50th Annual
Agricultural and Environmental Chemistry
Winter Colloquium

February 24 – February 25, 2022

Agricultural & Environmental Chemistry Graduate Group

EST. 1970

UC DAVIS

50th Annual Winter Colloquium Schedule

	Thursday, February 24th, 2022	Friday, February 25th, 2022
Time	**Speaker Name**	**Speaker Name**
9:15:00 AM		Alyssa Burns
9:30:00 AM		Jackie Lang
9:45:00 AM		*Break*
10:00:00 AM	Madi Mathers	Bofeng Pan
10:15:00 AM	David Bonnar	Anna Feerick
10:30:00 AM	Jiayin Dai	Stephen Corbett
10:45:00 AM	*Break*	*Break*
11:00:00 AM	Erik Rangel	Heather Lieb
11:15:00 AM	Ravi Kang	Elise Palombella
11:30:00 AM	Jeffrey Caudill	Stephanie Arciva
11:45:00 AM	*Break*	*Break*
12:00:00 PM	**Dr. Robert Kostecki (Keynote Speaker)**	**Dr. Jasquelin Peña (New AgChem Faculty Member)**
12:15:00 PM		
12:30:00 PM		
12:45:00 PM		*Lunch Break*
1:00:00 PM	*Lunch Break*	
1:15:00 PM		
1:30:00 PM		
1:45:00 PM		
2:00:00 PM		**Dr. Alex Chassy (UCD AgChem Alumni)**
2:15:00 PM		
2:30:00 PM		
2:45:00 PM		Angela Encerrado
3:00:00 PM	Brittany Saleeby	*Break*
3:15:00 PM	Ryan Farley	
3:30:00 PM	Austin Lourie	**Dr. Sieglinde Snapp (Keynote Speaker)**
3:45:00 PM	*Break*	
4:00:00 PM	Matthew Michel	
4:15:00 PM	Chris Niedek	
4:30:00 PM	Minyuan Wang	*Break*
4:45:00 PM		
5:00:00 PM		
5:15:00 PM		
5:30:00 PM		*Social Event*
5:45:00 PM		
6:00:00 PM		

50th Annual Winter Colloquium Abstracts

February 24, 2022

10:00:00 AM – Madi Mathers

Prevalence and composition of wetland sources to the non-algal particulate pool in a food-starved Delta

The Sacramento-San Joaquin Delta management is heavily driven by declining native fish populations, with the stressed lower food web suspected as a primary culprit. Food web limitations in the Delta are caused by a drop in primary productivity coinciding with an increase in filter feeders that have reduced particle concentrations and accompanied a decline in zooplankton. Solutions to increase available food are an obvious management target with needed emphasis on particulate material composed of detrital remains. Remains of wetland vegetation can help to enhance copepod survival in the presence of low algal concentrations. Wetlands are a critical but underappreciated feature in Delta food webs that have the potential to supply detrital material to recover declining fish species. However, little is known about the forms of exported wetland detrital material or how such particulates are distributed through the Delta's pelagic habitats. In this study, we collected particulate samples across the Sacramento-San Joaquin Delta over a two-year period to characterize and quantify export of wetland detrital particles and link these measurements to the lower food web. Lignin biomarkers and stable isotopes were the primary tools used to distinguish between vascular plant and algal organic matter. Other measurements include chlorophyll and optical characteristics. Preliminary data indicates variations in concentration greater than one order of magnitude for both chlorophyll and vascular plant material. This study is an assessment regarding the potential for restored tidal wetlands to support the lower food web and can provide guidance for future wetland restoration activities.

