

# Earth & Environmental Engineering Graduate Student Symposium 2017



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The Fu Foundation School of Engineering and Applied Science

## Introduction

The Department of Earth and Environmental Engineering is pleased to announce the 1<sup>st</sup> EEE Graduate Student Symposium will take place on October 27<sup>th</sup> 2017. The main objective of this symposium is to provide participants with broader insight of research being conducted within the department. The symposium is aimed towards graduate students in the department and will provide a forum to present their research and engage other students and faculty outside of their own research group. Two oral presentation sessions and a poster session will allow presenters to refine presentation skills and gain experience.

Highlights of the symposium include an opening keynote presentation given by a graduate of the EEE program, Dr. MaryTherasa Pendergast, who is now the director of research at OASYS Water in Boston, Massachusetts, as well as a closing keynote presentation that will be given by our department's own Prof. Pierre Gentine.

We warmly welcome all graduate students and faculty within the department to participate in this years symposium.

## Agenda Overview

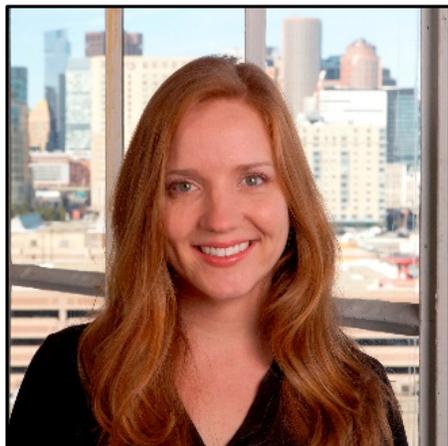
Date: Friday October 27<sup>th</sup> 2017  
 Time: 1:00 – 7:30 pm  
 Location: Oral Presentations: Davis Auditorium (412 CEPSR)  
 Poster session: 414 CEPSR

Davis Auditorium can be found on the Columbia University campus map here:  
<http://apam.columbia.edu/directions-davis-auditorium-cepsr>

The agenda for the workshop incudes opening and closing keynote presentations, 2 student presentation sessions and concludes with refreshments and a poster session.

Time	Event
1:00 PM	Welcome (Prof. Peter Schlosser & James Doss-Gollin)
1:15 PM	Opening Keynote: Dr. MaryTheresa Pendergast (pg. 3)
2:15 PM	Session 1: Water Resources, Sustainable Energy and Health Engineering (pg. 5)
3:30 PM	Break
4:00 PM	Session 2: Carbon Management and Hydrological Modeling (pg 5)
5:15 PM	Closing Keynote: Prof. Pierre Gentine (pg. 4)
6:15 PM	Closing Remarks
6:20 PM	Break
6:30 PM	Poster Session (pg. 6)
7:30 PM	Workshop Concludes

## Keynote 1: Dr. MaryTheresa Pendergast



Dr. MaryTheresa Pendergast has a range of experience in water treatment technology research, design, and project management focused on membrane-based systems and applications. As Director of R&D at Oasys Water, she is leading a team to develop forward osmosis enabled solutions for treatment of the world's most challenging waters through innovation in membrane performance, low energy draw solution recovery, and integrated systems design. MaryTheresa is a recognized and established author in the academic and water industry communities, and has published more than 24 journal articles and proceeding papers since 2007. She is an alumnus of the Earth & Environmental Engineering program, where she earned a B.S. in 2009, and holds an M.S. and Ph.D. from the University of California, Los Angeles.

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### Membrane-Based Solutions for Challenging Waters

MaryTheresa M Pendergast, Ph.D.<sup>1</sup>

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#### Abstract

The frontier of water treatment is being defined by hybrid approaches and thoughtful design integration. The use of increasingly sophisticated processes is driven by the need to treat dramatically impaired water supplies while maintaining low cost, high utilization, and high operational flexibility. Industrial wastewaters present an additional challenge, with increasing regulations and water scarcity driving the demand for novel approaches to treatment and reuse. Integrating membrane technologies into water treatment trains is one notable opportunity to realize substantial advantages in cost and performance compared to the use of more conventional processes.

Reverse osmosis is ideally suited to desalinate low fouling streams to moderate levels of recovery. Recent innovations in reverse osmosis membranes and process design have enabled higher levels of recovery, extending the possibilities for application. Beyond reverse osmosis, the traditional answer for high salinity wastewater concentration is thermal evaporation. Dryers and crystallizers are typically used to convert saturated or organic rich liquors to solid products when zero liquid discharge is required; however, these unit operations are energy intensive and require high capital investment. Today, forward osmosis based brine concentration, enabled by high performance draw solutions and materials, is challenging this traditional paradigm. The integration of forward osmosis provides the opportunity to do more work with membrane-based processes and lessen the reliance on thermal systems, thereby reducing energy demand and capital costs. Equally important as the proper selection of technologies, is the integration of the unit operations and design of tailored pretreatments to enable robust, reliable solutions.

In this discussion, we will cover membrane separations and explore how the integration of novel membrane technologies, in particular forward osmosis, provides new opportunities to deliver flexible and cost-effective solutions to treat difficult industrial wastewaters, minimize brine streams, and recover fresh reusable water.

## Keynote 2: Prof. Pierre Gentine



Prof. Pierre Gentine is a professor in the department of Earth and Environmental Engineering. He obtained his MSc and PhD from MIT. Pierre Gentine is working on land-atmosphere interactions, convection-clouds, and surface hydrology using conceptual models, numerical models and wide range of data analysis tools. His overall research objective is to understand how soil and atmospheric moisture organizes across different spatial and temporal scales and in particular how the interactions with the atmosphere, vegetation and landscape constrain this organization. Dr. Gentine has research interests in Land-atmosphere interactions, Hydrometeorology, Convection, Ecohydrology, Remote sensing, data assimilation of remote sensing measurements to estimate soil moisture and surface heat fluxes, Land-surface models, and Stochastic processes.

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### Impact from rising CO<sub>2</sub> on the hydrological cycle

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#### Abstract

The water and carbon cycles are ultimately coupled. I will discuss the implications of this coupling for climate change and our capacity to predict those two cycles. I will then present opportunities of fence remote sensing observations to better constrain their link.

