Fiscal Year:	FY 2021	**Task Last Updated:**	FY 01/21/2021
PI Name:	Farouk, Tanvir Ph.D.		
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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Zip Code:	29208-4104	**Congressional District:**	6
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:**	0
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
Contact Monitor:	Hicks, Michael C.	**Contact Phone:**	216-433-6576
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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:	February 2021 report: Mr. Sudipta Saha has been working on this project since last year; Ali Charchi has graduated so he is no longer CoInvestigator.		
COI Name (Institution):	Saha, Sudipta M.S. (University of South Carolina)		
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.
Task Progress:	Below are the abstracts from the two journal papers that were published during this reporting period. Due to Covid-19 related travel restrictions and closure we were unable to attend the typical conferences to present our research work. Due to the ongoing pandemic the labs at the university were closed for an extended period and also additional safety protocols were implemented so students were not allowed in the lab except only for designated time slots. We were expecting higher progress but were able to publish two papers during this reporting period. Some of the divergence issues of the code still need resolution. Journal abstracts below; See also Bibliography section below: “Initial diameter effects on combustion of unsupported equi-volume n-heptane/iso-octane mixture droplets: Experimental observations and detailed numerical modeling” Combustion and Flame 220, (2020), 82 – 91. This paper reports results of a detailed numerical model and an experimental effort to study 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. 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 onboard 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 for pure evaporation but lower than for 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. “Sub-millimeter sized multi-component jet fuel surrogate droplet combustion: Physicochemical preferential vaporization effects” Proceedings of the Combustion Institute (2020) https:// . 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, especially by including sooting effects in the computations. The interactions among the different liquid-phase components are modeled using UNIFAC activity coefficient methodology. 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.
Bibliography Type:	Description: (Last Updated: 03/08/2022)
Articles in Peer-reviewed Journals	Farouk T, Won S, Dryer F. "Sub-millimeter sized multi-component jet fuel surrogate droplet combustion: Physicochemical preferential vaporization effects." Proceedings of the Combustion Institute. 2021 Apr;38(2):3313-23. https://doi.org/10.1016/j.proci.2020.06.200 , Apr-2021
Articles in Peer-reviewed Journals	Xu Y, Farouk TI, Hicks MC, Avedisian CT. "Initial diameter effects on combustion of unsupported equi-volume n-heptane/iso-octane mixture droplets: Experimental observations and detailed numerical modeling." Combustion and Flame. 2020 Oct;220:82 – 91. https://doi.org/10.1016/j.combustflame.2020.06.012 , Oct-2020