Seed Grant Application Cover Page

PRINCIPAL INVESTIGATOR:

Name:	Tao Xing	Title:	Assistant Professor
Department:	Mechanical Engineering	Email:	xing@uidaho.edu

ADDITIONAL INVESTIGATORS:

Name:		Title:	
Department:		Email:	

Name:		Title:	
Department:		Email:	

Amount Requested:	$ 11,969.60

Proposal Title:	Numerical Simulation of Magnetic Nanoparticles Using Electromagnetic Separation Device

PROPOSAL CHECKLIST:

☒ Abstract
☒ 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

Has seed grant previously been awarded? ☐ Yes ☒ No

ELIGIBILITY:

☒ Early career faculty establishing scholarly program (5 years or less employment at UI)
☐ Established faculty transitioning into a new scholarly area

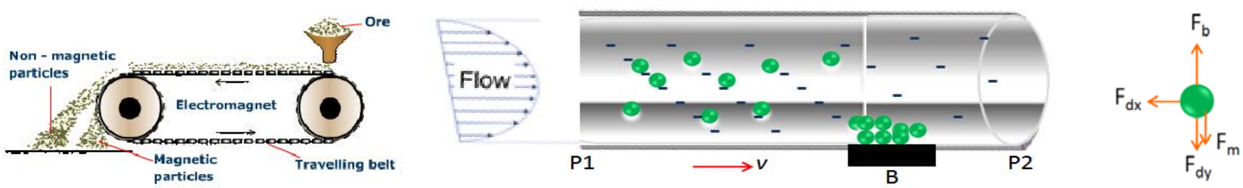
ABSTRACT

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).



(a) (b) (c)

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

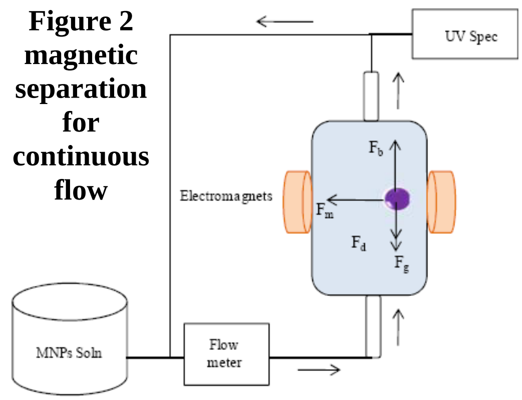
There are a few fundamental forces on a nanoparticle in solution/fluid. Based on the order of magnitude of analysis, the buoyant force (F_b), viscous drag force (F_{dx} and F_{dy}), and magnetic force (F_m) are more important than thermal kinetics, magnetic dipole interactions, and vander wall forces 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).

Figure 2 magnetic separation for continuous flow



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 sub-awarded 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.

Bibliography

1. H. Han, A. Johnson, J. Kaczor, M. Kaur, A. Paszczynski, and Y. Qiang, 2010, “Silica coated magnetic nanoparticles for separation of nuclear acidic waste,” *Journal of Applied Physics*, Vol. 107, no. 9, p. 09B520.
2. A. K. Johnson et al., 2011, “Highly hydrated poly(allylamine)/silica magnetic resin,” *Journal of Nanoparticle Research*.
3. S. Mohanty, B. Das, B.K. Mishra, 2011, “A Preliminary Investigation into Magnetic Separation Process Using CFD,” *Minerals Engineering*, Vol. 24, pp. 1651-1657.
4. Y. Qiang, M. Kaur, H. Han, A. Johnson, J. Kaczor, and A. Paszczynski, 2009, “Coated Magnetic Nanoparticles for Acidic Nuclear Waste Separation,” *Materials Research Society Symposium Proceedings*.
5. T. Xing and F. Stern, 2010, "Factors of Safety for Richardson Extrapolation," *ASME Journal of fluids engineering*, Vol. 132, No. 6, DOI: 061403.
6. T. Xing and F. Stern, 2011, Closure to "Discussion of 'Factors of Safety for Richardson Extrapolation,'"(2011, ASME J. Fluids Eng., 133, p. 115501), *ASME Journal of Fluids Engineering* (invited by the Editorial Office), Vol. 133, p. 115502.