10:15:00 AM – David Bonnar

The Partitioning Behavior of Oxyfluorfen in California Rice Field Conditions

Oxyfluorfen (trade name Goal) is a broad-spectrum, diphenyl ether herbicide used for pre- and post-emergent control of a variety of broadleaf and grassy weeds. Although registered over 40 years ago, the recent discovery of non-transgenic, oxyfluorfen-resistant rice strains in addition to demonstrated effectiveness on rice weeds has sparked a surge in interest, with researchers and herbicide manufacturers racing to bring a rice-field approved product to market. This process, however, faces the challenge that oxyfluorfen has historically been prohibited from use in or near aquatic sites due to its high toxicity to aquatic organisms. When rice fields are treated with herbicides, the potential exists for their discharge into receiving waters, risking exposure to wildlife, drinking water contamination, and transport to other agricultural fields. Thus, it is imperative that any decisions regarding registration of oxyfluorfen products for use in rice fields be supported by rice field-relevant fate data. Three of the most useful parameters used to predict how herbicides move around in the environment are the partitioning coefficients, K_d, K_{oc}, and K_H. These properties describe how an herbicide distributes itself across different environmental compartments, such as soil, water, and air, thus allowing for risk assessors to accurately estimate how much exposure and potential harm various biota face. In this presentation, preliminary data on the partitioning behavior of oxyfluorfen are shared and the potential implications to its overall fate in rice fields are discussed.

10:30:00 AM – Jiayin Dai

Effect of Flavorants on Chemical Composition of Electronic Cigarette Aerosols

Terpenes and terpenoids are present in nature and are used widely in commercial products as flavoring compounds, such as electronic cigarettes (e-cigarettes). The growing popularity of e-cigarettes raises concerns about the possibility of adverse health effects to primary users and people exposed to e-cigarette vapors. E-cigarettes are especially attractive to new young users due to the wide variety of flavors provided on the market, but how these flavoring compounds in e-liquids affect the toxicity and chemical composition of the vapor has not been well studied. In this study, high performance liquid chromatography coupled with high resolution mass spectrometry (HPLC-HRMS) is used to characterize and quantify carbonyl and acid products formed by thermal degradation. Terpenes and terpenoids are characterized and quantified by gas chromatography mass spectrometry (GC-MS). Since regulations on e-cigarettes in the U.S. do not provide guidelines on the chemical content of e-cigarette liquids, the results of this study can provide a more comprehensive understanding of aerosol composition from vaping e-liquid with different flavoring compounds, which could be a reference for policy guidance and further research.

11:00:00 AM – Erik Rangel

N-Nitrosamines from Postharvest Nitric Oxide Fumigation

Two nitrogenous organics used for postharvest preservation of fresh fruit, morpholine and diphenylamine, were sorbed to model surfaces and subjected to batch fumigations with nitric oxide at ca. 38,000 ppmv ($\mu L\ L^{-1}$) for 1 h. Capillary electrophoresis coupled to tandem mass spectrometry (CESI-MS/MS) was used to analyze the treatment byproducts, as it conveniently allowed for the quantification of (+) positively charged amine precursors and their neutral *N*-nitrosated products in the same sample, with minimal preparation and low potential for spectrometric interferents. The formation of *N*-nitrosodiphenylamine, *N*-nitroso-2-nitrodiphenylamine, and *N*-nitrosomorpholine were confirmed as residues. The work is presented in the context of forecasting the *N*-nitrosation of nitrogeneous organics, both anthropogenically- and naturally-derived, following nitric oxide fumigation of fresh fruit and other foodstuffs. In addition, the advantages of using CESI-MS/MS for the analysis of *N*-nitrosations are discussed and extended to other medicinal, toxicological, and environmental applications.

11:15:00 AM – Ravi Kang

Low-cost wastewater cultivation of microalgae for sustainable materials production

