Fiscal Year:	FY 2023	**Task Last Updated:**	FY 09/20/2022
PI Name:	Christov, Ivan Ph.D.		
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		
Program/Discipline:			
Program/Discipline--Element/Subdiscipline:	FLUID PHYSICS--Fluid physics		
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		
PI Email:	christov@purdue.edu	**Fax:**	FY
PI Organization Type:	UNIVERSITY	**Phone:**	765-496-3733
Organization Name:	Purdue University		
PI Address 1:	School of Mechanical Engineering		
PI Address 2:	585 Purdue Mall		
PI Web Page:			
City:	West Lafayette	**State:**	IN
Zip Code:	47907-2088	**Congressional District:**	4
Comments:			
Project Type:	Physical Sciences Informatics (PSI)	**Solicitation / Funding Source:**	2020 Physical Sciences NNH20ZDA014N: Use of the NASA Physical Sciences Informatics System – Appendix G
Start Date:	11/19/2021	**End Date:**	11/18/2023
No. of Post Docs:		**No. of PhD Degrees:**	
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:	Hasan, Mohammad	**Contact Phone:**	216-977-7494
Contact Email:	Mohammad.M.Hasan@nasa.gov		
Flight Program:			
Flight Assignment:			
Key Personnel Changes/Previous PI:			
COI Name (Institution):	Marconnet, Amy Ph.D. (Purdue University)		
Grant/Contract No.:	80NSSC22K0290		
Performance Goal No.:			
Performance Goal Text:			

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:

The proposed use of NASA's Physical Sciences Informatics (PSI) data repository, specifically the packed bed reactor experiment (PBRE) data, will enable new research on fluid physics across different gravity conditions. The 2011 National Academies decadal survey lists heat and mass transfer in porous media as a recommended research direction: ``TSES6—NASA should conduct research for the development and demonstration of closed-loop life support systems and supporting technologies. Fundamental research includes heat and mass transfer in porous media under full, partial and microgravity conditions and understanding the effect of variable gravity on multiphase flow systems." The proposed research aims to fill a knowledge gap in this area, which remains ``highest priority" in the midterm assessment of the decadal survey.
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, as well as terrestrial applications involving distillation, purification and separation, and catalytic reactions to enhance heat and mass transfer in convective flows, among other examples. However, gas-liquid flows through packed bed reactors have not been fully understood. Predictive modeling of these flows is challenging---even for terrestrial applications---and the lack of predictive simulation tools prohibits effective scaling up of systems to sizes required for future missions. To this end, we propose a computational fluid dynamics (CFD) approach for simulating gas-liquid flows in porous media across regimes: from bubbly, slug, core-annular flow to fully-dispersed gas phase. The CFD approach will be validated against the PBRE data from the PSI and extended to flows with heat transfer.

Task Progress:

The fluid physics of gas-liquid flows in packed bed reactors (PBRs) are challenging, in part due to the complex network of pore spaces giving rise to tortuous flow paths that fluid interfaces must traverse. The regime map of gas-liquid flows through packed beds depends on the gravity conditions under which the PBR is operating. Recently, experiments on the International Space Station (ISS) showed that two flow regimes are predominately observed at 0g: bubble and pulse (while other regimes, such as as trickle and spray flow, observed at 1g are not observed at 0g). Our goal is to develop a computational fluid dynamics (CFD) framework to simulate complex gas-liquid flows through PBRs under different gravity conditions. Towards accomplishing the project goal, our first task is to perform volume-of-fluid (VOF) simulations to track the interface between a gas and a liquid as they are displaced through a PBR. Through this task, we seek to enable resolved simulations of PBR flows in different regimes.
Our progress so far includes developing a workflow for generating a packing geometry using rigid body simulations in the open-source software Blender. Then, we extracted a representative volume element (REV or RVE) from the larger packed bed geometry that we generated in Blender. The idea is that this REV is more suitable for CFD analysis. The pore-space geometry was then meshed using a shrink-wrapping-based approach in order to generate bridges between adjacent spheres and avoid point-contacts. Next, VOF simulations were performed using ANSYS Fluent's solver. These fully-resolved simulations take into account the surface tension between the gas and liquid, as well as the contact angle between the liquid and the packing material. We simulated an example flow in the bubble regime by initializing the PBR flow domain with water and `patching in' a nitrogen bubble near the inlet of the geometry. We used a velocity inlet boundary condition for the water phase to push the bubble through the PBR, and observed its motion and deformation in our preliminary simulations so far.

Bibliography Type:	Description: (Last Updated: 11/24/2023)