Fiscal Year:	FY 2022	**Task Last Updated:**	FY 02/10/2022
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Project Title:	Validation of a CFD Model for Gas-Liquid Flows in Packed Bed Reactors to Enable Thermo-Fluid Analysis in Microgravity		
Division Name:	Physical Sciences		
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Program/Discipline--Element/Subdiscipline:	FLUID PHYSICS--Fluid physics		
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Comments:			
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COI Name (Institution):	Marconnet, Amy Ph.D. (Purdue University)		
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Task Description:	The proposed use of NASA's Physical Sciences Informatics (PSI), specifically the packed bed reactor experiment (PBRE) data, will enable new research on fluid physics in microgravity conditions. Two-phase gas-liquid flows are ubiquitous in life support and thermal control systems for spacecraft, space stations, and proposed habitats on the moon and Mars. Two-phase flows are impacted by microgravity conditions because while on Earth capillary forces are easily overcome by gravitational forces, the opposite is true in low-gravity environments. Predictive modeling of these flows is challenging -- even for terrestrial applications -- and the lack of predictive models limits the ability to scale up systems to sizes required for NASA missions. In the first year of the project, we will develop a computational fluid dynamics (CFD) approach for predicting dispersed gas-liquid flows. The CFD approach will be validated against the PBRE data from the PSI, specifically visual images of gas-liquid flows from videos, as well corresponding pressure drop information across disparate flow regimes. First, a suitable 3D flow geometry will be constructed from the specifications of the PBRE. The interFOAM solver in OpenFOAM will be adapted for interface-resolved simulation of gas-liquid flow through a packed bed. Using supercomputing resources at Purdue, we will perform large-scale simulations of gas-liquid flows across regimes (bubbly, slug, core-annular, stratified, etc.) at full and reduced gravity conditions. The flow-wise pressure gradient will be computed for different Reynolds numbers and gas volume fractions and compared to the PBRE datasets in the PSI. However, tracking the complex growing, merging, and rupturing gas-liquid interfaces in simulations is challenging. To address scale-up, two-fluid models, in which the gas and liquid phases are considered to be interpenetrating continua, have been proposed. Two-fluids models reduce computational cost by removing the need to track interfaces; however, they require calibration of parameters to become predictive. Specifically, a correlation for the interphase drag force must be developed. Using both fully resolved simulations and PBRE datasets, we will employ the physics-informed neural network (PINN) deep learning approach pioneered in 2019 to infer the parameters in the steady two-fluid model equations. The advantage of PINNs over other inverse methods is that PINNs work with limited measurements and noisy data. PINNs are not a "black box," as they build-in the underlying physical equations into the loss function to properly guide the learning process. Previous work has shown that the dimensionless parameter space consists of the Suratman number (a modified gas Reynolds number with the velocity set by the ratio of surface tension to viscosity) and the ratio of the gas and liquid phases' Reynolds numbers. We will determine the boundaries for flow regime transitions in this 2D space using interface-resolved simulations and compare to the predictions of a two-fluid model calibrated via a PINN. This regime diagram is critical for design and scale-up of packed bed reactors. While the flow physics alone is challenging to predict, such two-phase gas-liquid flows are often coupled with heat transfer and chemical reactions. In the second year of the project, we will consider flows coupled with heat transfer. Specifically, we will incorporate heat transfer into interFOAM and the two-fluid model. In parallel, we propose novel ground-based thermo-fluid experiments in a packed bed reactor against which to validate the extended models. Correlations for heat transfer coefficients for gas-liquid flows in packed beds will be calibrated (via PINNs) against these novel ground-based experiments, which we will perform based on the design of the PBRE. Ultimately, the proposed research will provide tools for accurately modeling coupled thermal-fluid systems for both terrestrial and low-gravity applications.
Rationale for HRP Directed Research:	
Research Impact/Earth Benefits:	
Task Progress:	New project for FY2022.
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