Fiscal Year:	FY 2022	**Task Last Updated:**	FY 02/15/2022
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Project Title:	Effect of External Thermo-Convective Perturbation on Cool Flame Dynamics: A Multidimensional Multi-Physics CFD Analysis		
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:	FLIGHT,GROUND,Physical Sciences Informatics (PSI)	**Solicitation / Funding Source:**	2015 Physical Sciences NNH15ZTT001N-15PSI-B: Use of the NASA Physical Sciences Informatics System – Appendix B
Start Date:	02/15/2017	**End Date:**	02/14/2022
No. of Post Docs:		**No. of PhD Degrees:**	1
No. of PhD Candidates:	1	**No. of Master' Degrees:**	
No. of Master's Candidates:		**No. of Bachelor's Degrees:**	
No. of Bachelor's Candidates:		**Monitoring Center:**	NASA GRC
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Flight Program:			
Flight Assignment:	NOTE: End date changed to 2/14/2022 per NSSC information (Ed., 1/26/21) NOTE: End date changed to 2/14/2021 per NSSC information (Ed., 9/9/2020) NOTE: End date changed to 2/14/2020 per NSSC information (Ed., 11/18/19)		
Key Personnel Changes/Previous PI:	No changes have occurred.		
COI Name (Institution):			
Grant/Contract No.:	NNX17AF97A		
Performance Goal No.:			
Performance Goal Text:			

Task Description:	The current proposal will explore the aspects of flame dynamics and ultimate fate of an already ‘established droplet cool flame’ under external thermal and convective perturbation through multi-physics based multi-dimensional computational fluid dynamics (CFD) analysis addressing the variability observed in the International Space Station (ISS) experiments. Here, we will investigate the two extremities of n-heptane droplet sizes pertaining to droplet combustion -- (a) large diameter (typical to that of NASA FLame Extinguishment Experiment (FLEX) experiments, 1-4 mm) and (b) small diameter (submillimeter dimension, ~0.5 mm). The discovery of n-heptane droplet ‘cool flame’ on board the International Space Station (ISS) has introduced new research thrust in understanding the intricate behavior of ‘cool flame’ for diffusion control environment. Even though these studies were targeted to be performed in near-absence external convection influence, perturbations in the experiments resulted in slow drift of the droplet thereby generating an unintentional convective field. The role of this convective field on the observed “cool flame” dynamics is not quantified and determined. Additionally, to address the design of next generation combustor deploying cool flame and/or low temperature (LT) kinetics, a better understanding about how quasi-steady ‘self-sustained’ cool flame behave in response to induced convective perturbation is important and critical. The objective of the proposed research is to determine the role of thermal and convection influence on the cool flame dynamics – analyzing and interpreting the ISS data and hence extending the interpretation to submillimeter sized droplets. In order to achieve the proposed objectives, multi-dimensional multi-physics OpenFOAM (Foam Optics And Mechanics) based CFD platform will be utilized incorporating detailed combustion chemistry and associated fluid physics under the influence of convection and thermal field. ISS FLEX cases performed under microgravity will serve as base comparison case. Subsequently, three possible fluid fields (with convection influence, with heat flux influence, and combination thereof) for single droplet will be considered. For initial model development in OpenFOAM, simplified reaction kinetics will be deployed and subsequently the computation effort will be casted towards the incorporation of reduced kinetics. The proposed hybrid multi-physics model will be developed to get deeper insight into the FLEX cool flame experimental observation exploring the influence of external perturbation to cool flame itself. Therefore, any constitutive analysis, conclusion, and/or hypothesis drawn from such numerical works will directly and coherently support the title objective of the NASA Research Announcement (NRA) Appendix B solicitation, i.e., ‘reusability’ of the available database. Furthermore, these detailed analyses will help NASA in developing test matrix for large diameter cool flame experiments under external perturbation. Lastly, ozone assisted small diameter investigations using the proposed computational strategies can assist NASA in designing experimental test matrix for observing first ever submillimeter sized droplet cool flame and its interaction with external perturbation.
