Fiscal Year:	FY 2023	**Task Last Updated:**	FY 04/26/2023
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Project Title:	PeleLM CFD of Ion Driven Winds from 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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Comments:			
Project Type:	GROUND,Physical Sciences Informatics (PSI)	**Solicitation / Funding Source:**	00-HEDS-02
Start Date:	01/20/2022	**End Date:**	01/19/2024
No. of Post Docs:	2	**No. of PhD Degrees:**	
No. of PhD Candidates:		**No. of Master' Degrees:**	2
No. of Master's Candidates:	1	**No. of Bachelor's Degrees:**	
No. of Bachelor's Candidates:		**Monitoring Center:**	NASA GRC
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Flight Program:			
Flight Assignment:			
Key Personnel Changes/Previous PI:			
COI Name (Institution):	Dunn-Rankin, Derek Ph.D. (University of California, Irvine)		
Grant/Contract No.:	80NSSC22K0364		
Performance Goal No.:			
Performance Goal Text:			
	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 investigation of the complex coupled system. PeleLM is a state-of-the-art reacting flow code tailored with a unique integration scheme that efficiently couples		

Task Description:	high-speed processes with the slower evolution of the flow structures using the adaptive mesh refinement (AMR) strategy. 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 coflow flames in the E-FIELD Flames dataset. Comparisons include V-I (voltage-ion current) curves and flame shapes (deduced from CH* images), varying with fuel 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 fields, and to evaluate the subsequent interactions with non-charged species, as well as to assess the potential 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 for beneficial purposes on earth and for a better understanding combustion control is compatible with the NASA objectives. 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-premixed 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 effectively separate their effects with any earth-gravity experiments where natural convection is a significant contributor to the combustion process. This rationale has been proven out by the E-FIELD flame experimental data now available as part of the PSI website. The Electric Field Effects on Laminar Diffusion Flames (E-FIELD Flames) experiment was completed in 2018, and with nearly 150 hours of operations over six months and the ignition of 250 electric field flames on the ISS, it was a very successful measurement campaign. The experiment aspect of this project is to extract and assemble a data portfolio that is ideally suited for validating numerical simulations. The simulation aspect of the project employs the PeleLM framework developed in the Lawrence Berkeley National Laboratory (LBNL), and recently transitioned to the National Renewable Energy Laboratory (NREL). This open-source code is for evolving chemically reacting flows at low Mach number with block-structured adaptive mesh refinement (AMR) using the AMReX library. It is the extension of this code that we exploit for comparison with E-FIELD Flames data, with the ultimate goal of understanding and then controlling hydrocarbon flames under the influence of electric fields. Control of combustion using electric fields has for decades been proposed for extending flammability limits, reducing emissions, and preventing instability and blowoff, as well as modifying soot production. Implementation of the concept has been difficult, however, because of the complex coupling between buoyant driven flows, ion production in the flame, ion acceleration by the electric field, and the resulting forces on the neutral gas. With an efficient and accurate simulation capability, it will be possible to explore temporal and geometric variations of the electric field to manipulate flames in a wide range of beneficial ways. Hence, the specific aims and objective of this project include: (1) Access, extract, and analyze ion current, voltage, and flame images from the PSI data base to serve as the benchmark microgravity data set for nonpremixed flames under the influence of an external electric field. (2) Modify PeleLM CFD software to approximate the physical boundary of an extruded tube coflow burner geometry with cylindrical symmetry (3) Extend PeleLM CFD software to include electrodynamics in the two-dimensional circular symmetric system (4) Implement PeleLM CFD with a reduced chemical mechanism that includes charged and excited species (5) Verify the fidelity of the PeleLM simulation of flames under the influence of electric fields by direct comparison with E-FIELD Flames data (6) Demonstrate validated PeleLM simulations of microgravity flames in steady conditions and during unsteady transitions in response to changes in the external electric field
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 can be seen from the objectives listing, this project has two major aspects, one associated with selecting and preparing an appropriate experimental data set, and the other with modifying and implementing the PeleLM computational fluid dynamics (CFD) code for simulating flames under the influence of an electric field. In the first year, significant progress has been made on items (1-4), with items (2) & (3) fully completed, and times (1) and (4) substantially completed. Specifically, the progress includes: Experimental Data (selection and analysis)--There are two major components of our using the E-FIELD Flames PSI dataset for effective validation of the computational models. First is the evaluation and regularizing the main features of the flame that will be used for the comparison. Second, is the selection of which data will serve as the baseline canonical dataset for comparison of computational findings. Computational Modeling (with and without electric fields)--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 reduced chemistry, including first modeling the same burner geometry (but without electric fields) to ensure robust simulation capability. Further details of the project progress through the first year in both the experimental and computational aspects are described in the following. Experimental Results and Discussion The experimental results and discussion part of the work (Chien, et al., 2022) described the preparatory and initial measurements of diffusion flames under the influence of an electric field aboard the International Space Station (ISS), as part of the Advanced Combustion via Microgravity Experiments (ACME) project. [Ed. Note: See References below and the Cumulative Bibliography in this Task Book record.] Intended as the foundation publication for the experimental