**Session #1: Water Resources, Sustainable Energy and Health Engineering**

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2:45	Chen, Xi	Sustainable Energy Production with Low-Temperature Heat using Vapor Pressure-Driven (VPD) Membrane Technology: Impact of Membrane Chemistry and Structure	9
3:00	Tian, Yixi	Production of structural concrete from waste to energy bottom ash	10
3:15	Tong, Zi-Xiang	Coarse-grained area-difference-elasticity membrane model coupled with IB-LB method for simulation of red blood cell morphology	11

**Session #2: Carbon Management and Hydrological Modeling**

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5:00	Massmann, Adam	When does vapor pressure deficit drive or reduce evapotranspiration?	16

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**Support**

This symposium would not have been possible without the dedication of the organizing committee: James Doss-Gollin, Martha Arellano and Kenneth Sinclair. Guidance from Prof. Yip and Elizabeth Allende's assistance was also highly appreciated. The symposium was made possible with generous support from the EEE department. Poster boards were graciously borrowed from the Columbia Nano Initiative.

# Assessing the effects of bisphenol-A exposure on the structure and function of microbial communities involved in nutrient removal

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<sup>2</sup> Black & Veatch

## Abstract

The environmental persistence and ecological impacts of trace organic contaminants (TOrcs)<sup>1</sup> are cause for growing concern. Because wastewater streams are significant sources of TOrcs in the environment,<sup>2</sup> wastewater treatment plants (WWTPs) hold the potential to serve as barriers for these contaminants of emerging concern. While biodegradation of a range of such compounds has been reported in WWTPs and nitrifying and denitrifying systems,<sup>3,4</sup> the roles of specific bacteria and biodegradation mechanisms remain unclear. Our research aims to understand which bacteria and metabolic mechanisms are involved in TOrc degradation by assessing effects of TOrc exposure on microbial community structure and function. In this work, we have investigated degradation and assimilation of the endocrine disrupting compound Bisphenol-A (BPA) by several microbial communities relevant to biological nutrient removal (BNR).

Separate batch BPA-exposure incubations were conducted with biomass from two suspended growth biological treatment reactors at a New York City wastewater treatment plant: one used for primary effluent treatment and the other used to treat reject water from anaerobic digestion after centrifugation. The biomass specific BPA biodegradation rate was higher in experiments with the microbial community previously treating primary effluent. DNA and RNA sequencing was used to interrogate whether differences in BPA biodegradation kinetics may be related to differences in community structure and metabolic versatility resulting from the diversity and availability of carbon substrates.

Batch experiments with biomass from a mixed culture nitrifying community resulted in incomplete BPA degradation along with decreased rates of nitrification during BPA exposure. 16S amplicon sequencing results reveal that three previously identified BPA-degrading classes were present in the nitrifying enrichment culture, though the potential role(s) of these bacteria in BPA degradation requires further study.

Preliminary results for aerobic batches of an axenic culture of the nitrate-reducing bacteria *Methyloversatilis universalis* FAM5 indicate limited degradation of BPA at an initial BPA concentration of 10 mg-BPA/L, both with and without a supplemental carbon source added. Ongoing research will assess BPA degradation under anoxic conditions relevant to denitrification.

These results suggest that TOrc degradation potential is influenced by treatment processes as well as TOrc exposure conditions. Our approach integrates techniques in molecular biology to probe microbial community structure and function along with substrate depletion analyses. Such fundamental research holds potential to identify opportunities for effective and sustainable TOrc attenuation in existing as well as to-be-developed next generation BNR systems.

# Flexible, Renewable-Powered, Variable-Salinity Reverse Osmosis Desalination

Adam A. Atia<sup>1\*</sup>, Vasilis Fthenakis<sup>1,2</sup>, Ngai Yin Yip<sup>2</sup>, William Becker<sup>1,3</sup>, Pablo Cassorla<sup>1</sup>

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<sup>2</sup> *Brookhaven National Laboratory*

<sup>3</sup> *Hazen & Sawyer*

## Abstract

Conventional reverse osmosis (RO) desalination plants remain costly and are designed to operate under steady-state conditions, drawing large amounts of energy from the grid at a fixed rate. As energy policy pushes towards the use of more renewables on the electric grid, the problems of over-generation and high ramp rates present significant challenges to grid operators, mainly in terms of resulting revenue losses and grid instability. Therefore, there is a need for the design of a novel integrated energy and desalination system that can provide drinking water and vary its energy consumption in a versatile manner to provide electricity system services, while also improving economic and environmental viability. An integrated energy and desalination design is proposed here, where access to seawater, treated wastewater effluent, and renewable energy resources can simultaneously mitigate water scarcity and facilitate services to the electricity system through time-shifting of energy usage, demand-response, and ancillary services. The proposed renewable energy and RO desalination design dynamically controls energy consumption under variable power and salinity conditions. The RO plant utilizes feedwater from low-salinity sources (e.g., treated wastewater) and concentrated sources (seawater). Variable-power pumping, variable feedwater salinity control, and flexible membrane flow configurations are used to enhance demand-response capabilities, compensating for stressors on the grid and fluctuations in renewable power generation, while continuously producing potable water. This system includes on-site renewable power and energy storage to operate the RO plant and supplies electricity to the grid during peak hours. Moreover, the proposed RO system can flexibly adjust its load setpoint in response to ancillary services to provide regulation capacity and spinning reserves when prices are favorable. In addition to flexible load response, this concept enables treatment of both low- and high-salinity feedwater which would ensure a higher system resilience, reduce costs and energy consumption, facilitate brine dilution, reuse wastewater, and could provide retrofitting potential for existing RO plants that lack flexibility in treatment capability and electric load controllability. This project was submitted for the US-Israel Integrated Energy and Desalination Design Challenge, issued by the Department of Energy (DOE). Our team was selected as one of three semi-finalists in the summer of 2016 and was subsequently awarded as the winner of the DOE Challenge in May 2017.

# Sustainable Energy Production with Low-Temperature Heat using Vapor Pressure-Driven (VPD) Membrane Technology: Impact of Membrane Chemistry and Structure

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## Abstract

Industrial waste heat and geothermal energy represent abundant and widely available clean energy sources that are currently underutilized. However, most of the industrial waste heat streams are at low temperatures (below 130 °C), while the temperature of accessible geothermal energy is constrained by the prohibitively high cost of drilling deep wells. The relatively low temperatures of the obtainable waste heat and geothermal energy thus pose considerable technical challenges for utilization by existing technologies. Recently, low-grade heat utilization by vapor transport through a hydrophobic membrane against a pressure difference was demonstrated. The pioneering study shows the promising potential of directly utilizing environmentally available heat resources below 80 °C for high power-density energy generation. A schematic of the process is depicted below.

