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| Fiscal Year: | FY 2024 | Task Last Updated: FY 10/03/2023 | |
| 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: | 11/17/2024 |
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| 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: | NOTE: End date changed to 11/17/2024 per NSSC information (Ed., 10/12/23) | | |
| Key Personnel Changes/Previous PI: | | | |
| COI Name (Institution): | Marconnet, Amy Ph.D. (Purdue University) | | |
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| Performance Goal Text: | | | |

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| | <p>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.</p> <p>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 as corresponding pressure drop information across disparate flow regimes. First, a suitable 3D flow geometry will be constructed from the specifications of the PBRE. Then, interface-resolved simulations will be performed 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 gas-liquid interface dynamics, as well as 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.</p> <p>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. 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.</p> <p>In second year of the project, we will calibrate two-fluid models, under the steady 1D flow assumption, by fitting the interphase drag coefficient to data from the PSI. In turn, two-fluid models will enable large-scale simulations, with unresolved pore-scale dynamics, towards scale up for packed-bed reactor properties. Specifically, two-fluid model simulations using the novel correlations learned from the PBRE datasets in the PSI will help determine the boundaries for flow regime transitions in the parameter space, leading to new regime diagrams, and specifically sharper transition boundaries between regimes, that address gaps in the current understanding.</p> <p>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 parallel, we propose to evaluate the feasibility of 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 can be calibrated against novel ground-based experiments, which we will explore 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.</p> |
| Task Description: | |
| Rationale for HRP Directed Research: | <p>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.</p> <p>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.</p> |
| Research Impact/Earth Benefits: | <p>Gas-liquid flows through packed bed reactors (PBRs) are challenging to predict due to the tortuous flow paths that fluid interfaces must traverse. The Packed Bed Reactor Experiment (PBRE) at the International Space Station showed that bubble and pulse flows are predominately observed under microgravity conditions, while trickle and spray flows, observed under terrestrial conditions, are not present in microgravity.</p> <p>Our progress in the last year is based on the groundwork from Year 1. Specifically, in Year 1, we developed the workflow for generating a packing geometry and extracting a representative volume element (REV) from the larger packed bed geometry for performing interface-resolved using the ANSYS Fluent's solver. In Year 2, we performed a detailed Computational Fluid Dynamics (CFD) study to understand the physics behind the measurements made during the PBRE. Specifically, we simulated bubble flow through a PBR for different packing-particle-diameter-based Weber numbers and under different gravity conditions. We demonstrated different pore-scale mechanisms, such as capillary entrapment, buoyancy entrapment, and inertia-induced bubble displacement. Then, we performed a quantitative analysis by introducing a new dynamic length scale, dependent upon the evolving gas-liquid interfacial area, to understand the dynamic trade-offs between the inertia, capillary, and buoyancy forces on a bubble passing through a PBR. This analysis led us to define new dimensionless Weber-like numbers that delineate bubble entrapment from bubble displacement suitable for microgravity research. This work has been submitted for review for publication. A preprint is freely available at https://arxiv.org/abs/2308.08075 while the supporting data is freely available in the Purdue University Research Repository at https://purr.purdue.edu/publications/4346/1 [Ed. Note: See Bibliography.]</p> <p>Further, in Year 2, we laid down the groundwork for using the PBRE data from the PSI towards novel data-driven</p> |
| Task Progress: | |

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| | calibration of two-fluid (Euler-Euler) models for these gas-liquid flows. |
| Bibliography Type: | Description: (Last Updated: 11/24/2023) |
| Articles in Other Journals or Periodicals | Nagrani PP, Marconnet AM, Christov IC. "Hydrodynamics of bubble flow through a porous medium with applications to packed bed reactors." arXiv preprint server. Posted August 16, 2023. https://doi.org/10.48550/arXiv.2308.08075 , Aug-2023 |
| Articles in Other Journals or Periodicals | Nagrani PP, Marconnet AM, Christov IC. "Simulations, data, and scripts for "Hydrodynamics of bubble flow through a porous medium with applications to packed bed reactors [data file]." Purdue University Research Repository: West Lafayette, IN. Posted August 31, 2023. https://purr.purdue.edu/publications/4346/1 , Aug-2023 |
| Papers from Meeting Proceedings | Nagrani PP, Marconnet AM, Christov IC "Bubble entrapment and displacement through packed-bed reactors." 76th Annual Meeting of the APS Division of Fluid Dynamics, Washington, DC, November 19-21, 2023. Bulletin of the American Physical Society. 2023 Nov. Abstract: T41.00007. https://meetings.aps.org/Meeting/DFD23/Session/T41.7 , Nov-2023 |
| Significant Media Coverage | Nagrani PP, Christov IC, Marconnet AM. (Selected contribution to art exhibit) "Computed Bubble Wrap." Summer Exhibition at Ringel Gallery, Purdue University: , Jun-2023 |