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)
i. Motivation: Electrodialysis metathesis (EDM) is an electrochemical membrane separation process that uses ion-exchange membranes and current to separate ions by double decomposition. The process can be applied to desalinate salty water. In order to obtain optimum desalination efficiency, appropriate parameter conditions and membrane types should be selected.
ii. Project Description: 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 time, 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 hand-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

"scale" (i.e., salts that precipitate from solution at the high temperatures and pressures in the shale formation). To address this concern, two major research questions will be examined in this project: 1) What is the chemical composition of the concentrate stream from a brackish groundwater desalination plant located in the Eagle Ford Shale, and 2) What is the potential for scale formation if this water is used as hydraulic fracturing fluid? The following activities will be conducted in this project to address these research questions: 1) Conduct a chemical analysis of the concentrate stream from the desalination facility; 2) Conduct an analysis of the geochemistry of the shale formation; and 3) Perform geochemical modeling to assess the potential for scale formation in the concentrate stream were to be used as hydraulic fracturing fluid.

iii. Undergraduate Research Opportunities: Undergraduate students will participate in all aspects of the proposed research activities. The students will learn 1) how to collect and preserve water samples; 2) how to perform various field water quality analyses (e.g., pH and conductivity), 3) how to conduct various laboratory water quality chemical analyses (e.g., alkalinity); and 4) how to perform basic water chemistry modeling. The students will also participant in the development of presentations.

3. Influence of SCIG and DFIG Based Wind Turbine on the Voltage Stability of a Weak Distribution Power Grid (Faculty Advisor: Dr. Masaud, Visiting Assistant Professor in Electrical Engineering)

i. Motivation: The integration of wind energy into the power grid has become a major concern for power system engineers today. Utilities are seeking to understand possible impacts on system operations when a variable and constant speed wind turbines are introduced into the electric power system. Voltage stability is a key factor to achieve a successful integration of wind power into power grid that needs to addressed and analyzed.

ii. Project Description: The project presents a comparative study of the impact of squirrel cage induction generator (SCIG) and doubly fed induction generator (DFIG) type wind turbine on the voltage stability of a distribution grid. Both static and dynamic analyses will be carried out to see the influence of two different wind turbine generators on the voltage stability of a weak distribution network.

iii. Undergraduate Research Opportunities: Undergraduate students will participate in all aspects of the proposed research activities. The students will be able to 1) understand and distinguish between fixed and variable speed wind turbine induction generators, 2) Under constant and variable speed wind turbines, what are the voltage stability, and reactive power support issues?, 3) participate in computer model simulations to aid them pertaining to understanding of complex electric power systems.

4. Two-Axis Position Control of Solar Panels for Maximum Efficiency (Faculty Advisor: Dr. Ozcelik, Professor in Mechanical and Industrial Engineering)

Fixed solar panels do not receive sunrays in a direction to generate maximum current (power) throughout the day due to sun movement. To increase the efficiency of a solar panel (large scale), a mathematical model for the dynamics of a two-axis (rotating along elevation and azimuth angles) large scale solar panel will be studied and developed. Based on historical data and sun's movement, a control system is to be designed to track sun's position so that solar panels can receive sun rays in a perpendicular direction so that current generated is maximized, hence efficiency is increased. A prototype is to be designed and tested.

5. Dynamics and Control of Wind Turbines (Faculty Advisor: Dr. Ozcelik, Professor in Mechanical and Industrial Engineering)

Study the modeling and control of vibrations in wind turbines due to change in the rotational speed of the blades. Review the basic structure of wind turbines and then describe wind turbine control systems and control loops. Focus on generator torque and blade pitch control systems for performance improvements. Plan to perform simulations using Matlab/Simulink.

6. Regeneration of Toxic Vapor-Saturated Activated Carbon via Microwave Energy (Faculty Advisor: Dr. Ramirez, Associate Professor in Environmental Engineering)

i. Motivation: Energy conservation is important for a sustainable societal development. Reduced energy consumption through conservation can benefit not only energy consumers by reducing their cost but also the society in general by reducing the use of energy resources and consequently the reduction in emissions of air pollutants. Microwave regeneration can be an energy efficient technology for the capture and recover of toxic vapors emitted from industrial sources.

ii. Project Description: The desorption efficiency of activated carbon using microwave energy will be investigated by considering operating parameters such as volumetric flow rate and temperature on a laboratory scale experimental set up. The microwave energy will be generated at a frequency of 2.45 GHz and used to maintain the temperature range of 150°C to 200°C to heat activated carbon previously saturated with hazardous air pollutants (HAPs). Examples of HAPs to be used include benzene, toluene, ethylbenzene and xylene isomers (BTEX). The research activities to be conducted are 1) set up and test a microwave-assisted adsorption-desorption system for the capture and recover of BTEX mixtures, 2) to conduct tests that will help elucidating the effects of gas flow rate and temperature on the regeneration of BTEX captured on activated carbon, and 3) analysis of microwave energy consumption over conventional regeneration systems. It is expected that the BTEX mixtures are recovered as liquid by condensation. Microwave energy has the advantage of not inducing unwanted chemical reactions because the energy of microwaves is lower than the ionization energies of van der Vaals intermolecular interaction among BTEX molecules and lower than the energy associated with the Brownian motion of HAPs molecules.

iii. Undergraduate Research Opportunities: The undergraduate student participant will conduct the proposed research activities with a doctoral student. The undergraduate researcher will 1) be trained on setting up and testing a microwave-swing adsorption system, 2) get hands-on training on gas-phase generation of BTEX mixtures, use of a portable air toxic monitoring instrument based on gas chromatography-flame ionization detector, and a photoionization detector, and 3) learn how to use data analysis tools for the comparison of energy consumption of different regeneration technologies.