This study further investigates the impact of membrane chemistry and structural parameters on mass and heat transfer in vapor-pressure-driven (VPD) membrane processes. Membrane materials with different surface hydrophobicity and transport structures are studied. Gradients of temperature difference and operational pressure are also applied to further study the system's potential and analyze the energy consumption/generation tradeoff. A complex indicator,  $bm$ , is also proposed for the first time for better evaluating membrane performance and fabrication for this technology. The findings of this study will enhance understanding of the fundamental principles of the novel VPD membrane technology, and the insights can inform the development of greater conversion efficiency and higher power-density clean energy generation.

# Production of structural concrete from waste to energy bottom ash

Yixi Tian

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<sup>2</sup> Prof. S. Kawashima

## Abstract

Waste-to-energy (WTE) is a widely accepted municipal solid waste (MSW) management technique, applied in over 1,000 plants in the world. The major by-product of the full combustion of mixed MSW with excess air is the incinerator bottom ash (IBA), representing 20-25% of the weight of the MSW combusted. IBA is typically quenched in a water vessel under the discharge end of the moving grate. After recovery of ferrous and non-ferrous metals, IBA is often used in civil engineering applications. The use of IBA in construction requires that it passes leaching tests to ensure that the IBA eluate will not contaminate surface and ground waters. The aim of the project was to assess the viability of using WTE bottom ashes in civil engineering applications and identify the optimum mixture composition for the production of concrete blocks. The raw materials used were three different fractions of IBA: the fine (<0.0787 inches), medium (0.0787-0.375 inches) and coarse (0.375-1 inches). The fine fraction was used to replace sand by 10, 30 and 100%. The medium and coarse fractions were used for the replacement of the aggregates, by 10%, 30%, and 100%. The as-received IBA samples were obtained from two different sources. The water to cement ratio for the production of concrete was 0.5 and the samples were cured for 7 and 28 days. Concrete testing involved the characterization of the mechanical properties, i.e. compressive strength, max load, elastic modulus, standard physical testing, i.e. void content, and leaching behaviour of the samples based on the Leaching Environmental Assessment Framework (LEAF). The results indicated that increasing the use of the fine fraction of IBA in the cement production decreased the mechanical properties of concrete. Concrete samples produced with the medium and coarse fraction of IBA indicated similar or improved properties as compared to concrete blocks produced with naturally derived aggregates. The main finding of the research is that the mechanical properties of samples produced with the various fractions of IBA are higher as compared to the residential and commercial concrete values. Therefore, these materials can be safely used in the construction and replace the naturally derived materials.

# Coarse-grained area-difference-elasticity membrane model coupled with IB-LB method for simulation of red blood cell morphology

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## Abstract

The morphological evolutions of red blood cells (RBCs) in fluid environment have attracted many research interests, which cannot be effectively revealed by continuum elastic membrane models. We propose a coarse-grained membrane model based on the area-difference-elasticity (ADE) model, and integrate the immersed boundary (IB) method and lattice Boltzmann (LB) method for the simulations of vesicles and RBCs. The membrane's energy is composed of bending energy, ADE energy, area energy and the elastic energy of the membrane skeleton. The automatic difference is used to calculate the derivatives of the energy and therefore the forces. The fluid environment is solved by the LB method, and the membrane and fluid models are coupled by the IB method.

During the simulations, the cell is initially spherical and then the membranes are enlarged. Since the fluid is incompressible, the volume of the cell is constant and the shape of the cell will deform. The energy of the system will decrease, the cells will evolve through quasi-stable states and finally reach stable states. The reduced volume  $\nu$  is defined by the ratio between the volume of a sphere with the enlarged surface area and the volume of the original cells. The morphology of cells is studied with different  $\nu$  and energy components.

In 2D condition, the cells finally become peanut-like profiles. In 3D conditions, if only bending energy are considered, the cells show the prolate-oblate-stomatocyte transition with decreasing reduced volume (Fig. 1). If all energy components are included, the stomatocyte–discocyte–acanthocyte transition of the cell morphology is recovered with increasing area difference between the two leaflets of the membrane (Fig. 2-3). Therefore, the proposed numerical model is capable to simulate the morphology of the RBC in various scenarios. This model can be further employed to study the deformation of cells in blood flows.

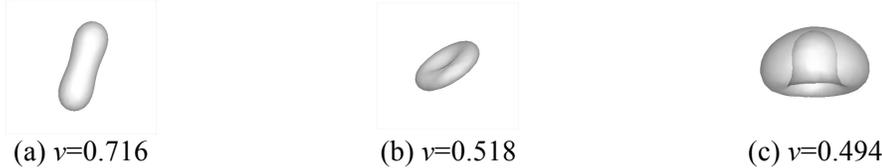


Fig. 1 The final equilibrium shapes of the 3D membrane for different reduced volume

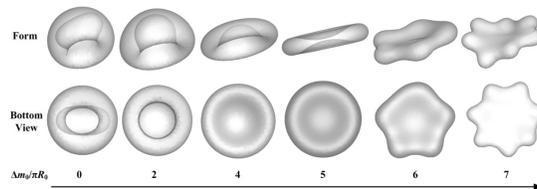


Fig. 2 The shapes of the membrane when  $\nu=0.414$  and  $\Delta m_0=0 \sim 7\pi R_0$

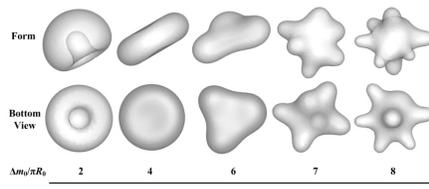


Fig. 3 The shapes of the membrane when  $\nu=0.716$  and  $\Delta m_0=2\pi R_0 \sim 8\pi R_0$

