Fiscal Year:	FY 2018	**Task Last Updated:**	FY 05/10/2018
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:**	02/14/2020
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 2/14/2020 per NSSC information (Ed., 11/18/19)		
Key Personnel Changes/Previous PI:	May 2018 report: There have been no changes in the key personnel.		
COI Name (Institution):	Alam, Fahd Ph.D. (University of South Carolina) Charchi, Ali 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 extend 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 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 first phase of this project encompasses three different studies pertaining to smaller droplet (Do = 0.5 mm), those that are amenable to perform terrestrial drop tower based tests-- (1) Initiation of directly established cool flame for sub-millimeter sized droplet utilizing selective ambient O3; (2) Mechanistic understanding of direct cool flame initiation for higher flash point fuels; (3) Dynamics of continuously expanding oscillatory cool flames. In the first study, isolated n-alkane droplet combustion was numerically studied for different initial diameters (Do = 0.1, 0.5 mm), ambient pressures (1, 25 atm) with selected levels of O3 in the surrounding. This study primarily focuses on the exploration pathway to introduce directly established cool flame for sub-millimeter sized n-alkane droplets. It was found that the required initiation energy for igniting low and high flashpoint (relative to ambient temperature) fuel droplets differ due to the difference in fuel vapor accumulation near the liquid surface vicinity as a result of disparate flash point temperature. This results in a different strength (fuel mole fraction) of combustible partially premixed flammable vapor mixture. The rapid combustion of the premixed mixture provides additional energy feedback to sustain combustion during the transition from partially premixed to diffusive burning. In the case of high flash point fuel, the condensed phase droplet must be heated above its flash temperature by the initiation energy, which must also provide the energy to sustain the transition to diffusive burning. In the second study, we extended the concept of ozone-assisted, directly induced cool flame combustion of the submillimeter-sized droplet (Do = 0.5 mm) for n-C10H22 and n-C12H26. It is found that simply modulating the ignition energy alone, especially for low flash point fuels, is an ineffective means of directly establishing cool flame burning. However, a combination of selective O3 loading and ignition energy have the potential to directly initiate cool flame for all three fuels at atmospheric pressure and temperature condition and for droplet sizes commensurate with ground-based experimental techniques. The absence of sufficient fuel vapor around the droplet for heavier n-alkanes compared to its low flash point counterpart prohibits the direct establishment of cool flame. Upon ignition, the fuel vapor is quickly consumed, which is inadequate to supply necessary energy feedback to the droplet, triggering multiple dumped cool flame oscillation before entering quasi-cool flame burning. In addition, the computational comparison among three different kinetic models for n-C12H26 demonstrated significant model to model prediction discrepancies suggesting the future need for large scale reevaluation of kinetic coefficients. The findings from these two studies were presented at the 10th US national Combustion Meeting 2017 and 33rd ASGSR Annual Meeting 2017. As a continuation of the aforementioned two studies, we then explore the dynamics of oscillatory cool flames for n-C7H16 droplet. The dynamics of the near-limit cool flame burning of isolated submillimeter sized n-heptane droplets was numerically investigated. To provide the necessary near limit condition, the oxygen in the ambient was set to a value that is lower than the limiting oxygen index for n-C7H16, and ozone was seeded to the ambient to accomplish cool flame combustion initiation. The predictions show that at low oxygen indices, a quasi-steady cool flame burn is unattainable and the system transitions to a continuously pulsing, cool flame droplet combustion mode. Analyses further indicate that the dynamic interaction of degenerate chain branching and chain termination/propagation reaction classes

	of QOOH associated with the low temperature and negative temperature coefficient (NTC) kinetic regimes, and continuous fuel leakage across the flame location contribute to the ever-increasing trends of the oscillation magnitude.
Bibliography Type:	Description: (Last Updated: 06/13/2025)
Abstracts for Journals and Proceedings	Alam F, Dryer F, Farouk T. "Cool Flame Combustion of Sub-Millimeter Sized Higher n-Alkane Droplets at Atmospheric Condition." 2017 10th U.S. National Combustion Meeting, College Park, MD, April 23-26, 2017. 2017 10th U.S. National Combustion Meeting, College Park, MD, April 23-26, 2017. , Apr-2017
Abstracts for Journals and Proceedings	Alam F, Dryer F, Farouk T. "Non-Premixed - Partially Premixed to Diffusive Burning: Initial Transient of Direct Cool Flame Burn." Combustion Science forum. 33rd Annual Meeting of the American Society for Gravitational and Space Research, Seattle, WA, October 25-28, 2017. 33rd Annual Meeting of the American Society for Gravitational and Space Research, Seattle, WA, October 25-28, 2017. , Oct-2017
Papers from Meeting Proceedings	Alam F, Charchi A, Dryer F, Farouk T. "Oscillatory Cool Flame Combustion Behavior of Submillimeter Sized n-Alkane Droplet under Near Limit Conditions." To be presented at 37th International Symposium on Combustion, Dublin, Ireland, July 29-August 3, 2018. 37th International Symposium on Combustion, Dublin, Ireland, July 29-August 3, 2018. In press as of May 2018. , May-2018