Klaipėdos universiteto strateginės mokslo krypties
„Tvarių technologijų, mėlynojo bei žaliojo augimo ir sveikos jūros link“
podoktorantūros stažuotės temos paraiška (2025-2027)

Title of traineeship topic	**Advanced AI-CFD modelling for scaling-up of all-weather flow battery**
Field(s) of study, unit, start date, duration	Information Technology and Chemical Engineering Research activities under this fellowship will take place at the Department of Informatics and Statistics, Klaipeda University. Two years program will be started from not later than 31.12.2025.
Brief description of the research and the results to be achieved (aim and objectives, keywords)	Redox Flow Batteries (RFBs) have been in the top of the list for large-scale energy storage system development; are adaptable for remote mines, war zone, coastal areas, tourist spots, and other locations where they can be positioned in closed and open spaces. Although existing RFBs been verified to operate perfectly within laboratory environment, any substantial deviations from the controlled environment can severely impact their stability. For example, chemical species used in RFBs are characteristically steady at temperatures vary between 5 to 40 °C and can (i) precipitate beyond the range, (ii) affects the fluid (electrolyte) flow and (iii) uneven species distribution which results the unstable energy outcomes. Thus, it is imperative to develop an RFB system adaptable to wider range of temperature variation. Therefore, it is important to understand and predict the nonlinear fluid dynamics of RFBs accurately under various climate conditions. Additionally, the computation of electrical power distribution and discharging range changes due to nonlinear fluid dynamics are significant engineering challenges when the scaling up of RFBs is the main purpose. The CFD (Computational Fluid Dynamics) code is considered as one of the most functioning computational tools to analyse complex particulate-fluid dynamics in various conditions. Whereas, advancements in Artificial Intelligence (AI) will surely be very effective to calculate the electrical power distributions in the various phases of electrolytic fluids by developing a novel algorithm. AI-driven approaches can significantly enhance CFD-based modeling by improving computational efficiency, predicting complex interactions, and optimizing energy distribution. Integration of machine learning (ML) algorithms with CFD simulations will allow to accelerate convergence in complex fluid flow simulation, improve real-time prediction of power output variations under different operational conditions. Deep Neural Networks (DNNs) and Convolutional Neural Networks (CNNs) will be explored for their ability to model the complex, high-dimensional relationships governing electrolyte flow and energy distribution in Redox Flow Batteries (RFBs). DNNs, with their multi-layered architecture, can approximate the nonlinear behaviour of fluid dynamics and predict electrolyte flow patterns beyond the scope of traditional numerical simulations. CNNs, on the other hand, are particularly effective in recognizing spatial patterns in fluid flow and electrochemical reactions by processing image-based data from CFD simulations. These networks will be trained using experimental and simulated datasets to enhance the accuracy of electrolyte species distribution predictions, optimizing system stability under varying environmental conditions. In parallel, Reinforcement Learning (RL) will be investigated to dynamically optimize electrolyte flow and power distribution in real-time. By treating flow control as a decision-making problem, RL algorithms such as Deep Q-

	Networks (DQN) and Proximal Policy Optimization (PPO) will be implemented to continuously adjust flow rates, pressure, and temperature based on real-time feedback. These models will learn optimal policies by interacting with CFD-generated environments, gradually improving performance to ensure stable and efficient energy generation. The combination of RL with CFD simulations will allow the system to adaptively respond to environmental fluctuations, minimizing energy losses and improving the large-scale feasibility of RFB technology. The aim is to develop an advanced AI-integrated CFD model for optimizing electrical power distribution in electrolytic fluids, enabling the commissioning of a large-scale RFB battery system with a capacity exceeding 500 MWh. Objectives: 1. Develop a controlled RFB geometry and implement CFD simulations to model multiphase fluid dynamics using advanced computational techniques. 2. Create an AI algorithm capable of integrating with the CFD model to optimize energy generation predictions and enhance computational efficiency. 3. Utilize machine learning techniques to process, train, and validate CFD simulations with experimental and collected data, ensuring model accuracy and reliability. Keywords: Large-scale energy storage; Artificial Intelligence; Redox Flow Battery, Machine Learning for CFD, High-Performance Computing (HPC), AI-Integrated Simulation
Relevance of the topic to the objectives and priorities of the strategic research thrust	The proposed fellowship activities are closely aligned to the research theme "Towards sustainable technologies, blue and green growth and a healthy sea" proposed by Klaipeda University. The outcomes from this research will result an advanced and user-friendly computational tool be applicable in decision making and bringing quick and affordable solution for energy sector in EU and globally to reach the decarbonization benchmarks with the alignment of REPowerEU and Green Deal concepts.
Planned intermediate and final outputs (scientific outputs: publications, presentations, etc.)	1. Scientific Publications The research aims to contribute to the scientific community by publishing findings in high-impact journals. The planned outputs include: • First Scientific Article (Q1-Q2 Journal, Year 1-2. Development of the AI-integrated CFD model for simulating multiphasic fluid flows in an RFB system. • Second Scientific Article (Q1-Q2 Journal, Year 2): AI-driven predictive modeling and experimental validation of large-scale RFB system performance. 2. Conference Participation • To disseminate research findings and engage with the scientific community, participation in at least one international conference is planned. 3. Additional Potential Outputs • Engaging with industry partners and academic collaborators for future projects and funding opportunities.
Requirements for the trainee	Candidate must hold a PhD in Information Technology, Chemical Engineering, or Computer Engineering The preferred experience in computational modelling and simulation using tools such as ANSYS, Open-

	FOAM, or MATLAB. A solid background in programming, coding, and Artificial Intelligence (AI) is also preferred.
Provisioning of the subject (infrastructure, link to ongoing projects)	The candidate will get the opportunities work with a team of scientists and researchers with extensive experience in CFD, AI, Electrochemical Reaction Engineering and multidisciplinary expertise. The research will utilize the laboratory infrastructure accumulated by ISK and IK, which includes various types of sensors, actuators, data acquisition, and processing equipment. Equipment purchased through the "University Excellence Initiative" project for the establishment of the Center of Excellence for Coastal Sustainable Development will also be used. The project is linked to ongoing projects such as Thermochemical Heat Recovery and Upgrade for Industrial Processes and Horizon EU-CONEXUS Enables.
Expected traineeship supervisor	Supervisor: Doc. Dr. Mindaugas Kurmis Co-supervisor: Dr. Khan Mohammad Jakir Hossian (CFD, modelling, Data Analysis) ; email: Khan.mohammad-jakir-hossian@ku,lt ; cell:+37069603676
Supervisor's experience on the proposed topic	Dr. Mindaugas Kurmis, is the head of the Department of Informatics and Statistics, specializing in the application of informatics in various engineering fields. Together with co-authors, he has published 13 CA WoS publications and has led or participated in more than 10 interdisciplinary national and international projects. Currently, he is leading HORIZON projects WP, including Thermochemical Heat Recovery and Upgrade for Industrial Processes in Lithuania, R&D development at UAB Gutsaga Technologies, and serving as the project manager for Klaipėda University as a partner institution. Dr. Khan has extensive experience in CFD simulation, Scale-up, Optimization, electrochemical system designing and process control. He has participated several project applications under HORIZON, M-ERA.NET, EIC Pathfinder and Interreg Baltic programs.