Fiscal Year:	FY 2020	**Task Last Updated:**	FY 02/04/2020
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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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:**	02/14/2021
No. of Post Docs:		**No. of PhD Degrees:**	1
No. of PhD Candidates:	2	**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 2/14/2021 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 2020 report: PhD student Fahd Alam, who was involved in the project, has graduated. We have a new PhD student, Sudipta Saha, who has been working on this project since last year.		
COI Name (Institution):	Charchi, Ali M.S. (University of South Carolina) Saha, Sudipta M.S. (University of South Carolina)		
Grant/Contract No.:	NNX17AF97A		
Performance Goal No.:			
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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:

The contributions to this specific research are to utilize the FLEX experimental dataset to develop and validate sub-models and utilize these models to obtain fundamental insight on the coupled physicochemical processes resulting in cool flame behavior for multicomponent liquid fuel droplets. Our transient modeling efforts utilize large detailed kinetic mechanisms for n-heptane and iso-octane mixture (Primary Reference Fuel – PRF) and they also include coupled, convective diffusive transport in the gas and liquid phases, and a statistical narrow band radiation model to resolve radiative effects in the gas phase. In addition, 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. A specific target has been to test and validate the multicomponent liquid phase submodel. 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 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 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. We had used computations over the past year to:

• characterize the dynamics of cool flame for a Primary Reference Fuel (PRF) droplet containing 50% n-heptane and 50% iso-octane mixture

• investigate the effect of droplet diameter on the cool flame behavior of PRF droplets

• analyze the role of multicomponent liquid droplet on the overall combustion behavior

• investigate the influence of sooting behavior on multicomponent droplet combustion.

Bibliography Type:	Description: (Last Updated: 03/08/2022)
Abstracts for Journals and Proceedings	Farouk T, Won S, Dryer F. "Investigating the role of preferential vaporization during submillimeter sized multicomponent jet fuel surrogate droplet combustion." Presented at the 11th U.S. National Combustion Meeting, Pasadena, CA, March 24-27, 2019. 11th U.S. National Combustion Meeting, Pasadena, CA, March 24-27, 2019. , Mar-2019
Abstracts for Journals and Proceedings	Farouk T, Won S, Dryer F. "Multi-component jet fuel surrogate droplet combustion: Preferential vaporization behaviors under spray relevant conditions and effects on combustion behaviors." Presented at 35th Annual Meeting of the American Society for Gravitational and Space Research, Denver, CO, November 20-23, 2019. Program and Abstracts. 35th Annual Meeting of the American Society for Gravitational and Space Research, Denver, CO, November 20-23, 2019. , Nov-2019
Articles in Peer-reviewed Journals	Alam F, Aghdam AC, Dryer F, Farouk T. "Oscillatory cool flame combustion behavior of submillimeter sized n-alkane droplet under near limit conditions." Proceedings of the Combustion Institute. 2019;37(3):3383-91. https://doi.org/10.1016/j.proci.2018.05.151 , Jan-2019
Articles in Peer-reviewed Journals	Ju Y, Reuter C, Yehia O, Farouk T, Won S. "Dynamics of cool flames." Progress in Energy and Combustion Science. 2019 Nov;75:100787. https://doi.org/10.1016/j.pecs.2019.100787 , Nov-2019