effort, the work comprehensively included the space experiment methods, the capabilities of the ACME insert, experiment procedures, data, and limitations and constraints. The measurements presented included images and ion currents of small diffusion flames of methane (in air), subjected to a ramping electric field in microgravity. While there have been prior microgravity studies of Electric Field Effects on Laminar Diffusion Flames (E-FIELD Flames) using a drop tower, the published measurements represented the first mapping of the effects of an ion-driven wind on flame behavior under an electric field in the absence of the confounding influences of buoyancy. The paper described the challenges of remote measurement and manipulation of flames on the ISS and presented preliminary results from the first set of coflow flames. The results showed clearly that the flame is most compact at saturation while the measured voltage-current characteristic (VCC) curve demonstrates parabolic behavior after saturation which differs from observations in 1 g on Earth (shown in Chein, et al., 2022, figure 6). The flame images in microgravity of methane coflow conditions (in Chien, et al., 2022, figure 9) corresponding to the same comprehensive set of results. Identifying these images is nontrivial because the camera time stamp is not directly coincident with the scalar data information. Hence, one of the key accomplishments has been the linking of these two disparate data outcomes into a single unified comparison set. The flame images with different fuel flow rates 19 or 15 cm/s, and concentrations at 100%, 70% and 40% also show how different flames can look while still producing the same ion current as shown in Chein, et al., 2022 figure 11. The above scientific results provided the information that permitted the selection of 70% methane 30% nitrogen with a positive electric field applied as the most distinct condition to serve as the first comparison data set for the modeling.

The PSI data set is complete and the tools for extracting images and scalar data from that data set are achieved. Evaluating all of the different conditions showed that the 70% methane fuel case, with a positive electric field has the most consistent and distinct features while also providing a complete range of field strengths to use as the first comparison data set for the modeling efforts. The experiments also highlight the very clear first peak (called the acme point in Chien, et al., 2022) where the ion current reaches a saturation apex before decreasing, which is distinctly different from what happens in 1-g Earth gravity where a saturation plateau is seen. It is this feature that provides the clearest challenge to the computational model – to both demonstrate the validity of the model and to explain the physical processes that lead to this distinct acme point behavior in zero-g.

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 a recent publication (Chien, et al., 2023). 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.

(a) Using PeleLM with various pressures and fuel dilution – no electric field

This part of the progress investigates high pressure methane diffusion flames with water addition using PeleLM simulation. The study used the same geometry coflow burner as for E-FIELD Flames but examined its behavior under the pressure conditions of previous ground-based experiments. This work provides a comprehensive preliminary understanding of how combustion changes when dilution (water vapor in this case) is introduced into the fuel flow from 0% - 60% mole fraction. It provides the detailed temperature, CO, and CO2 concentration distribution using the PeleLM adaptive mesh refinement (AMR) code. The results showed that the peak temperature in the flame reduces with water addition and increases with pressure increase. The general conclusion is that the pressure influence dominates over the dilution effect. This computational result helps to understand the scope of change when dilution is introduced into the high pressure flow and helps the next step of experiment planning (for possible future high pressure zero-g combustion studies). An example of these results appears in Chien, et al., 2023, figure 4.

Task Progress:

This work concludes that the pressure has the most dominance over the water dilution conditions, while the flame is observed to lift at the 60% limit close to extinguishment. The work also plots the peak concentration of the species CO2, CO, O2 and OH at atmospheric pressure, to observe the relationships not only on OH + CO -> CO2, but also the O2 peak value change with the increase of dilution with water. The peak value of CO2 does not change throughout all the conditions but OH and CO are both decreased. O2 peak value remains similar with water dilution. Therefore, further analysis on how water vapor addition affects or participates in the reaction particularly on hydroxyl, carbon monoxide, water, and carbon dioxide is needed for understanding the influence from water addition, while the role of elevated pressures remains significant with the density change.

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.