Rationale for HRP Directed Research:	
Research Impact/Earth Benefits:	Low temperature combustion (LTC) and its association with cool flame kinetics have recently become leading research topics of interest due to their relevance to achieving high thermal efficiency, fuel flexibility, and low pollutant emissions for both advanced and legacy internal combustion engine applications. Despite promising lab-scale demonstrations of LTC technologies (e.g., homogeneous charge compression ignition (HCCI) and reactivity controlled compression ignition (RCCI) engines)), the lack of fundamental understanding of the associated chemical kinetics continues to limit implementation of LTC technology in reciprocating engines and the interpretation of near-limit behaviors in gas turbine engines (e.g., lean blow off). A clearer understanding of the kinetics on pressure, temperature, equivalence ratio, and fuel structure is critical for enabling these new technology developments. Considering the fuel injection techniques commonly utilized in the aforementioned engine technologies, understanding how the dynamics and chemistries of LTC depend on fuel physical properties and distillation characteristics is also critical for these multi-phase, multi-component applications.
	The tasks completed resulted in 5 papers (4 published and 1 in review). The major tasks accomplished: Task 1: Oscillatory cool flame combustion behavior of submillimeter sized n-alkane droplet under near limit conditions This task reports simulation results of oscillatory cool flame burning of an isolated, submillimeter sized n-heptane droplet in a selectively ozone seeded nitrogen-oxygen environment at atmospheric pressure. An evolutionary one-dimensional droplet combustion code encompassing relevant physics and detailed chemistry was employed to explore the roles of low temperature chemistry, ozone seeding, and dynamic flame structure on burning behaviors. For XO2=21% and a range of selective ozone seeding, near-quasi-steady cool flame burning is achieved directly (without requiring hot flame initiation and radiative extinction). Under low oxygen index conditions, but with significant ozone seeding, a nearly quasi-steady cool flame is initially established that then transitions to a dynamically oscillating cool flame burning mode until the droplet is completely consumed. It is found that the oscillation is initiated by the depletion of a fuel vapor-oxidizer layer evolving near the droplet surface and its dynamic re-establishment through liquid vaporization and vapor/oxidizer transport. A kinetic analysis indicates that the dynamic competition between the reaction classes – (a) degenerate chain branching, and (b) chain termination/propagation – along with continuous fuel and oxygen leakage through the flame location contributes to an oscillatory burning phenomena of ever-increasing amplitude. Analysis based on a single full-cycle of oscillatory burning shows that the reaction progression matrices (evolution of heat and species) for hydroperoxy alkyl (QOOH) chain propagation/termination reactions directly scale with the gas phase temperature field. On the contrary, the hydroperoxy alkyl (QOOH) degenerate branching reactions undergo three distinct stages within the same cycle. The coupled flame dynamics and kinetics suggest that in the oscillatory burning mode, kinetic processes dynamically cross through conditions characterizing the negative temperature coefficient (NTC) turnover temperature separating low temperature and NTC kinetic regimes. In addition, a parametric study is conducted to determine the role of ozone seeding level on the observed oscillation phenomena. Task 2: Dynamics of cool flames Cool flames play a critical role in ignition timing, burning rate, burning limits, engine knocking, and emissions in conventional and advanced combustion engines. [Ed. Note. Reference: Ju Y, Reuter CB, Yehia OR, Farouk TI, Won SH. “Dynamics of cool flames.” Progress in Energy and Combustion Science. 2019 Nov;75(100787):1-39.] This paper provides an overview of the recent progress in experimental and computational studies of cool flames. First, a brief review of low temperature chemistry and classical studies of cool flames is presented. Next, the recent experimental and computational findings of cool flames in microchannels, microgravity droplet combustion, counter-flow flames, and turbulent combustion environments are reviewed. The flammability diagrams of different low temperature flames and their relations to hot flames in premixed and nonpremixed systems are discussed. The impact of cool flames on turbulent combustion and knock formation is also highlighted. Finally, future avenues in cool flame research, including the use of cool flames as a new platform for low temperature kinetic model validation, are presented. It is concluded that the

