Seed Grant Application Cover Page

Has seed grant previously been awarded?

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Amount Requested:	\$ 11,969.60		
Proposal Title:	Numerical Simulation of Magnetic Nanoparticles Using Electromagnetic Separation Device		
PROPOSAL CHECKLIST:		ELIG	IBILITY:
 Narrative (2 single-spaced pages) Budget Page Biographical Data Publications/Exhibits/Performances (5 years) Proposals Submitted/Funded (5 years) Summary of Previous Seed Grant(s) Applicable animal/human requests for approval are attached 		⊠ Ea	arly career faculty establishing scholarly program (5 years or less employment at UI) istablished faculty transitioning into a new scholarly area

ABSTRACT

This project aims to use computational fluid dynamics (CFD) to design and optimize the magnetic separation system used in spent nuclear fuel recycling. The project will develop advanced models for both the fluid and particles such that the accuracy of predicting the removal efficiency of particles will be significantly improved. The model will be validated using data measured by a research team at the Department of Physics, University of Idaho, and other experimental data when available. The validated model will be used to elucidate the best combination of flow rate, concentration, magnetic field gradient, and types of particles to achieve the highest removal efficiency of particles. The research results/findings will be published in refereed Journals and conference proceedings. The model can be easily transformed to be used for many disciplines such as nuclear engineering, chemical engineering, and mineral engineering.

Narrative

Magnetic separation is one of the ancient ways to separate magnetic materials based on the fact that materials with different magnetization experience different forces in presence of field gradient. Magnetic separation can also be used to separate two types of non-magnetic particle by selectively coating magnetic particles on a particular type. Magnetic separation has been applied in biotechnology, chemistry, and medicine. Compared to other separation methods, magnetic separation has the following advantages: (1) fast and clean separation, (2) easiness of analysis and monitoring samples, (3) high removal efficiency, and (4) cost effective. It can be used for separation of magnetic from non-magnetic waste, waste water treatment, and cell to processing of minerals (Figure 1a).

Of interested herein is the use of functionalized magnetic nanoparticles (MNPs) in spent nuclear fuel separation technology. It has shown great advantages as it minimally generate secondary waste stream, high separation efficiency, selective separation of various chelators, and cost-effective process with reusable MNPs. Additionally, it is environmentally benign and do not generate secondary solid waste (Qiang et al. 2009; Han et al., 2010; Johnson et al., 2011).



Figure 1. applications of magnetic separation: (a) mineral processing, (b) spent nuclear fuel separation, (c) forces on magnetic nanoparticles

There are a few fundamental forces on a nanoparticle in solution/fluid. Based on the order of magnitude of analysis, the buoyant force (F_b), viscous drag force (F_{dx} and F_{dy}), and magnetic force (F_m) are more important than thermal kinetics, magnetic dipole interactions, and vander wall forces such that the latter is ignored (Fig. 1c). In order to understand the separation process and address design issues, a robust and accurate mathematical model of the process is very important. However, a careful review of the literature indicates that very little work has been carried out on the development of such a model. Due to the complexity of the motions of fluid and particles, most of previous studies made invalid assumptions, use inaccurate empirical formulas, and ignore important flow physics. For instance, the flow is assumed to be laminar (fluid velocity is very low) whereas almost all flows in are turbulent (fluid velocity is high). Previous studies also ignored the following factors: (1) nonlinear two-way coupling between the particles and fluid; (2) particle-particle and particle-wall interactions; (3) trajectory of individual particles; and (4) unsteadiness of the fluid flow. These limitations prevented the mathematical model to be used on design and must be resolved.

Recently, researchers have shown some preliminary but interesting results of using computational fluid dynamics (CFD) to simulate the flow behavior of slurry of magnetic and non-magnetic particles between two plates of a magnetic separator (Mohanty et al., 2011). The predicted concentrations of the two-type particles agree reasonably with what observed in experiments. However, most of the limitations discussed still exist and new models that account for the motions of individual particles and turbulent flow are needed.

The objective of the project is to develop and implement new CFD models to simulate MNPs motions in fluid for accurate prediction and optimization of the spent nuclear fuel separation. The model includes magnetic field simulation, three-dimensional unsteady turbulent fluid simulation using Navier-Stokes Equations, and Lagrangian simulation to predict the motions of individual particles.

The objective will be achieved through completion of the following tasks: (1) develop a CFD model on the platform of ANSYS FLUENT (months 1-2); (2) validate the model for static separation using experimental data from Dr. You Qiang's research team at Department of Physics of University of Idaho, including separation time for un-functionalized and functionalized MNPs under different magnetic field gradients (months 3-5); (3) parametric studies for static separation using different particle sizes and shapes with experimental validation (month 6); (4) extend the model for dynamic separation involving unsteady fluid flow with validation by experimental data when available (months 7-9); (5) system simulation and optimization (months 10-11). A prototype of the system is show in Fig. 2. A known volume and

concentration of colloidal solution will be allowed to flow through the region with magnetic field. Concentration of solution flowing out of the tube in each cycle will be measured using Ultraviolet visible spectroscopy, which will be used for validation of the CFD model. Optimization of the system will focus on identifying the best combination of flow rate, concentration, magnetic field gradient, and types of particles to achieve the highest removal efficiency of particles; and (6) summarize research results/findings, prepare for papers and presentations (month 12). Additionally, for each task, quantitative verification



(estimation of source and magnitude of numerical errors) and validation (estimation of modeling errors) will be conducted using the factor of safety method (Xing and Stern, 2010, 2011).

The project will give new challenges but also opportunities for the PI to develop new CFD models and numerical methods. Successful completion of the project will enable the PI to extend CFD for solving problems in other discipline areas including physics, minerals engineering, and nuclear engineering, etc. It will help me build real collaborations with researchers in those areas.

The findings of the research will be published in refereed Journals or conference proceedings. In addition to the research data produced by the research, the models developed in the form of user defined subroutines for ANSYS FLUENT can be easily transformed for other disciplines due to the popularity of this software.

The research results produced by this project will be incorporated into research proposals that will likely be externally funded by the Nuclear Engineering University Program (NEUP) of U.S. Department of Energy or National Science Foundation (NSF).

The PI has a grant from National Science Foundation with a total of \$118,998 from 2012 to 2014, which was originally awarded to the PI at Tuskegee University at \$200,000 and subawarded to University of Idaho in Jan. 2012. However, the grant is for designing offshore wind turbines. The proposed research herein is for a completely new research area. It will synergize the talents from both Department of Mechanical Engineering and Department of Physics. The model developed can be easily extended to be used by nuclear engineering, chemical engineering, and mineral engineering, etc.