7. Seed Grant Application Budget Form

Salaries (It covers half of a graduate student* at $6,240 for academic year (390 hours at $16/hour) and $2,080 for summer (130 hours at $16/hour). Part of the startup money may be used to contribute to this project so that a full time graduate student can be supported.	$8,320.00
Fringe Benefits (if applicable) (This is the fringe benefits for a graduate student at rates 1% for academic year and 9% for summer).	$249.6
Travel* (travel to field sites or other locations to perform research is permitted; travel to professional conferences is limited to $500) (N/A)	$0.00
Other Expenses (e.g., field or lab supplies, software, etc) (The license fee for Commercial CFD software ANSYS FLUENT (Academic Research Version) will be purchased at a cost of $3,400. The software is needed to develop the new models and run the proposed simulations.	$3,400.00
Capital Outlay (e.g., field equipment, computers, etc) ($8,387.14 from my startup money has been used to purchase a DELL Precision T7500 with 12 cores and 48 GB RAM in the PI's office, which is sufficient to complete the most expensive simulations proposed. The startup money will also be used to purchase other necessary software such as Pointwise Gridgen for CFD grid generation and Tecplot 360 for post-processing CFD results).	$0.00
Trustee Benefits (Describe)	$0.00
Total Requested	$11,969.60

*The graduate student will be selected from the students who are taking my course on computational fluid dynamics (ME 404/504).

Other Information

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a. Professional Preparation

Xi'an Jiaotong University	Mechanical Engineering	B.S. (1995)
Xi'an Jiaotong University	Mechanical Engineering	M.S. (1998)
Purdue University	Mechanical Engineering	Ph.D. (2002)
Postdoctoral Associate (The University of Iowa)	Ship hydrodynamics	2002~2005 (3 yrs)

b. Appointments

Assistant Professor	**University of Idaho**	**2011 (Aug. 14) – present**
Assistant Professor	Tuskegee University	2009 – 2011
Adjunct Assistant Professor	The University of Iowa	2006 – 2008
Assistant Research Scientist	The University of Iowa	2005 – 2008

c. Selected Publications (Journal papers)

(1) Li, Y.W., Paik, K.J., **Xing, T.**, Carrica, P.M., 2012, "Dynamic Overset CFD Simulations of Wind Turbine Aerodynamics," *Renewable Energy*, Vol. 37, Issue 1, pp. 285-298.
(2) **Xing, T.**, Bhushan, S., and Stern, F., 2011, "DES for a Tanker at Drift Angles with Analogy to Delta Wings, " *Computers & Fluids*, under review.
(3) Bhushan, S., **Xing, T.,** Stern, F., 2011, "Vortical Structures and Instability Analysis for Athena Wetted Transom Flow with Full-scale Validation," *ASME Journal of Fluids Engineering*, under review.
(4) **Xing, T.** and Stern, F., 2011, Closure to "Discussion of 'Factors of Safety for Richardson Extrapolation,'"(2011, ASME J. Fluids Eng., 133, p. 115501), *ASME Journal of Fluids Engineering* (invited by the Editorial Office), Vol. 133, p. 115502.
(5) **Xing, T.** and Stern, F., 2010, "Factors of Safety for Richardson Extrapolation," *ASME Journal of fluids engineering*, Vol. 132, No. 6, DOI: 061403.
(6) Pinto, H., A., **Xing, T.**, Stern, F., 2010, "URANS and DES for Wigley Hull at Extreme Drift Angles," *Journal of Marine Science and Technology*, DOI 10.1007.
(7) Ismail, F., Carrica, P., **Xing, T.**, Stern, F., 2010, "Evaluation of Linear and Nonlinear Convection Schemes on Multidimensional Non-Orthogonal Grids with Applications to KVLCC2 Tanker," *International Journal of Numerical Methods in Fluids*, Vol. 64, Issue 8, pp. 850-886.

(8) Bhushan, S., **<u>Xing, T.</u>**, Carrica, P., Stern, F., 2009, "Model- and Full-scale URANS Simulations of Athena Resistance, Powering, Seakeeping, and 5415 Maneuvering," *Journal of Ship Research*, Vol. 53, No. 4, pp. 179-198.

(9) Kandasamy, M., **<u>Xing, T.</u>**, Stern, F., 2009, "Unsteady Free-Surface Wave-Induced Separation: Vortical Structures and Instabilities," *Journal of Fluids and Structures*, Vol. 25, Issue 2, pp. 343-363.

(10) **<u>Xing, T.</u>**, Carrica, P., Stern, F., 2008, "Computational Towing Tank Procedures for Single Run Curves of Resistance and Propulsion," *ASME Journal of Fluids Engineering*, Vol. 130, No.1, 101102.

(11) **<u>Xing, T.</u>**, Kandasamy, M., Stern, F., 2007, "Unsteady Free-Surface Wave-InducedSeparation: Analysis of Turbulent Structures Using Detached Eddy Simulation and Single-phase Level Set Method," *Journal of Turbulence*, Vol. 8, No. 44, pp. 1-35.

d. Selected Publications (conference proceedings/reports)

(1) Xing, T., Carrica, P., Stern, F., 2011, "Developing Streamlined Version of CFDShip-Iowa-V4.5," IIHR Technical Report No. 479.

(2) **Xing, T.**, Burge, L.L. Jr., Aglan, H.A., 2011, "Integration of Mobile Technology into Undergraduate Engineering Curriculum," ASEE 2011 Annual Conference & Exposition, June 26-29, 2011, Vancouver, BC, Canada.

