Research Development Fund – Fall 2023 Application Template
Submission Deadline: *12:00PM CDT Monday – October 23, 2023,* to rdf@tamu.edu

*****Applications exceeding page limits for any section or do not follow the template will not be reviewed*****

Application Title: FastScan Atomic Force Microscope for Microscale Particle Detachment Force Measurements at the Materials Characterization Facility to Develop Resuspension Models for Improved Mitigation

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Key Participating Units: TAMU: Material Characterization Facility (MCF), Civil and Environmental Engineering, Mechanical Engineering, Atmospheric Science; Sandia National Laboratories, Department of Energy (DoE) Pantex

RDF Amount Requested ($): $553,440 (Bruker Dimension FastScan Closed Loop Atomic Force Microscopy)

Executive Summary

Include the overall scope/objective of the application. What research infrastructure enhancement is proposed? How will research at Texas A&M be improved? Who (units) will benefit at the Brazos County locations? How will external funding be enhanced? What outcomes are anticipated? Explain clearly how this investment supports Texas A&M research infrastructure for broad campus benefit.

Our objective is to create a multiscale, multiphysics model suite which can more accurately predict particle resuspension and improve inhalational dose assessments for radiological, chemical, and biological Consequence Management (CM). In funded collaboration with DoE and Sandia National Laboratories (Sandia NL) we will utilize advanced surface physics models along with Large-Eddy-Simulation (LES) of the Atmospheric Boundary Layer to develop a predictive computational capability rather than rely solely on empirical data which is the basis of current technology.

An important aspect of this work will be the experimental validation at Texas A&M University. PI King's team working with Dr. Wilson Serem has gained significant experience with macroscale resuspension measurements and has recently developed microscale and macroscale techniques including protocols with custom probes to characterize adhesion force probability distributions using Atomic Force Microscopy (AFM) at the Materials Characterization Facility (MCF), a core user facility at Texas A&M. The currently available Icon AFM instrument at MCF has enabled the generation of preliminary data for proof-of-concept evaluation. However, to create a computational model, large datasets are required that can be achieved using the Bruker Dimension FastScan Closed Loop AFM instrument. These microscale data are needed to calibrate the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) molecular dynamics resuspension models and assess how much input data is needed to accurately predict hazardous particle adhesion and resuspension. This assessment is important since, ultimately, we want to extrapolate to scenarios with sparse or no data such as plutonium and bioparticles. **The goal of this proposal is to apply for the acquisition of the FastScan Atomic Force Microscope at MCF to enable the collection of large datasets for the generation of predictive resuspension models.**

This project strategically aligns TAMU with the DoD, DoE and Sandia NL strategy to radically improve mission delivery through increasing the use of experimentally validated modeling and simulation, as well as enhancing research and use of emerging technologies. The direct Fuego/LAMMPS program coupling is an emerging research tool (implemented in FY23) which will be used to enhance the performance of operational consequence management assessments. This advanced research methodology can be used for the resuspension of radionuclides, chemical particles and bioaerosols and will be enabled by microscale and macroscale experimental validation data collected uniquely by TAMU. Major users at TAMU will include the users of the current AFM instrument at MCF and faculty at Biological and Agricultural Engineering (Sandun Fernando, Sergio Capareda), Mechanical Engineering (Jaime Grunlan, Michael Pate), Civil and Environmental Engineering (Xingmao Ma, Qi Ying) and Atmospheric Science (Sarah Brooks, Yue Zhang).