(b) Preliminary Results including Electric Fields - PeleLMeX

The first step was to select the conditions most appropriate for comparing simulations with experiments. The selected case from the 70% methane coflowing with air conditions starting from the acme point, already identified above as the 70% positive field situation. The first results of a zero gravity flame simulation with temperature plot, and the flame is subjected to an electric field influence is computed. The simulation shows clearly that the electric field pulls the flame upward and narrows it as would be expected. The detailed comparison of the ion current with the calculated ion current has the same order of magnitude but is not yet quantitatively matching. There are many avenues yet to explore, including the reduced chemistry mechanism. The current work is using the only published reduced mechanism for ions but that reduced mechanism was created for turbulent flames and may not provide the best performance for laminar flames. Continued work is needed on identifying the best mechanism to use. Another challenge with the simulations is the computational time needed. 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.

Computational Conclusions

The computational progress has been substantial, with the conversion of PeleLM to a version that functions in cylindrical symmetry and one that includes the appropriate equations for the electric field and the ion mobility in that field (PeleLMeX). The code has also been exercised under different coflow flame conditions with different levels of fuel dilution and different pressures to demonstrate the validity of the boundary condition implementation, the ignition and steady state achievement in the code, and the capability of simulating an extruded tube geometry with a flat boundary by adjusting the inlet flow profile.

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.

Reference:

Chien, Y.-C., Stocker, D., Hegde, U. and Dunn-Rankin, D. (2022) "Electric-Field Effects on Methane Coflow Flames Aboard the International Space Station (ISS): ACME E-FIELD Flames," Combustion and Flame, Vol. 246. DOI: 10.1016/j.combustflame.2022.112443

Chien, Y.-C., Girodon, H., Esquivias Rodriguez, B. (2023), "Modeling of elevated pressure diffusion flames with water addition," Combustion Science and Technology, Special issue of ICDERS 2022. doi: 10.1080/00102202.2023.2182205

Invited Technical Lectures/Presentations for this PSI Project:

1. 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).

2. Technical talk and dinner at SWE Holiday Soirée (Society of Women Engineer – Orange County), Microgravity E-FIELD Flames Aboard the International Space Station (ISS): Research, Education and Embracing Diversity," Irvine, California. December 8th, 2022.

3. Seminar in Institute Pprime - CNRS/ISAE-ENSMA (Centre national de la recherche scientifique - Institut P', Université de Poitiers – ISAE-ENSMA), Microgravity E-FIELD Flames on the ISS and Gas Hydrates for Combustion Research, November 24, 2022.

4. Seminar in ICARE - CNRS Orléans Campus (Centre national de la recherche scientifique - Institut de Combustion, Aérothermique, Réactivité et Environnement), Microgravity E-FIELD Flames on the ISS and Gas Hydrates for Combustion Research, Orléans, France, November 18, 2022.

5. Seminar for SIRiPods (Samueli Interdisciplinary Research in Pods) Junior Engineering Students at University of California, Irvine, hosted by Christine King — My Research Experience for E-FIELD Flames: Experiment Operation on the ISS from Earth, August 10, 2021.

6. Guest Speaker for the EXpanding Communities and Encouraging Leadership (EXCEL) students, 1st and 2nd year STEM undergrads in Bio/Chem at University of California, Irvine, hosted by Dr. Harris, the Director of CAMP, February 16, 2021.