Microalgae are photosynthetic organisms applied for wastewater bioremediation and as feedstock for high-value bioproducts such as algae-derived biofuels and pigments for use in the nutrition and cosmetics industries. Microalgae biomass is of interest for infrastructure materials since microalgae can sequester atmospheric CO_2 as compared to traditional materials processing which generally requires large energy and CO_2 inputs. To apply microalgae to infrastructure materials, it is important to understand the structural strength of microalgae, particularly when grown on wastewater. My research aims to optimize biomass productivity and quantitate protein, lipid, and carbohydrate content in microalgae species to understand their applications for infrastructure materials. Structural parameters will be investigated for microalgae grown in food waste permeate (FWP) and stripped food waste permeate (SFWP) from the UC Davis READ facility. Our previous research has also demonstrated that this digestate contains toxic levels of ammonia and low levels of phosphorus that are not optimal for microalgae cultivation. Therefore, my current research focuses on pre-treatment methods and using nitrifying bacteria to adjust nutrient levels where I hypothesize that a one-step co-treatment of the FWP with microalgae and nitrifying bacteria could support growth and increased biomass. Currently, I am investigating this hypothesis in *Chlorella sorokiniana* and will expand to include other species of interest; specifically, *Chlorella vulgaris*, *Tribonema minus*, *Phaeodactylum tricornutum*, and *Scenedesmus acuminatus*.

11:30:00 AM – Jeffrey Caudill

Assessing impact of select herbicide application on Delta Smelt embryos and phytoplankton community

Delta Smelt (Hypomesus transpacificus) is an endangered species in the California Sacramento-San Joaquin River Delta and Suisun Marsh and the potential effects that may adversely impact hatching success is not very well known. Adult Delta Smelt exposed to an aquatic herbicide, fluridone (liquid formulation), showed signs of endocrine disruption, oxidative stress, and neurotoxic effects (Jin et al. 2018). In addition, fluridone exposure significantly affected hatching success of a model fish species, Japanese Medaka (Jin et al. 2020). Given the pellet form of fluridone is used to treat the habitat, there is a risk that Delta Smelt embryos, which have adhesive grand and attach to substratum, are exposed to high concentrations of fluridone in the benthic environment. Another concern is impacts of fluridone on phytoplankton. Fluridone kills plants by inhibiting phytoene desaturases, which prevents carotenoid production, leading to treated plants to bleaching. The phytoene desaturases are conserved in various types of phytoplankton including diatoms, therefore fluridone exposure can inhibit phytoplankton growth as well (Lam et al. 2019). Lam et al. (2019) also reported that susceptibility of phytoplankton on fludidone can vary among different phytoplankton taxa. The goals of this study are (1) to assess whether sediments collected from fluridone application sites in the Delta cause adverse effects on Delta Smelt embryos and (2) to investigate whether fluridone application reduces phytoplankton biomass and/or alter phytoplankton community structure in the habitat.

12:00:00 PM – Dr. Robert Kostecki (Keynote Speaker)

Rechargeable batteries – from fundamental research to large scale applications

The past 200 years of engineering of electrochemical energy storage systems have been explicitly focused on understanding the fundamental limitations of energy density and power density and optimizing these metrics for a given application. Because of the current world-wide emphasis on the importance of energy conservation, and in part because of tremendous technical advances in battery performance, large numbers of people are entering the battery field who have expertise in experimental and theoretical approaches that have not traditionally been applied to batteries. Completely new battery chemistries and formats are being demonstrated at an increasingly rapid pace. In the last decade, capital cost, operating cost, cycle life and calendar life have become equally important metrics. But while energy and power studies have roots in fundamental chemistry and physics, the latter metrics were typically relegated to manufacturing and warranty concerns. Although commercial batteries have been available for over 150 years there are still many fundamental gaps in understanding the atomic- and molecular-level processes that determine and govern their function, operation, performance limitations and failure. Moreover, designing batteries is a highly empirical process, where the chosen solution is often simply to greatly overdesign the battery. This presentation will discuss various aspects of the secondary battery R&D within its current and historical science and technology context.