# A Kinetic study on the dissolution of heat-treated Serpentine for Permanent CO<sub>2</sub> storage

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## Abstract

The ever increasing atmospheric CO<sub>2</sub> concentration is becoming a more and more significant environmental issue, which leads to an increasing risk and uncertainty to the climate and the ecology. In order to reduce the atmospheric CO<sub>2</sub> concentration, people have developed different technologies to capture, utilize and store CO<sub>2</sub> (CCUS), either from concentrated CO<sub>2</sub> emission point sources or from air. One of the CCUS technologies to permanently immobilize CO<sub>2</sub> and keep CO<sub>2</sub> away from atmosphere is called mineral carbonation, which reacts CO<sub>2</sub> with Mg or Ca-bearing silicate to produce stable, environmentally benign and insoluble carbonates where CO<sub>2</sub> is firmly fixed. Serpentine ((Mg, Fe)<sub>3</sub>(OH)<sub>4</sub>Si<sub>3</sub>O<sub>5</sub>) is a hydrated magnesium silicate, which has a large CO<sub>2</sub> mineralization capacity to mineralize a significant quantity of the anthropogenic CO<sub>2</sub> emissions. However, it cannot be neglected that the low reactivity of Serpentine makes a large difficulty to extract Mg from the mineral and thus the kinetics for CO<sub>2</sub> to be mineralized is largely limited. In order to enhance the reactivity of the mineral, the researchers have put forward the method of heat treatment to activate the mineral in the previous studies. The reason serpentine can be activated in this way is that lattice can be disordered and the previously confined Mg in the lattice with low chemical potential can be released during the heat treatment process. As a result, a reliable method to evaluate the reactivity of the heat-treated Serpentine (HT Serpentine) mineral is important to study the effect of the heat treatment on mineral activation and optimize the heat treatment conditions. In a typical mineral carbonation process, Mg is first extracted from the HT Serpentine mineral and then employed to produce carbonates. Thus, the reactivity of the HT Serpentine should be evaluated by its dissolution kinetics. However, the research on the kinetics of HT Serpentine dissolution is still rather limited. The fact that the ash layer of silica can build up during the dissolution process and the rate control mechanism can change from the chemical reaction to mass transfer makes it relatively complicated to model the dissolution kinetics and distinguish different stages of this process. Without a clear recognition and understanding of different stages of the dissolution process, the calculation of the kinetics parameters and the evaluation of the mineral reactivity cannot be very instructive. The comparison of the reactivity of different minerals can also be challenging. In this study, we will study the dissolution kinetics of HT Serpentine to evaluate the reactivity the HT Serpentine. We'll first build up the kinetics model based on previous studies to depict the dissolution process with different stages controlled by different rate-limiting mechanisms. Then, the results of the HT Serpentine dissolution experiments with a differential bed reactor (DBR) setup will be reported. The kinetics model will then be applied on the experimental data to observe the different stages of the dissolution process. The values of the critical ash layer thickness at the turning points between different stages are also calculated. The validity of our method will be checked by comparing the ash layer thickness visualized with the SEM-EDS test and that predicted by our model. Then, the kinetics parameters of different stages, including the reaction order, the reaction activation energy and the apparent activation energy at the mass transfer control stage, will also be calculated so that the reactivity of the HT Serpentine sample can be comprehensively evaluated for the entire dissolution process. Hopefully, our study can provide new insights into the evaluation of the HT Serpentine reactivity and can help us to better understand the kinetics of the HT Serpentine dissolution process.

# CO<sub>2</sub> Capture and Conversion on Ru-Na Dual Functional Materials (DFM)

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## Introduction

Increasing demand of energy obtained from fossil fuel combustion and other processes induces accumulative impacts of emitted CO<sub>2</sub> contributing to the green-house gas effect. The “state-of-the-art” is CO<sub>2</sub> capture and sequestration (CCS), using aqueous amine solutions having the major drawback of an energy-intensive regeneration step to separate the CO<sub>2</sub> and H<sub>2</sub>O from the amine. Dual Functional materials (DFM) solids, first disclosed by Duyar et, al <sup>[1]</sup> offers a unique solution by capturing and catalytically converting chemisorbed CO<sub>2</sub> in situ to CH<sub>4</sub> or synthetic natural gas (SNG) from a simulated industrial flue gas. The source of H<sub>2</sub> is water electrolysis from excess renewable energy (solar and/or wind). By capturing and converting CO<sub>2</sub> in the hot flue gas no external heat is required. The process is carried out at the same temperature in one solid material thereby circumventing the energy penalty of CCS. The SNG produced is then recycled to the inlet of the power plant thereby approaching carbon neutrality. The original DFM with a composition of 5% Ru, 10% CaO/Al<sub>2</sub>O<sub>3</sub> has been investigated and shown to have stable cyclic performance of CO<sub>2</sub> adsorption and methanation in a simulated flue gas containing oxygen and steam. <sup>[2]</sup>

We have now demonstrated that sodium and/or potassium carbonate, in concert with 5% Ru on gamma Al<sub>2</sub>O<sub>3</sub>, enhance CO<sub>2</sub> capture capacity and methanation by nearly two fold that relative to the original materials under the same experimental conditions. <sup>[3]</sup> Cyclic aging tests in simulated flue gas, using 5\*5 mm particulates, have successfully demonstrated stable performance.

The carbonates not only adsorb CO<sub>2</sub>, but can also be catalytically hydrogenated to CH<sub>4</sub> at 320°C, 1 atm. resulting in increased CO<sub>2</sub> adsorption and enhanced methane production. Using Ru-Na<sub>2</sub>CO<sub>3</sub> on Al<sub>2</sub>O<sub>3</sub>, as the DFM, the rate limiting step appears to be hydrogenation of the bulk carbonate while methanation of adsorbed CO<sub>2</sub> on the Ru and on the carbonate surface is rapid. We are reporting a parametric kinetic study for methanation of adsorbed CO<sub>2</sub> as a function of hydrogen partial pressure, temperature, and carbonate loading to optimize the process and composition of the DFM.

## Materials and Methods

The DFM studied is 5% Ru, 10% Na<sub>2</sub>CO<sub>3</sub>/Al<sub>2</sub>O<sub>3</sub> prepared via a precipitation from aqueous solution. The data presented was obtained using thermogravimetric analysis (instruments: TG 209 F1 Libra NETZSCH and/or SAT 449 F3 Jupiter NETZSCH) and a large scale fixed bed reactor (analyzer: Enerac-700) containing 5\*5 mm particulate materials. The data used to generate the empirical rate law for carbonate hydrogenation is shown in Table 1. The hydrogenation conditions for the kinetic study were derived from the cyclic aging tests in the large scale fixed bed reactor shown in Figure 1.