(3) **Xing, T.**, Carrica, P., Stern F., 2010, "Large-Scale RANS and DDES Computations of KVLCC2 at Drift Angle 0 Degree," Gothenburg 2010: A Workshop on CFD in Ship Hydrodynamics, December 8-10 2010, Sweden.

(4) **Xing, T.** and Stern F., 2010, "Factors of Safety for Richardson Extrapolation," IIHR Technical Report No. 476.

(5) **Xing, T.** and Stern F., 2009, "Factors of Safety for Richardson Extrapolation," IIHR Technical Report No. 469.

(6) **Xing, T.** and Stern F., 2008, "Factors of Safety for Richardson Extrapolation for Industrial Applications," IIHR Technical Report No. 466.

(7) **Xing, T.**, Shao, J., and Stern, F., 2007, "BKW- RS-DES of Unsteady Vortical Flow for KVLCC2 at Large Drift Angles," the 9th international conference on Numerical Ship Hydrodynamics, Ann Arbor, Michigan.

e. Grants Awarded

(1) **PI and leading organization**, "Collaborative Research: Simulation Based Design for Deep Water Offshore Wind Turbines Including Wave Loads and Motions," 2011–2014, National Science Foundation (NSF), Division of Chemical, Bioengineering, Environmental, and Transport Systems, Award #1066873, **$200,731** (May-Dec. 2011) awarded at Tuskegee; **$118,998** (Dec. 2011- Apr. 30, 2014) subawarded to University of Idaho.

(2) **PI,** "Transition CFDShip-Iowa to Create Ship Hydrodynamics Program," the Office of Naval Research (ONR) and the University of Iowa, 2009–2011, **$30,500**.

(3) **PI,** "Developing Streamlined Version of CFDShip-Iowa-V4," ONR and The University of Iowa, 2008–2009, **$50,290**.

(4) **Co-PI**, "6DOF Viscous Ship Hydrodynamics," ONR, 2000–2009 (N00014-01-1-0073), **$4,227,643**.
(5) **Co-PI**, "URANS/DES Code Development for Ship Hydrodynamics Simulation Based Design: CFDSHIP-IOWA," funded by ONR, 2006–2009 (N00014-06-1-0420), **$6,589,048**.
(6) **Co-PI**, "Two-Phase URANS/DES Simulations of Large Scale/RE Air Layer Drag Reduction," funded by ONR, 2008, **$300,000**.

f. Proposal Submitted

(1) **PI, "**Collaborative Research: From Ion Channel Mutations to Blood Flow: Development of A Multiscale Mechano-Electrical-Fluid Interaction Model for Three-Dimensional Excitable Tissues," Biomechanics and Mechanobiology, Division of Civil, Mechanical, and Manufacturing Innovation, NSF, Oct. 3 2011.
(2) **Co-PI**, "NSF MRI: Acquisition of an Adaptive Computation Server for Support of STEM Research at the University of Idaho," NSF, Feb. 2012.

g. Synergistic Activities

(1) Development of teaching modules for integration of computational fluid dynamics (CFD) into undergraduate and graduate engineering courses and laboratories. Teaching modules include hands-on CFD educational interface in the product name "FlowLab 1.2.10 with NSF templates," CFD lectures, CFD lab exercise notes, CFD pre- and post-tests, CFD report templates, Pre- and Post-surveys for course and experimental fluid dynamics (EFD) and CFD. For more information, please visit: http://css.engineering.uiowa.edu/~fluids and http://css.engineering.uiowa.edu/~me_160
(2) Implementation of detached eddy simulation (DES) model into CFDShip-Iowa
(3) Moderator for the CFD Workshop "0413: Integrating CFD into the Undergraduate Curriculum," held on June 18, ASEE 2006 Annual Conference at Chicago
(4) Worked with Fluent Inc. (http://www.fluent.com) on developing the CFD Educational Interface (funded by National Science Foundation #0126589).

h. Collaborators & Other Affiliations

(1) **Collaborators and Co-Editors:** Antonio Pinto-Heredero (Technical University of Madrid), Farzad Ismail (Universiti Sains Malaysia), Frederick Stern (The University of Iowa, UI hereinafter), Mani Kandasamy (UI), Pablo Carrica (UI), Shanti Bhushan (UI),
(2) **Graduate Advisors and Postdoctoral Sponsors**
Graduate and Ph.D. Thesis advisor: Steven H. Frankel (Purdue University)
Postdoctoral sponsor: Frederick Stern (UI)/Office of Naval Research
(3) **Thesis advisor**
(total of 2 graduate students, both at University of Idaho)
Current: Sean Quallen (Ph.D. Student); Landon Owen (Master's Student)