3:00:00 PM – Brittany Saleeby

Addressing Public Health Concerns of Yurok Tribe Using Non-Target Analysis

The objective of current research activities is to apply non-targeted workflows for the analysis of high-resolution mass spectrometry on affected environmental samples, with prioritizing compounds identified by analysis via in-vitro assay for biological activity (bioassay). In collaboration with UC-Davis, the Yurok Tribe Environmental Program (YTEP) collected sediment suspected of contamination from previous logging and agricultural industry activity for non-target analysis of compounds linked to the community's adverse health issues. Scientist from YTEP collected sediment from affected regions between 2018-2020. At UC-Davis, the sediments were extracted, analyzed on multiple MS platforms, and vetted for QA/QC information derived from target analytes and internal standards. All sample extracts and blanks that were prepared for analysis were also submitted to collaborators for bioassay results. Complete sample datasets have been compiled and optimized on MS-Dial application, and the resulting alignment compound features have been exported for statistical analysis. From the exported MS-Dial alignment data and bioassay data from collaborators, Spearman's rank correlation coefficients were calculated for ordinal correlation between bioassay activity and ion intensity. Some of these features are automatically identified by spectral libraries, but others will require identification via non-target molecular formula generating programs like MS-Finder and SIRIUS.

Unlike traditional targeted and suspect analytical workflows where compounds of concern are known, the non-targeted analytical workflow supports compound discovery by broader and systematic methods of detecting unknown analytes. A benefit but also a challenge to this methodology is that non-target workflows result in a list of molecular features typically in the order of thousands even after filtering and post processing steps. Due to the immense number of compounds that could be detected in any given chemical space, these biological indicators are necessary to guide action for regulation of these contaminants. Ultimately, by using Spearman's rank correlation coefficients to highlight molecular features of interest, the list can be reduced to hundreds, rather than thousands, of compounds.

3:15:00 PM – Ryan Farley

Impacts of Aging on Aerosol Chemistry within Wildfire Plumes – From Near-Source to the Regional Scale

The atmospheric processing of biomass burning organic aerosol (BBOA), and the resulting implications on tropospheric aerosol composition and physicochemical properties is still uncertain. This study investigates the transformation of BBOA in the U.S. Pacific Northwest based on measurements of the submicron particulate matter (PM_1) concentration and chemical composition between <1 and ~10 hours of equivalent photochemical using a high-resolution soot particle aerosol mass spectrometer (SP-AMS) aboard the DOE G-1 aircraft. Additionally, a second standard vaporizer HR-AMS at the Mt. Bachelor Observatory (MBO) ground site allowed for measurements of BBOA from wildfires that had undergone at least 6 hours and up to multiple days of processing. The strategically combined airborne and mountaintop measurements provide an opportunity to investigate the near-field (< 1 hr) and regional evolution of BBOA properties in wildfire emissions located in the western U.S. A clear increase in the degree of oxidation of the OA is seen throughout the course of aging. Positive matrix factorization analysis is used to disentangle the contribution of primary BBOA from secondary BBOA formed through atmospheric reactions of volatile organic compounds. Five distinct BBOA types were observed, including two fresh BBOA factors, an intermediate BBOA factor and two oxidized BBOA factors. Wildfire plumes are dynamic environments, and these results can be used to better understand and model the evolution of aerosols and the formation of secondary organic aerosol (SOA) within these systems.

3:30:00 PM – Austin Lourie

Investigating Hydrogen Cyanide Fumigation Treatments to Control Brown Marmorated Stinkbug and Other Invasive Insects

Hydrogen cyanide provides a new alternative for controlling pests such as brown marmorated stinkbug (BMSB), *Halyomorpha halys* (Stål) (*Hemiptera: Petatomidae*), Mexican fruit fly (MFF) (*Anastrepha Lumens)*, and Spotted lanternfly (SLF) (*Lycorma Delicatula)*. These invasive insects have detrimental effects on invaded countries in various ways especially through the destruction of agricultural products. They also affect multiple regions across the globe; specifically, BMSB is of primary concern to Australia and New Zealand while SLF and MFF are of concern to North and Central America amongst many other countries. Fumigation of both non-horticultural and horticultural consignments plays a major role in preventing these insects from hitchhiking into new countries. While dangerous, HCN is already registered in countries like New Zealand, and preliminary data suggest it requires lower doses and shorter fumigation times to control BMSB. A dose between 2-4 mg/L for a length of 30 minutes to 2 hours showed to be a highly effective treatment for both diapausing and non-diapausing BMSB. Data collection for MFF inside of mandarin oranges and SLF eggs is currently ongoing. This research will help establish HCN as another alternative to methyl bromide alongside others such as ethyl formate and sulfuryl fluoride.