## **A combination of catalysts and adsorbents for in-situ conversion of CO<sub>2</sub> to synthetic natural gas**

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### **Abstract**

We report the advantages of a Dual Function Material (DFM) that combines a CO<sub>2</sub> adsorbent in combination with a catalyst that captures and converts CO<sub>2</sub> in situ to synthetic natural gas (CH<sub>4</sub>) with the addition of H<sub>2</sub> produced from excess solar or wind energy via water electrolysis. This technology offers a new approach towards managing CO<sub>2</sub> emissions while producing a useful fuel while closing the carbon cycle. Different loadings of adsorbents (CaO, MgO, K<sub>2</sub>CO<sub>3</sub> and Na<sub>2</sub>CO<sub>3</sub>) and catalysts (Ru, Rh, and Ni) were compared for CO<sub>2</sub> adsorption and conversion to synthetic natural gas production. All materials rapidly adsorb CO<sub>2</sub> but hydrogenation to CH<sub>4</sub> is highly dependent on the adsorbent and catalyst material. Ni based DFMs cannot completely hydrogenate adsorbed CO<sub>2</sub> at 320°C. Excellence in performance was observed for CO<sub>2</sub> captured on 5%Ru-10%Na<sub>2</sub>CO<sub>3</sub>/Al<sub>2</sub>O<sub>3</sub>.

## Addressing the water-agriculture-ecosystem nexus in a large endorheic river basin using a new ecohydrological model

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### Abstract

Inner-basin water use conflicts are common in arid and semi-arid areas. As the second largest endorheic river basin in China, the Heihe River Basin (HRB) is exemplary of such conflicts between agriculture and ecosystem preservation. The densely distributed agriculture in the midstream consumes a large amount of water for irrigation, which has directly threatened the fragile and water-limited ecosystem in the downstream. To alleviate the conflict between the mid- and downstream and prevent the trend of continuing ecological deterioration of the downstream, an Ecological Water Diversion Project (EWD) has been implemented since 2000 to ensure that enough water is released to the downstream. With the water diversion, an increase in the leaf area index (LAI) has been observed in the downstream. However, to ensure the annually allocated streamflow discharge to the downstream, more groundwater has been pumped for irrigation in the midstream, which has led to declining groundwater levels. How to make water management more sustainable for both agriculture and ecosystem has thus become an urgent issue. Crops and natural vegetation play vital roles in affecting the water cycle, hence it should be well integrated into a hydrological model for water management.

A new Hydrological and Ecological Integrated watershed-scale FLOW model (HEIFLOW) has been developed as part of a major ecohydrological research initiative in the Heihe River Basin. HEIFLOW is based on an improved version of the GSFLOW developed by the U.S. Geological Survey and a General Eco-Hydrological Module (GEHM) developed in this study to simulate plant growth kinetics. The integrated model can represent both hydrological variables including streamflow and groundwater level, and ecological variables including leaf area index (LAI), biomass, and partitioned evapotranspiration (ET). The model has been applied to simulate the ecohydrological conditions in the middle and downstream. It was independently checked by remote sensed LAI and ET products from 2000 to 2012. The model results show a consistently good agreement with the observation data.

Analysis using the new integrated model indicates that the midstream groundwater system is not sustainable under current water use methods. To assess the impact of possible more rigorous water management policy for promoting ecological restoration of downstream, we further set up 2 series of scenarios that represents the reduction of midstream irrigation with and without water-saving agricultural technique respectively. Results of scenario analysis show increasing trends of streamflow discharge to downstream, and midstream storage has a maximum recovery when same quantity of irrigation are all reduced from groundwater, rather than from surface water or proportionally from both sources. Furthermore, midstream storage has trivial changes with evaporative water-saving agricultural technique implemented, mainly due to accordingly increased transpiration(T) and streamflow to downstream. This study could be a paradigm for water-agriculture-ecosystem nexus analysis in other arid and semiarid river basins globally.

## When does vapor pressure deficit drive or reduce evapotranspiration?

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### Abstract

Depending on plant response (e.g. stomatal closure), ecosystem- scale evapotranspiration can either increase or decrease with changes in vapor pressure deficit. This ecosystem response drives evapotranspiration and atmospheric moisture feedbacks. We use data from 75 FluxNet sites within a Penman-Monteith framework to examine when ecosystem evapotranspiration is suppressed or enhanced by increases in vapor pressure deficit. Evapotranspiration response is quantified as a function of soil moisture, atmospheric conditions, and plant functional type. The framework is designed so model and observational uncertainties are represented in the results. This in-situ observation-based analysis aids understanding for how ecosystems will respond and/or contribute to future shifts in atmospheric water demand.

## RE-ENGINEERING the Nitrogen Cycle: A Novel Microbial Treatment Process for Highly Resource-Efficient Denitrification

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Historically, energy and cost-intensive nitrification and denitrification were used to treat industrial waste streams containing high concentrations of ammonium ( $\text{NH}_4^+$ ) and nitrate ( $\text{NO}_3^-$ ), and municipal waste streams containing  $\text{NH}_4^+$ . The discovery of anaerobic ammonium oxidation (anammox) bacteria led to implementation of nitrification or partial nitrification to oxidize  $\text{NH}_4^+$  into nitrite ( $\text{NO}_2^-$ ) for use by anammox to oxidize remaining  $\text{NH}_4^+$  to dinitrogen ( $\text{N}_2$ ) gas. This approach can be challenging depending on waste stream and process characteristics. Instead, this study presents a novel approach using partial denitrification (denitratation) to reduce  $\text{NO}_3^-$  to  $\text{NO}_2^-$  in pre-nitrified waste streams before being fed into an in-line anammox reactor.

Based on previous studies, glycerol has high potential for  $\text{NO}_2^-$  accumulation compared to other carbon sources since it favors higher kinetics of  $\text{NO}_3^-$  to  $\text{NO}_2^-$  reduction than for  $\text{NO}_2^-$  reduction. This is likely based on selection for microorganisms that contain only enzymes to reduce  $\text{NO}_3^-$  to  $\text{NO}_2^-$  or with rapid glycerol uptake and storage, potentially leading to electron donor limitation for further  $\text{NO}_2^-$  reduction. Herein, glycerol was used as the external carbon source to achieve partial denitrification by controlling the solids retention time and limiting the influent glycerol dosage. Integrating this process with downstream anammox will achieve significant energy and cost savings over conventional processes. For instance, when treating industrial waste streams, conventional nitrification and denitrification aeration energy and COD requirements are reduced by 100% and 80%, respectively. The benefits extend to municipal treatment with decreases in aeration energy and COD requirements of 50% and 80%, respectively.

## Silicon Oxide Nanofilms for Energy and Water Applications

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### Supervising Faculty, Sponsor, and Location of Research

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### Abstract

Since the mid-twentieth century, the global average surface temperature has risen by 1°C and is projected to continue to increase in the coming decades. In order to prevent further global warming, effective sustainable energy systems must be instated. A major challenge is that renewable energy is produced intermittently and in limited locations. To overcome this issue, fuel cells can convert renewable energy into solar fuels that can be stored and transported, where electrolyzers revert the fuel to electricity. However, these technologies are not yet efficient enough to be widely implemented. A second issue this project seeks to address is water scarcity; one in ten people worldwide lack access to clean water, and these conditions will worsen as global warming progresses. Reverse osmosis (RO) desalination, involving the membrane-based separation of ions from water, can produce clean water sustainably, but inefficiencies make large-scale use of the process difficult.

