REU Site: Integrating Research in Sustainable Energy and the Environment across Disciplines
(IR-SEED)

Summer 2015 IR-SEED REU Program: June 1 to August 7, 2015

1. Impact of Membrane Material in the Electrodialysis Metathesis Process for Desalination of Salty Water (Dr. Camacho, Assistant Professor in Environmental Engineering)

The main goal of this project is to produce drinking water by EDM. A major question to be answered during the course of this experimental research study is if commercially available ion-exchange membranes are suitable for selective separate monovalent and divalent ions and cations to generate drinking water as final product. Answering this key question will allow select additional parameters accordingly. The EDM separation process depends not only of the type of membrane but also on process conditions such as feed composition, feed concentration, pH, flow rate and voltage. In this research study, process parameter conditions will be maintained constants while different types of membranes will be tested. Initially, seawater will be simulated to test the membranes. Real seawater samples will be tested once the optimal membrane is selected. Seawater contains monovalent as well as divalent ions. During the separation process a diluted and a concentrated stream will be generated. Depending on the properties of the membrane used, the ions concentration of the diluted stream can be reduced to its minimum to produced drinking water.

iii. Undergraduate Research Opportunities: An Undergraduate student will conduct laboratory research experiments for 10 weeks during the summer, sponsored by the NSF-REU program and under the supervision of a Ph.D. student in the Department of Environmental Engineering. The student will have the opportunity to 1) learn about cutting edge technologies for desalination of water; 2) have hands-on experience on EDM technology; and 3) learn about laboratory techniques applicable to environmental engineering.

2. Feasibility of Using Desalination Concentrate for Hydraulic Fracturing Fluid (Faculty Advisor: Dr. Clapp, Professor in Environmental Engineering)

i. Motivation: The oil and gas industry uses large amounts of water for hydraulic fracturing operations in the Eagle Ford Shale. Currently, freshwater is primarily used for hydraulic fracturing operations; however, other sources of water, including wastewater effluent and brackish groundwater, could be substituted for freshwater. This would preserve freshwater resources for other uses.

ii. Project Description: Desalination is becoming more common in South Texas. When brackish groundwater is desalinated, a residual high-salinity "concentrate" stream is produced. This project is evaluating the feasibility of using desalination concentrate streams as make-up water for hydraulic fracturing fluid. If feasible, this would result in two benefits: 1) a low-cost source of water for the oil and gas industry, and 2) a low-cost concentrate disposal option for inland desalination facilities. However, the oil and gas industry is concerned about the formation of

grid by 2025. The integration of photovoltaic thermal systems in residential buildings is a promising solution to achieve this goal. Nevertheless, existing researches mainly evaluate the energy savings potential without considering the impact of occupancy behavior or optimized system design matching real energy requirement. This project investigates the system in a holistic manner.

<u>ii. Project Description:</u> The objective of the proposed project is to establish a ‘benchmark’ for integration of photovoltaic thermal systems in residential buildings and investigate their energy and environmental impacts. Specifically, the following activities describe the tasks required to achieve the objective and bridge the research gaps previously mentioned.

Task 1: Establish energy use pattern and occupancy behavior model. A comprehensive questionnaire will be developed to collect energy consumption information in various local families. Based on the questionnaire results, one or several typical energy use patterns will be established. Then one representative family will be selected (for each pattern) to perform real time monitoring of energy consumption and occupancy behavior. The ultimate result for this task will be a practical energy use profile and occupancy behavior model.

Task 2: Solar energy resource analysis and photovoltaic system design. This task is

Task 1: Measurement of water temperature of Corpus Christi Bay. The National Oceanographic Data Center [1] provides useful water temperature information at sea surface. However, these data cannot be used in assessing WSHP performance because the water temperatures at intake are generally different from the surface temperatures. So the first task of this project will be to measure the water temperature at several depths under surface possible to be water intake for WSHP system.

Task 2: Predictive model for water temperature. In practice, water temperatures are often including core definition, meshing, calculation, and visualization. This innovative extension of commercial FEA software to nuclear engineering will bridge ME and NE and provide an alternative and versatile tool for nuclear reactor simulations.

10. Kinetic Monte Carlo Simulation of Hydrogen Diffusion in Tungsten Bulk (Faculty Advisor: Dr. Yang, Assistant Professor in Mechanical and Industrial Engineering)

<u>i. Motivation:</u> Tungsten is one of the most promising divertor plate candidate materials to be used in ITER fusion reactor. Low hydrogen isotopes constantly impinge the tungsten surface. Some of them will be bounced back, while the others will be trapped in the tungsten bulk. For safety and economic reasons, it is important to understand the behavior of the hydrogen isotopes in tungsten bulk.

<u>ii. Project Description:</u> Based on the success of kinetic Monte Carlo (KMC) simulation of the hydrogen diffusion on tungsten surface [1]. This methodology can be extended/applied to 3-D hydrogen diffusion in tungsten bulk modeling. The students involved in this project will first find the hydrogen trapping sites and energy barriers using nudged elastic band calculation, or acquire this information from existing DFT literatures. Then, the student will design KMC algorithm for 3-D hydrogen diffusion in tungsten and write corresponding code and perform KMC simulations. The simulation results will be verified against existing experiment measurement. The student shall have basic knowledge of crystallography and one programing or scripting language, like MATLAB.

<u>iii. Undergraduate Research Opportunities</u>: Undergraduate students will participate in all aspects of the proposed research activities. The students will practice literature survey to study the background and the existing related work. The students will learn the KMC method and design the KMC algorithm for the simulation of 3-D hydrogen diffusion in tungsten bulk. The students will also sharpen their scientific computing skills, and learn how to validate their simulation results with previous experiment data.