Task Progress:	understanding and control of low temperature combustion is critical for the development of future advanced engines and new fuels. Task 3: Initial diameter effects on combustion of unsupported equi-volume n-heptane/iso-octane mixture droplets Combustion of stationary fuel droplets comprised of an equi-volume mixture of n-heptane and iso-octane with initial diameters (Do) ranging between 1 mm and 6 mm was studied under this task. The intent was to show that by increasing Do to large enough values the burning mode would transition to a “Cool Flame” (CF) regime. The principle mechanism for the transition is radiative losses from the droplet flame that dominate the thermal field for large droplets. Unsupported or free-floating and droplets were probed in experiments carried out on board the International Space Station to promote spherical symmetry and a one-dimensional transport process in the standard atmosphere. The simulations employed a kinetic mechanism comprised of 298 species and 1916 reactions which included radiation, variable transport properties, and unsteady liquid and gas phase transport. Radiative losses from the droplet flame were unimportant for Do < 3 mm with no evidence of extinction. Larger droplets extinguished during burning and passed through a CF regime characterized by a non-visible flame and a burn rate which was higher than that of pure evaporation but lower than that of the initial hot flame burning. The simulations showed this transition occurring when radiative losses from the flame would drive the system to a burning mode controlled by low temperature combustion kinetics. The evolution of droplet diameter was well-predicted by the simulations. Predicted flame stand-off ratios were independent of Do early in burning and a transition to CF occurred later in the burning history as Do was increased. The average droplet burning rates of the mixture prior to extinction showed a power-law dependence on Do that was well predicted by the simulations. Measured mixture extinction diameters varied linearly with Do and were also well-predicted by the simulations. Task 4: Sub-millimeter sized multi-component jet fuel surrogate droplet combustion Isolated droplet burning behaviors of real jet fuel surrogates that all share the same kinetic behaviors for predicting fully pre-vaporized combustion behaviors of “global” Jet-A real fuel are investigated numerically. The three multi-component surrogate fuels (Surrogate-1: n-decane/iso-octane/toluene 42.7/33.0/24.3, Surrogate-2: n-dodecane/iso-octane/1,3,5 trimethyl benzene 49.0/21.0/30.0 and Surrogate-3: n-hexadecane/iso-octane/1,3,5 trimethyl benzene 36.5/31.0/32.5 molar ratios) have disparate distillation curve and other physical properties. Isolated droplet burning computations are used to compare and analyze the coupled effects of physical and chemical properties on predictions in comparison to microgravity data previously published in the literature. Simulations are performed using a transient one-dimensional sphero-symmetric model, involving numerically reduced detailed chemical kinetics, and multi-component gas-phase diffusive transport. Predictions agree well with microgravity experimental data published previously for surrogates 1, especially by including sooting effects in the computations. The interactions among the different liquid-phase components are modeled using UNIFAC activity coefficient methodology. [Ed.Note: UNIFAC is the UNIversal quasichemical Functional group Activity Coefficients method.] Stagnant and internally mixed liquid-phase behaviors are considered. The roles of preferential vaporization behavior are comprehensively evaluated by varying fuel composition, droplet size and ambient pressure conditions. Impacts of preferential vaporization on observed behaviors are highly sensitive to the droplet size, and thermodynamic conditions of the surrounding ambient. An expression for the degree of preferential vaporization effects is proposed, expressed in terms of average, maximum, and ignition burning rate. Preferential vaporization was found to have a strong non-linear dependence on initial droplet diameter, as well as operating pressure conditions. This implies that the preferential vaporization might have significant and dominant impact on multiphase/spray combustion of multicomponent fuels. Task 5: Extinction characteristics of isolated n-alkane fuel droplets during low temperature cool flame burning in air Large carbon number n-alkanes are notable components in all real transportation fuels, and their chemical structures foster substantial low temperature kinetic reactivity. Normal alkanes have been studied in various canonical configurations but rarely in systems with strong coupling between low temperature chemistry and transport for pure as well as for multi-component n-alkane mixtures. The Flame Extinguishment (FLEX) experiments on board the International Space Station have provided a unique platform for investigating low temperature multi-phase n-alkane and iso-alkane combustion. Among the many interesting phenomena experimentally observed, cool flame extinction can occur, accompanied by the concurrent formation of a surrounding cloud of condensed vapor. In this work, we conduct numerical simulations of high and low temperature combustion of large, initially single-component n-heptane, n-decane, and n-dodecane droplets. The role of initial droplet diameter, operating pressure, and n-alkyl carbon number on the extinction of hot and low temperature flames is investigated and compared against the available experimental data. While all three fuels exhibit similar hot flame behavior, cool flame activity increases with the carbon number, resulting in an increased cool flame temperature and decreased extinction diameter. Multi-cyclic “hot/cool flame transitions” are found in air as pressure is slightly increased above one atmosphere. The cyclic behaviors correspond to continuously varying hot and cool flame transitions across the high, low, and negative temperature coefficient (NTC) kinetic regimes. Further increase in pressure results in a second stage steady “Warm flame” transition. The extinction of hot and cool flame has a strong non-linear dependence on ambient pressure; but as the hot flame extinction diameter increases with pressure, the extinction diameter of the cool flame decreases. The computational results are compared with a recent asymptotic analysis of FLEX n-alkane cool flames.
Bibliography Type:	Description: (Last Updated: 03/08/2022)