Research in Esposito lab uses an ultrathin silicon oxide ( $\text{SiO}_x$ ) overlayer on catalytic nanoparticles in fuel cells and electrolyzers to improve stability of the devices. Within this context, a  $\text{SiO}_x$  overlayer seems to enhance selectivity against metal ions. Better understanding the transport properties of silicon oxide could inform further development of the  $\text{SiO}_x$  overlayer model. As such, one goal of this study is to characterize and analyze the transport of water and solutes across a membrane with a  $\text{SiO}_x$  overlayer deposited upon it.

A prominent issue in RO desalination is biofouling on the membrane surface, and damage to the membrane from chlorine used to clean it. Thus, our second goal is to determine whether the  $\text{SiO}_x$  overlayer confers fouling-resistant or chlorine-resistant properties on the membrane. In this study, we tested different methods of deposition of  $\text{SiO}_x$  in order to achieve a uniform layer. Then, we used a diffusion cell and RO system to characterize the transport properties of  $\text{SiO}_x$ . Preliminary results from the diffusion cell suggest the  $\text{SiO}_x$  overlayer decreases permeability of the membrane to NaCl. We will continue by fine-tuning our deposition process, measuring transport for various solutes, and testing  $\text{SiO}_x$  resistance to biofouling and oxidizing agents.

### Keywords

*Silicon oxide, fuel cell, electrolyzer, desalination, reverse osmosis, diffusion cell*

# Enabling Ultrahigh Salinity Desalination at Moderate Hydraulic Pressures with Cascading Osmotically-mediated Reverse Osmosis

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## Abstract

Advancing the science and technology of desalination is vital to sustainably meet the world's water challenges. Reverse osmosis (RO) is the most energy efficient desalination method. However, conventional RO is confined to purifying seawater and lower salinity sources, and is unable to desalt hypersaline streams, such as produced water from oil and gas operations, and also cannot obtain high recovery rates in seawater desalination. This is because the elevated hydraulic pressure,  $\Delta P$ , requirement for high salinity and high recovery desalination imposes considerable material, system design, and operational challenges that cannot be readily surmounted. Here, we propose an innovative "cascading osmotically-mediated reverse osmosis (COMRO)" technology to overcome the limitations of conventional RO and enable energy efficient desalination with reduced hydraulic pressurizations. The technique utilizes the novel design of bilateral countercurrent reverse osmosis stages to substantially lower the osmotic pressure difference across the RO membrane, thus lessening the  $\Delta P$  needed and additionally achieve considerable energy savings. Instead of the 137 bar  $\Delta P$  required for conventional RO desalination of 70,000 ppm TDS produced water, the highest operating pressure in COMRO is only 68.3 bar (-50%). Furthermore, up to ~17% saving in specific energy consumption is attained by COMRO compared to traditional RO (3.16 kWh per cubic meter of product water, instead of 3.79 kWh/m<sup>3</sup>). The analysis further underscored the promise of COMRO for boosting the recovery rate of seawater desalination to 75%, from the typical 40-50%. Again, COMRO can operate at a lower  $\Delta P$  of 102 bar (-25% compared to conventional RO) and achieve substantial energy savings of up to 38% (~2.4 kWh/m<sup>3</sup> with COMRO, compared to 3.79 kWh/m<sup>3</sup>). This study highlights the highly encouraging potential of energy efficient COMRO desalination to access unprecedented high recovery rates and treat ultrahigh salinity streams at moderate hydraulic pressures that are within current technical reach.

## Effect of film thickness on stokes flow past a spherical particle along the fluid-fluid Surface of a thin liquid film

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### Abstract

Modeling Stokes flow around small particles of the order of nanometers to tens of microns in size, on the surfaces of thin liquid layers is important, for example, in understanding their capillary-driven self-assembly into crystalline monolayers on thin evaporating films on solid supports. On the other hand, modeling the motion of particles on the surfaces of free interfaces is critical for understanding the colloidal stabilization of foams and the transport of particles along the lamellar interfaces in particle-laden foams developed in flotation processes. We study the hydrodynamics of particles moving along the gas/liquid surface of a thin planar liquid film situated on either a solid substrate, or bounded from below by a second gas/liquid interface (a free lamella). Finite element numerical solutions were developed for inertia-less (Stokes) flow of a spherical particle translating and rotating on a Newtonian liquid film of finite thickness. Our analysis indicates that for liquid films on a solid substrate and a fixed contact angle, the drag coefficient for translation and the cross coefficients increase as the film thickness decreases but the resistive torque for rotation only increases marginally due to the weaker hydrodynamic interaction in the vicinity of a wall. For a free interface, the decreased hydrodynamic interaction of translating and rotating spheres with the stress-free lower surface causes all the drag and torque coefficients to be less than their values when the particle is on a semi-infinite liquid.

## **Regional intense precipitation: inference from credibly simulated GCM variables**

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Many authors have demonstrated that extreme precipitation is often biased in ocean-atmosphere General Circulation Models (GCMs). Given this GCM bias, and the nonstationarity of extreme precipitation, projecting future changes in extreme precipitation frequency is difficult. One potentially fruitful strategy is to identify potential circulation patterns that are both predictive of the likelihood of extreme precipitation events and are well simulated by the GCMs. The frequency of these patterns can then be evaluated in the historic and future GCM runs and used to infer future changes in the frequency of extreme precipitation. We demonstrate such a methodology for springtime regional extreme precipitation events in the Ohio River Basin with a coupled Geophysical Fluid Dynamics Laboratory GCM. We show that the GCM simulates too many springtime events in the historic record but does credibly simulate the distributional and persistence properties of a large-scale atmospheric pressure gradient index. Further, we show that this index modulates the likelihood of regional extreme precipitation events in the reanalysis/observational record. We construct a conditional simulation model with the GCM pressure gradient index, which improves the simulation of the extreme precipitation events from the GCM. We then use the GCM pressure gradient index from a future simulation to project extreme precipitation frequencies to 2100. The proposed approach is broadly applicable and provides promise as a robust alternative to grid-cell bias correction schemes.