4:00:00 PM – Matthew Michel

Characterizing the Vacuolar Transport of Lignin Monomers Using Isolated Vacuoles from Model Plant Species

Lignin is a complex heteropolymer and the second most abundant organic polymer on Earth. It forms an integral part of the secondary cell wall in vascular plants, providing structural support and playing roles in pest resistance, drought and salt stress tolerance and temperature acclimation. Despite its abundance and importance to plant life it is unclear how the building blocks of lignin, called monolignols, are transported from within the plant cell to the cell wall where they are polymerized. It is known that monolignols also become glycosylated and sequestered in the central vacuoles of plant cells for reasons not fully understood. Previous literature contains disagreements over the likely mechanism of transport into the vacuole. In this project, we aim to characterize the mechanism by which glycosylated monolignols enter the plant vacuole. To achieve this, we are isolating whole, intact vacuoles from *Arabidopsis thaliana* and *Medicago sativa* to obtain an unaltered membrane environment which mimics the *in vivo* environment as much as possible. Once reliable purification of intact vacuoles is achieved, kinetics studies using pharmacological inhibitors of transporter proteins will be performed to classify the transport mechanism. This project additionally seeks to demonstrate that intact plant vacuoles are a powerful tool for characterizing the function of vacuolar transporter proteins and the transport of compounds across the vacuole membrane as well.

4:15:00 PM – Chris Niedek

Offline Aerosol Mass Spectrometry Analysis of Ambient Particles Collected Via Uncrewed Aerial Systems (UASs)

Ambient aerosols play key roles in human health, air quality, and the climate and the chemistry of the particles has a large impact on their radiative and toxicological properties. Continuous air quality monitoring and improved techniques for aerosol measurements are needed to more fully understand the effects aerosols may have in the atmosphere. Offline analytical techniques have been critical for the advancement of our understanding of atmospheric aerosol chemistry, particularly for organic aerosols (OA), as field deployment of the instrumentation necessary for real-time analysis of particles can be prohibitively expensive and technically demanding. In addition, small, uncrewed aerial systems (UASs) have been increasingly used for meteorological and air quality monitoring over the past few decades as they offer a way to fill the measurement gaps left between ground-based, traditional crewed aircraft, and satellite measurements of atmospheric species. Detailed chemical analysis of PM samples collected via UASs has not been previously performed partially due to analytical challenges involved with extracting and analyzing the low amount of PM mass that can be collected during typical UAS flight times combined with the relatively high PM concentration and volume requirements of common atomization systems. In this study, we develop and validate a novel micronebulization technique capable of nebulizing microliter volumes of liquid. The chemical composition of ambient PM samples collected via UASs were then analyzed using a soot particle aerosol mass spectrometer (SP-AMS).

4:30:00 PM – Minyuan Wang

Organizational Chirality of Nanostructures by Design

Surface chirality is an area of growing interest with many potential applications, such as chiral sensors, enantiomeric separation, and enantioselective heterogeneous catalysis. This work reports production of organizational chiral structures using Atomic Force Microscopy (AFM) based nanolithography in conjunction with surface reactions that include the intentional use of mechanochemistry. This presentation will reveal a variety of organizational chiral features produced with high spatial precision. Individual chiral features include a series of Archimedean spirals with right and left-hand rotations, defined by parametric equations. These chiral spirals were produced in two different systems: an alkane thiol self-assembled monolayer (SAM) on an Au surface, and maleimide-anthracene (MA) mechanophores on Si wafers. Complex chiral features were also designed using parametric equations, and rendered via a tip directed retro-[4+2] cycloaddition reaction (retro-Diels-Alder reaction), resulting in multi-shade chiral blades with anthracene functionality. Finally, hierarchical chiral features were designed and then produced using this AFM tip directed mechanochemistry based nanolithography method. In comparison to the current methods to produce chiral features, such as using self-assembly, our new approach has the technical advantage of high spatial precision and enables production of organizational chiral structures by design.