7. Integration of Photovoltaic Thermal Systems in Residential Buildings for Energy Saving (Faculty Advisor: Dr. Shen, Assistant Professor in Civil and Architectural Engineering)

i. Motivation: Residential buildings in U.S. consume a large amount of energy. They are one of the heaviest consumers of natural resources and account for a significant portion of the greenhouse gas emissions that affect climate change. DOE is taking ongoing efforts to develop marketable Net-Zero Energy Buildings, which use state-of-the-art efficiency technologies and on-site renewable energy generation to reduce consumption and offset their energy use from the 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.

ii. Project Description: 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 committed to analyze the available annual solar energy resource and estimate the capacities of different photovoltaic systems including electricity production, water heating and solar cooling (space heating is not considered for the hot local climate). Real-time measurement of solar radiation and photovoltaic efficiency will be performed under real operation conditions. Simulations with professional tools will also be employed to model system capacities.

Task 3: Customize optimal photovoltaic systems. In this task, an optimized multi-functional photovoltaic system will be developed for each residential building type combining results from task 1 and task 2. Annual analysis of energy consumption and greenhouse gas emission will be simulated and compared with the current building conditions. A payback time will also be calculated upon market available prices of system components, labor cost, utility prices and potential energy rebate and incentives.

iii. Undergraduate Research Opportunities: Undergraduate students will participate and learn during the whole period of the proposed project. Expected learning experiences include 1) development of a comprehensive questionnaire, analysis of the results and drawing conclusions; 2) hands-on experimental skills; 3) solar energy calculation and 4) professional software operation. The students will also participate in the dissemination activities.

8. Application of Seawater-Source Heat Pump in Hot Climate (Faculty Advisor: Dr. Shen, Assistant Professor in Civil and Architectural Engineering)

i. Motivation: Water-source heat pump (WSHP) has gained considerable interest in recent years for its potential of energy and environmental savings. There have been many successful applications in North Europe, Korea and Japan. The city of Corpus Christi is bordered by a long coastline and therefore has the natural advantage to utilize this type of system. The performance of WSHP is greatly influenced by water temperature at intake, but this information is usually missing for system designers. This research will study the seawater temperature variation and investigate the applicability of WSHP in hot climate area like Corpus Christi.

ii. Project Description: The objective of the proposed project is to develop a predictive model for seawater temperature of Corpus Christi Bay and investigate the potential of WSHP application. The following activities will be conducted to achieve the objective.

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 obtained from regression equation based on measurement if long-term measurement is not available. In fact, even if an annual measurement can be performed, the data are not universal for different year utilizations. So a reliable model predicts water temperature is essential and valuable. Existing models in literature will be examined against measured data and then improvements will be made to develop a new model. Additionally, water temperature at different depths will be investigated as well.

Task 3: Assess the potential of using WSHP in hot climate area. In this task, the annual performance of WSHP system will be simulated and compared with traditional air-conditioning systems. Water temperatures at different depths will be investigated to identify the proper system water intake location and evaluate the energy and environmental saving potential.

iii. Undergraduate Research Opportunities: Undergraduate students will participate and learn during the whole period of the proposed project. Expected learning experiences include 1) hands-on experimental skills; 2) data processing and model development and 3) professional software operation. The students will also participate in the dissemination activities.

9. Bridging FEA Software in Mechanical Engineering to Nuclear Reactor Neutronics Simulations (Faculty Advisor: Dr. Yang, Assistant Professor in Mechanical and Industrial Engineering)

i. Motivation: The neutron diffusion equation, the simplified form of Boltzmann neutron transport equation, is adequate to accurately determine the neutron flux in present thermal-neutron reactors, and can be solved by finite element analysis (FEA) method for various 1-D, 2-D, and 3-D reactor geometries. However, this task is rarely done by the commercial FEA software widely used in mechanical engineering (ME), despite their superior capabilities for solving multiphysics engineering problems. Therefore, the goal of this project is bridging FEA Software in ME to reactor neutronics simulations.

ii. Project Description: The student of this project shall have working knowledge of one of the FEA software, such as ANSYS, and some background of numerical methods for partial differential equation. The goal of this research is to solve the neutron diffusion equation to acquire the multiplication factor and neutron flux profiles of 2-D and 3-D nuclear reactors using one of the commercial FEA software. This outcome can be achieved by the following major steps: 1) Review the numerical methods for neutron diffusion equation and the capabilities of the FEA software. 2) Define the geometry and material properties of a 2-D/3-D reactor. 3) Use the built-in meshing module to discretize the reactor geometry. 4) Define the differential equation over each mesh. 5) Perform the calculation and verify the results with the references.

iii. Undergraduate Research Opportunities: Undergraduate students will participate in all aspects of the proposed research activities. The students will learn the numerical methods associated with neutron diffusion equation, explore how to use FEA commercial software to model nuclear reactors, design parallel computing algorithm, and produce eye-popping neutron flux images/animations. The success of this project will unify all reactor simulation processes 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)

i. Motivation: 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.

ii. Project Description: 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.

iii. Undergraduate Research Opportunities: 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.