## **Novel Liquid-like Nanoparticle Organic Hybrid Materials (NOHMs)-based Electrolyte for Combined CO<sub>2</sub> Capture and Conversion**

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### **ABSTRACT**

Carbon Capture, Utilization and Storage (CCUS) has imposed a new demand for utilizing captured CO<sub>2</sub> as a chemical feedstock for value-added products. However, CO<sub>2</sub> capture and CO<sub>2</sub> conversion, though have been well demonstrated in the past few decades, are still two separate processes. The parasitic high energy consumption associated with the two steps is one urgent problem to solve. Thus, a medium for carbon capture with the ability of hosting subsequent CO<sub>2</sub> conversion is proposed as referred to Nanoparticle Organic Hybrid Materials (NOHMs)-based electrolyte. NOHMs are comprised of silica nanoparticle, grafted with task-specific polymers. NOHMs have exhibited excellent thermal stability, negligible vapor pressure and chemical/physical tunability. In this study, NOHMs-based electrolyte is developed where NOHMs, a secondary fluid and salt are mixed at a certain ratio. In this way, an electrolyte with a high CO<sub>2</sub> solubility can be obtained for subsequent electrochemical conversion of CO<sub>2</sub>, with renewable energy. Preliminary studies via Ultra-Small Angle X-ray Scattering (USAXS) have revealed a fractal structure within NOHMs-based electrolyte, which is crucial to the electrochemical properties and CO<sub>2</sub> transport. A further investigation of the chemistry between NOHMs, secondary fluids and salts is also conducted to better design the fractal structures and optimize the electrolyte for combined carbon capture and conversion. A tentative combined carbon capture and conversion is also performed with tunable products and yield. It is believed that this novel approach has the potential in offering a new way for carbon management.

# Understanding The Permeability Selectivity Tradeoff Of Salt Rejecting Polymeric Membranes

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## Abstract

Water, the most essential component for human health and well-being, is becoming increasingly difficult to access, even with the technological advancements of the twenty-first century. With the threat of water scarcity looming large, membranes, in particular, have received much attention for their ability to cost-effectively treat and purify water sources, such as seawater and wastewater. Although reverse osmosis and nanofiltration membranes have seen strong improvements in performance over the past decades, these enhancements have leveled off in recent years. Efforts toward identifying candidates for next-generation membrane material are hindered by an incomplete understanding of the fundamental transport phenomena in polymers and its relationship with intrinsic material properties. Therefore, we present a systematic evaluation of the transport properties of a range of commercial thin-film composite membranes, in order to elucidate the intricate relation between water permeability and solute selectivity. The intrinsic water and solute permeability of seawater, brackish water, and nanofiltration membranes are carefully characterized with four distinct ionic salts, NaCl, MgCl<sub>2</sub>, Na<sub>2</sub>SO<sub>4</sub>, and MgSO<sub>4</sub> in a custom-built high-throughput cross-flow reverse osmosis laboratory test setup. Analysis utilizes the experimental results in a semi-empirical model to define the permeability-selectivity tradeoff of these membranes. A membrane that allows a higher passage of water is often associated with higher passages of salt, a detriment to overall performance. Furthermore, we establish connections to this relationship and solute properties, namely hydrated ionic radii and salt diffusion coefficients. Across all membrane types, salt rejection tended to generally increase with larger hydrated ionic radii. In addition, results suggest that the water and solute permeability coefficients, A and B, respectively, are linked to the diffusion coefficients by the relation  $A^x B^y \approx D$ , in which x and y represent empirical parameters. The findings of this study aim to advance the understanding of transport in salt-rejecting membranes, and guide the development of next-generation materials for reverse osmosis and nanofiltration in water purification and treatment applications.

# The impact of mineral particles of zooplankton carbon assimilation and implications for the efficiency of the biological pump

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## Abstract

A major sink of CO<sub>2</sub> is the ocean “biological pump” – the process of C fixation by phytoplankton and sinking of organic matter to the deep ocean. Dust deposition is a source of limiting nutrients and other minerals to the ocean affecting phytoplankton productivity as well as community structure. It has been suggested to facilitate the flux of carbon to the deep ocean through both chemical and physical effects. However, these effects are not well constrained and preliminary experiments suggested a possible feedback mechanism that has been completely overlooked: the presence of dust may significantly reduce the carbon assimilation of marine grazers, resulting in enhanced carbon transport to the deep ocean via fast-sinking, carbon-rich fecal pellets.

Preliminary work indicated that zooplankton ingestion of mineral material increased organic carbon content in fecal pellets, as well as size and density. Based on these observations, sinking rates of fecal pellets and associated carbon transport to depth via fecal pellet export were hypothesized to increase with increasing dust deposition. To test this, mesocosms were designed to conduct feeding experiments in the Red Sea and the Mediterranean Sea. Ambient assemblages using locally collected phytoplankton and mineral sources were fed to pre-concentrated ambient zooplankton grazers. These bioassays delineated ecological interactions and better represented realistic conditions. Fecal pellets generated were collected and analyzed for their carbon content.

Results from mesocosm experiments were compared with data collected from field observations from locations representing a range of oceanic regimes and atmospheric depositions. Data from field observations can be used to further investigate relationships between mineral dust and fecal pellet characteristics, placing results from the mesocosm experiments into a more clearly defined context. Data documenting this process limited, and no quantitative or mechanistic understanding for these relations is currently available. Investigation of this interaction will offer significant contribution to the understanding of carbon sequestration via the biological pump.

## Correlation And Reliability Analyses On Wind Farm Energy Production

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### Abstract

Wind farm installations show an increasing trend since wind energy is a renewable, sustainable, environmentally friendly and profitable energy source. However, the intermittent and unpredictable nature of wind and the reliability of the entire farm make harder for the operators to get the best out of the wind source. Cultivated wind power at a wind farm depends on different parameters such as wind speed, wind direction, site topography, reliability of individual turbines and the characteristics of the wind turbines. In this study, we address the unpredictable nature of wind by applying correlation analysis to data of wind speed, wind direction and wind turbine power output from the Sotavento Wind farm, in Spain. We used 20 data sub sets categorized by 18-degree direction intervals. We also analyzed the availability of the wind farm by using real time high resolution data. We concluded that there is a higher correlation in wind speed than in wind turbine power through the time intervals considered. Power generation strongly depends not only on the wind speed but also on the wind direction although the wind turbines have yawing systems to catch the maximum wind and this can potentially be attributed to wind direction changes and/or imperfect correlation between the wind speed measurements at the meteorological stations and the speeds experienced by the wind turbines because of the topographic and wake effects. Also, we found that  $\sim 1/3$  of the wind turbines were unavailable at any given time and this may be in part a result of wind direction changes that are not reflected in the energy production data.