50th Annual Winter Colloquium Abstracts

February 25, 2022

9:15:00 AM – Alyssa Burns

Terrestrial Organic Carbon Transport and Transformation from the Yukon River to the Arctic Ocean

Due to rapidly changing Arctic environmental conditions, increasing impacts to carbon cycles are underway within the land-ocean continuum. Coastal erosion and permafrost thaw can be attributed to a warming climate and may influence the concentration and composition of organic carbon discharged into the Arctic Ocean. A poorly defined spatial relationship in Arctic regions is how riverine organic carbon changes through deltas and across salinity gradients. While there is existing data characterizing salinity effects at lower latitudes, we cannot assume the same phenomena occur in Arctic regions due to differing carbon sources. In this study, Yukon River delta samples were collected to investigate changes in dissolved organic carbon (DOC). Preliminary data suggests that there could be decreases in DOC and lignin with increased salinity, potentially due to DOC conversion to particulate organic carbon (POC) via flocculation. Sampling along a salinity gradient allows for comprehensive understanding of the form and fate of organic carbon as it's transported from freshwater rivers to the open ocean, but there are sampling challenges in remote areas like the Arctic that highlight the need for laboratory-simulated salinity mixing experiments. Field samples will be compared to results from laboratory experiments to determine feasibility for mimicking estuarine processes. With a validated mixing model, and an improved understanding of salinity effects on flocculation, we will be able to make predictions from the long-term USGS dataset at Pilot Station about terrestrial organic carbon released into the Arctic Ocean and establish a baseline for the upcoming NASA Arctic-COLORS field campaign.

9:30:00 AM – Jackie Lang

6ppd-Quinone Physicochemical Property Estimation and Environmental Fate Predictions from Molecular Structure

Tire wear emissions in the USA are estimated at 1.5 billion kg per year, enough to fill 500 Olympic-size swimming pools. Approximately 20% of these emissions pollute stormwater with particulates, leached additives, and transformation products. One recently discovered transformation product of a globally ubiquitous tire additive, 6PPD-quinone, has caused decades of stormwater-associated acute mortality events in coho salmon. For this project, molecular descriptors were derived from the molecular structure of 6PPD-quinone using the UFZ-Linear Solvation Energy Relationship (LSER) Database. From these descriptors, physicochemical properties were estimated and used as default parameters in a level III fugacity model to predict partitioning between environmental compartments. The model's default environment was used with some modifications to better represent an urban Sacramento River environment. Environmental parameters including water temperature and fraction of organic carbon were varied for sensitivity analysis. The results of this project indicate that 6PPD-quinone will primarily partition into water but will migrate into soil or sediment with high organic carbon content. There is also potential for 6PPD-quinone to accumulate in fish with high lipid content. This work provides an initial schema for the environmental fate of 6PPD-quinone and highlights future areas of research for improving current environmental fate models. Future work will use quantitative structure-activity relationship (QSAR) modeling to identify other potentially toxic tire additives and transformation products. The environmental fate of the potentially toxic compounds identified will be predicted using methods similar to this study.

10:00:00 AM – Bofeng Pan

Study of SARS-CoV-2 Spike Protein Affinity Peptides for Colorimetric Nanofiber COVID-19 Biosensors

The COVID-19 pandemic revealed the shortage and demands for accessible, reliable, and flexible diagnosis approaches for household use to combat the pandemic more effectively. Despite the approval of several PCR-based and affinity-based in-home COVID-19 testing kits, many of them suffer from problems such as higher false-negative rate, long waiting time, and short storage period. Based on One-bead-one-compound (OBOC) high-throughput screening, we successfully discovered several peptides with nanomolar binding affinity towards SARS-CoV-2 spike protein, the characteristic surface proteins of the SARS-CoV-2 virus. These peptides allow us to fully leverage the advantages of the high specific surface area of porous nanofibers as immobilized peptides on nanofiber can enrich the viral analytes to achieve ppb-level sensitivity in saliva, which is 10-fold more sensitive than typical enzymatic-linked immunosorbent assay (ELISA) in use. The affinity peptide-coated nanofiber biosensor could be a promising approach for in-home COVID-19 diagnosis with high accuracy and flexibility in maneuver.

