirical data, this part of the work is to evaluate potential mechanism candidates: (A) 30 species and 86 reaction using Coffee mechanism as foundation (1993) by Pederson and C. Brown, (B) 26 species and 134 reactions but only 4 ionic species using GRI Mech 3.0 by Renzo et al., and (C) the recent published 45 species and 216 reactions using San Diego reduced mechanism, by López-Cámara et al This task is to implement the recently published reduced San Diego mechanism in microgravity. These mechanisms are chosen for their comprehensive coverage of ionic and exited species within the flame compared to the mechanism currently used by Renzo et al. which is not able to capture the ion current behavior in microgravity condition as part of work from the previous fiscal year.
	The main difference lies in the (C) reduced San Diego mechanism chemical model which includes 11 charged species, including H3O+, HCO+, C2H3O+, CH5O+, O2-, OH-, e-, CO3-, CHO2-, O-, and CHO3- (in comparison to the previous used (B) H3O+, HCO+, O2- and e-) and included excited species CH and OH. This mechanism includes many species and as the electric field is introduced the calculation became extensive and the computation time increased substantially. With various tests and approaches for launching the mechanism at various stages, the simulation remains computing with extended calculation time, unresolved and/or unstable with inconsistent results. The heat release from the calculation can be massive at a single cell and that can lead to a relatively large local flow, and/or the chemical solver may fail to sort through the reaction and lead to confusion. Further tests on the mechanism particularly on sorting through how the solver processes each step in the calculation, as well as how the mechanism works with a relatively newer version of the simulation is needed.
	Conclusions
	The modeling work are progressing with the newer version of PeleLMeX using the same reduced mechanism in gravitational environment. The experiments are conducted, and data are measured using ISS conditions. Locally with PeleLM non-subcycling version, the code has also continued to be exercised under different coflow flame conditions with different levels of fuel dilution with carbon dioxide and different pressures to demonstrate the validity from the previous work with water addition of the boundary condition implementation. Challenges remain for implementing a relatively large newer mechanism including more ions and charged species into the newer version of PeleLMeX. Continuing work on this project focuses more heavily on the computations with detailed assessment of the ion current prediction and the role the chemical mechanism plays in that prediction.
	References:
	Esquivias, B., Girodon, H. and Chien, YC. (2023)."A Comparison Between Water Addition and CO2 Addition to a Diffusion Jet Flame," abstract 263, International Colloquium on the Dynamics of Explosions and Reactive Systems, Siheung, Korea, July 23-28.
	Donzeau, M., Esclapez, L., Day, M. S. and Chien, YC. (2023). "Recent Progress on Numerical Modeling for Microgravity Electric Field Flames Results," 13th U.S. National Combustion Meeting, March 19-22, 2023, College Station, Texas.
	Invited Technical Lectures/Presentations for this PSI Project:
	National Academies of Sciences Speaker, "Sustainability & ADEI – Research Scientist in Higher Education Academic Setting", and Early-Career Panelist for the Committee on Biological and Physical Sciences in Space (CBPSS), Space Science Week 2023, Washington D.C., March 29th, 2023 (this project was presented).
Bibliography Type:	Description: (Last Updated: 02/05/2025)
Abstracts for Journals and Proceedings	Deu Morel R, Day M, Chien Y-C. "Investigation of mechanisms for microgravity ion-driven wind using simulation." 39th Annual Meeting of the American Society for Gravitational and Space Research, Washington, DC, November 13-18, 2023. Abstracts. 39th Annual Meeting of the American Society for Gravitational and Space Research, Washington, DC,
	November 13-18, 2023. Graduate poster presentation., Nov-2023
Abstracts for Journals and Proceedings	Chien Y-C et al. "Electric field flames 1g experiment validation for PeleLMeX simulation using microgravity conditions." 39th Annual Meeting of the American Society for Gravitational and Space Research, Washington, DC, November 13-18, 2023. Abstracts. 39th Annual Meeting of the American Society for Gravitational and Space Research, Washington, DC, November 13-18, 2023. Graduate poster presentation. , Nov-2023
Articles in Other Journals or Periodicals	Esquivias Rodriguez B, Chien Y-C. "A comparison between water addition and CO2 addition to a diffusion jet flame." Combustion Science and Technology. International Colloquium on the Dynamics of Explosions and Reactive Systems (ICDERS) Special Issue, under review as of March 2024. , Mar-2024
Dissertations and Theses	Dru L. "Electric field flames 1g experiment validation for PeleLMeX simulation using microgravity conditions." M.S. Thesis for Engineering Internship from ISAE-ENSMA, University of California, Irvine, 2023. , Dec-2023

Dissertations and Theses	Deu Morel R. "Simulating microgravity E-FIELD flames using a mechanism including chemiluminescence species." M.S. Thesis for Engineering Internship from ISAE-ENSMA, University of California, Irvine, 2023. , Dec-2023
Papers from Meeting Proceedings	Chien Y-C, Donzeau M. "Recent progress on microgravity E-FIELD flames and simulation." 19th Annual AIAA Southern California Aerospace Systems and Technology (ASAT) Conference, May 20, 2023, Irvine, California. Abstracts. 19th Annual AIAA Southern California Aerospace Systems and Technology (ASAT) Conference, May 20, 2023, Irvine, California. , May-2023
Papers from Meeting Proceedings	Dru L, Chien Y-C. "Electric field flames 1g experiment validation for simulation." University California Irvine Combustion Institute-Summer School (UCI CI-SS), Irvine, CA, August 20-25, 2023. Abstracts. University California Irvine Combustion Institute-Summer School (UCI CI-SS), Irvine, CA, August 20-25, 2023. Unofficial poster session. , Aug-2023
Papers from Meeting Proceedings	Deu Morel R, Day M, Chien Y-C. "E-Field flames simulation in microgravity." University California Irvine Combustion Institute-Summer School (UCI CI-SS), Irvine, CA, August 20-25, 2023. Abstracts. University California Irvine Combustion Institute-Summer School (UCI CI-SS), Irvine, CA, August 20-25, 2023. Unofficial poster session. , Aug-2023