# Circulation pathways and spreading rates of the Atlantic Water in the Arctic Ocean: Results from 25 years of tracer observations

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## Abstract

The Atlantic Ocean supplies heat to the Arctic Ocean along two pathways: one entering through Fram Strait (Fram Strait Branch) and one entering through the St. Anna Trough after seasonal modifications on the Barents Sea shelf (Barents Sea Branch). Although shielded from direct contact with the sea ice cover by the cold mixed layer and halocline, some of the heat reaches the sea ice via turbulent exchange and thus has impact on sea ice extent and thickness. This raises the question of the stability of the Atlantic Water circulation in the Arctic Ocean in a rapidly changing Arctic system and the consequences of potential changes in its position within the water column.

The presently accepted circulation scheme of Atlantic Water in the Arctic Ocean was first depicted by Rudels *et al.* (1994) based on hydrographic data and dynamical considerations and has been extensively discussed in the literature and widely used in many studies. Although the general circulation patterns seem to be robust, so far not all of its branches have been verified by direct observations such as current meter measurements or geostrophic flow estimates. Additionally, there are few direct measurements of the spreading velocities of the individual components of the overall circulation scheme. We present tritium/<sup>3</sup>He data and discuss how they add to our understanding of the circulation patterns and spreading velocities..

Specifically, we use <sup>3</sup>H/<sup>3</sup>He and hydrographic data from 21 expeditions spanning 25 years of Arctic Ocean section work (1987 and 2013) to estimate spreading velocities and flow paths of Atlantic Water branches on a pan-Arctic scale. Our tracer data corroborate and add a time dimension to previously estimated circulation schemes. The results confirm the presence of a well-organized boundary current that cyclonically flows along the continental slope and add insights on the other, typically topographically steered, circulation branches of Atlantic water, most notably those following the Lomonosov Ridge. The tracer data also show that within the limits of our method the current system has been stable over the 25 years of observation.

## Two-step Mineral Carbonation of Heat-treated Serpentine using Dilute CO<sub>2</sub> Stream

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### Abstract

Carbon capture, utilization, and storage is an essential technology for greenhouse gas reduction in the future. Ex-situ mineral carbonation process that magnesium or calcium silicate mineral is chemically reacted with CO<sub>2</sub> to form value-added product in the form of thermodynamically stable solid carbonate is one of the most promising CO<sub>2</sub> sequestration technology. However, there is a challenge in transportation of mineral and CO<sub>2</sub> for developing of the process. If CO<sub>2</sub> source and mine are located far from each other, the ex-situ process would generate significant CO<sub>2</sub> from transportation. Consequently, the net amount of CO<sub>2</sub> sequestered would become negative and it could make the process impractical. One possible option is to directly capture CO<sub>2</sub> from the air and use it for the process. The usage of diluted CO<sub>2</sub> stream from a direct air capture unit which is located at the vicinity of the mineral source will be able to make the ex-situ mineral carbonation process practical. Therefore, developing of mineral carbonation process using diluted CO<sub>2</sub> stream is necessary. In this study, two-step mineral carbonation process using low partial pressure CO<sub>2</sub> stream was tested in batch system. Two-step process consists of dissolution and precipitation part. Relatively higher pCO<sub>2</sub> stream is used for dissolution of mineral and lower pCO<sub>2</sub> stream is used for precipitation at a higher temperature condition. The precipitation of solid carbonate is obtained via temperature and pCO<sub>2</sub> swing. In dissolution batch reactor, the effect of temperature, slurry density and ligand on dissolution behavior of heat-treated serpentine was studied. Also, degassing and precipitation behavior were studied at different temperature and pCO<sub>2</sub> condition to optimize precipitation process. The experiment results showed a possibility of two-step mineral carbonation process using diluted CO<sub>2</sub> stream.

## **Polymer Hybrid Material For Sustainable Water Treatment Solution**

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### **ABSTRACT**

Water contamination by heavy metals such as Pb is one of the major environmental concerns and a serious problem due to the adverse effects caused by these heavy metals, a concern which has additionally be raised by the recent Flint disaster. The purpose of this study is to develop polymer based hybrid material for sustainable water treatment solution. Existing methods for water treatment solutions to remove lead, are either expensive, such as membranes or are disposable after one use. For this study, the idea is to create a robust, reusable and cost effective composite to remove lead from water, even at low concentrations(<30ppb). In this case, A conducting polymer, PEDOT (Poly-(3, 4-ethylenedioxythiophene)) was synthesized on a glassy carbon sponge (GCS) along with Manganese Dioxide(MnO<sub>2</sub>) and was used for water treatment purposes. Manganese has been traditionally known to have high affinity for Pb<sup>+</sup> ions, and PEDOT too due to the conjugation present in its structure. The basic idea is to electrochemically synthesize MnO<sub>2</sub> and PEDOT on the GCS surface. The composite hence prepared will then act as a lead adsorbent from water. Re-usability of this system will be implemented by discharging the adsorbed lead ions on the surface by immersing in a wash solution (HCl typically) and applying a potential difference. Techniques such as Zetasizer, XRD, Atomic adsorption Spectroscopy(AAS), SEM were used to characterize and study the material and it's performance.

## **Nanoparticle emissions from residential wood combustion: A literature review, characterization, and recommendations**

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### **Abstract**

The increased use of wood as a heating fuel in residential and small commercial buildings has increased concern about potential environmental and safety impacts, specifically particulate matter (PM) emissions in the nanometer range. Larger particles ( $> 2.5 \mu\text{m}$ ) can be effectively removed from exhaust streams by emission control devices. However, nanoparticles (NP), due to their size, are more difficult to capture in exhaust flue gases. In addition NPs have a higher surface to volume ratio, allowing them to absorb organic compounds, causing them to be more reactive than their larger counterparts.

Current emission regulations do not reflect the NP count or type produced from residential wood combustion, although studies show that a significant portion of the particles produced during combustion is in the nano size range. Fuel type, device type and combustion periods have all shown to impact the NPs produced; some conditions more favorable than others. This literature review also offers suggestions for future testing, monitoring and environmental impact studies as the use of wood combustion devices continues to be the largest source of particulate emission in NYS. The information gathered from writing this review paper will stress the importance and need for additional nanoparticle emission research from residential wood heaters.