Bibliography Type:	Description: (Last Updated: 03/20/2024)
Abstracts for Journals and Proceedings	Chien Y-C, Dunn-Rankin D. "Recent progress in preparation for PeleLM CFD of ion-driven winds from diffusion flames." 37th Annual Meeting of the American Society for Gravitational and Space Research, Baltimore, MD, November 3-6, 2021. Abstracts. 37th Annual Meeting of the American Society for Gravitational and Space Research, Baltimore, MD, November 3-6, 2021. Selected PSI project, Combustion 3 short talk. , Nov-2021
Abstracts for Journals and Proceedings	Esquivias B., Girodon H, Chien Y-C. "A comparison between water addition and CO2 addition to a diffusion jet flame." 29th International Colloquium on the Dynamics of Explosions and Reactive Systems, Siheung, Korea, July 23-28, 2023. Abstracts. 29th International Colloquium on the Dynamics of Explosions and Reactive Systems, Siheung, Korea, July 23-28, 2023. Abstract 263. , Jul-2023
Abstracts for Journals and Proceedings	Esquivias Rodriguez B, Girodon H, Chien Y-C. "Numerical simulation of water-vapor addition into a laminar diffusion methane/air flame at elevated pressures using PeleLM." 39th International Symposium on Combustion, Vancouver, Canada, July 24-29, 2022. Abstracts. 39th International Symposium on Combustion, Vancouver, Canada, July 24-29, 2022. Work-in-Progress poster 2P092. , Jul-2022
Abstracts for Journals and Proceedings	Chien Y-C, Stocker D, Hegde U, Dunn-Rankin D. "Microgravity E-FIELD flames results on CH4/air coflow burner." 39th International Symposium on Combustion, Vancouver, Canada, July 24-29, 2022. Abstracts. 39th International Symposium on Combustion, Vancouver, Canada, July 24-29, 2022. Work-in-progress poster 2P091. , Jul-2022
Articles in Peer-reviewed Journals	Escofet-Martin D, Chien Y-C, Dunn-Rankin D. "PLIF and chemiluminescence in a small laminar coflow methane-air diffusion flame at elevated pressures." Combust Flame. 2022 Sep;243:112067. https://doi.org/10.1016/j.combustflame.2022.112067 , Sep-2022
Articles in Peer-reviewed Journals	Chien Y-C, Stocker D, Hegde U, Dunn-Rankin D. "Electric-field effects on methane coflow flames aboard the International Space Station (ISS): ACME E-FIELD Flames." Combust Flame. 2022 Dec;246:112443. https://doi.org/10.1016/j.combustflame.2022.112443 , Nov-2022
Articles in Peer-reviewed Journals	Chien Y-C, Girodon H, Esquivias Rodriguez B. "Modeling of elevated pressure diffusion flames with water addition." Combustion Science and Technology. 2023 May 19;195(7):1666-80. https://doi.org/10.1080/00102202.2023.2182205 , May-2023
Awards	Chien Y-C. "American Society for Gravitational and Space Research (ASGSR) Thora W. Halstead Young Investigator Award, November 2021." Nov-2021
Dissertations and Theses	Esquivias Rodriguez B. "Numerical simulation of water-vapor addition into a methane diffusion flame at high pressure using PeleLM." Thesis, University of California, Irvine, 2021. https://escholarship.org/uc/item/4474s0v6 , Jan-2021

Dissertations and Theses	Girodon H. "CFD modeling of pressurized laminar coflow (non premixed) diffusion flames with water addition." Thesis report for Engineering internship at University of California, Irvine, 2021. , Nov-2021
Dissertations and Theses	Donzeau M. "PeleLM CFD of ion driven winds from diffusion flames." Thesis report for Engineering internship at University of California, Irvine, 2022. , Nov-2022
Papers from Meeting Proceedings	Girodon H, Dunn-Rankin D, Chien Y-C. "CFD modeling of pressurized laminar coflow (non-premixed) diffusion flames with water addition." 28th International Colloquium on the Dynamics of Explosions and Reactive Systems, Naples, Italy, June 19-24, 2022. Abstracts. 28th International Colloquium on the Dynamics of Explosions and Reactive Systems, Naples, Italy, June 19-24, 2022. Paper 162. , Jun-2022
Papers from Meeting Proceedings	Esquivias B, Dunn-Rankin D, Chien Y-C. "Numerical simulation of water-vapor addition into a methane diffusion flame at high pressures." 12th U.S. National Combustion Meeting, College Station, TX, May 24-26, 2021. Abstracts. 12th U.S. National Combustion Meeting, College Station, TX, May 24-26, 2021. Laminar Flames. Paper 2F08. , May-2021
Papers from Meeting Proceedings	Donzeau M, Esclapez L, Day MS, Chien Y-C. "Recent progress on numerical modeling for microgravity electric field flames results." 13th U.S. National Combustion Meeting, College Station, Texas, March 19-22, 2023. Abstracts. 13th U.S. National Combustion Meeting, College Station, Texas, March 19-22, 2023. Paper 1D04. , Mar-2023
Significant Media Coverage	Christopher L. "Graduate students meet Astronaut Harrison Schmitt at national conference." UC Irvine (UCI) Samueli School of Engineering News article, April 6th, 2023. https://engineering.uci.edu/news/2023/4/graduate-students-meet-astronaut-harrison-schmitt-national-conference , Apr-2023
Significant Media Coverage	NASA Science Editorial Team. "NASA selects proposals to provide new insights from openly available data." NASA news release, June 16, 2021. https://science.nasa.gov/science-news/bps/nasa-selects-proposals-to-provide-new-insights-from-openly-available-data , Jun-2021
Significant Media Coverage	Brandt L. (Chien Y-C interview). "NASA funds E-FIELDS flames simulation project." UC Irvine (UCI) Samueli School of Engineering News article, Sept 27, 2021. https://engineering.uci.edu/news/2021/9/nasa-funds-e-fields-flames-simulation-project , Sep-2021
Significant Media Coverage	Brandt L. (Chien Y-C interview). "Chien recognized for gravitational and space research and mentoring." UC Irvine (UCI) Samueli School of Engineering News article, March 14, 2022. https://engineering.uci.edu/news/2022/3/chien-recognized-gravitational-and-space-research-and-mentoring , Mar-2022