10:15:00 AM – Anna Feerick

HLB Retainability in the Context of Chemical Space

Hydrophilic Lipophilic balanced (HLB) cartridges are widely used in solid-phase extraction for sample cleanup and concentration for nontarget analysis. Their ability to retain a diverse set of compounds while simultaneously removing interferences makes them a preferred step in many workflows. Despite the diverse set of compounds that HLB is capable of recovering, inevitably, many are not successfully retained. The boundaries of chemical space, i.e., the set of known and possible compounds, covered by HLB extraction remains undefined, limiting identification confidence of suspect and unknown contaminants annotated during nontarget analytical workflows. Defining the "*HLB detectability domain*", an area of chemical space where HLB is capable of extracting versus not based on a multitude of molecular descriptors, is crucial for improving the confidence of feature annotation. We propose using computational machine learning-based models to predict detectability domains of nontarget methods by examining the extraction potential of HLB sorbents. For this purpose, a dataset consisting of 414 priority and emerging pollutants in water was used. Classification algorithms (i.e., classification and regression trees, support vector machines) were evaluated for their potential in developing a quantitative structure-property relationship model that describes which molecular descriptors most affect HLB retainability. Knowing the range of compounds that can be readily recovered by HLB resins confines nontarget annotations to this area of chemical space. Understanding the bounds of HLB extraction (nontarget space) is an important step in nontarget method standardization and reproducibility, both of which are necessary for improving regulatory acceptance of the methods for environmental monitoring and assessment.

10:30:00 AM – Stephen Corbett

Development of eFUME to Safely Disinfest Key Pests of Citrus

Asian citrus psyllid's (ACP) *Diaphorina citri* was first detected in Florida, 1998, and has since established populations throughout the southern United States. ACP is a pest of concern to citrus due its capacity to efficiently vector the bacterium Huanglongbing (HLB), and the feeding damage it causes to new shoot growth. California has taken aggressive measures to control their spread within the state, quarantining large areas of southern California where the pests have been detected, adopting "spray and pray", and regulating the transportation of citrus between production districts. To help relieve the burden upon the citrus industry, research is being conducted to disinfest bulk citrus, before the fruit leaves the field, with applications of 250 gm^{-3} of eFUME (42 gm^{-3} ethyl formate active ingredient). These applications are operated under "total utilization" so that headspace concentrations are compliant with California/OSHA 8-h TWA PEL levels of ethyl formate (less than 100 ppmv), and safe for applicator/worker reentry into the fumigation space. Studies have been conducted on laboratory and commercial-scale trials to assure efficacy of the treatment and the kinetics of ethyl formate with various citrus varieties. This novel application of eFUME coupled with standard packing/export procedures allow for a system-based approach to control additional pests of concern: California Red Scale (CRS) *Aonidiella aurantia*, bean thrips *Caliothrips fasciatus*, and the mite *Brevipalpus californicus.*

11:00:00 AM – Heather Lieb

Understanding the Spatial Variation of Poor Air Quality in Imperial Valley

Nitrogen oxides (NO_x) are precursors of particulate matter and ozone, persistent air pollutants throughout California due to the climate. Although regulatory policies in California have successfully mitigated NO_x pollution from transportation sources, several of the United States' worst-air quality districts remain in rural regions of the state, including Imperial Valley. This region is vital for California's agricultural industry due to its perennial sunny climate but depends on irrigation to maintain its steady farming practices. As a result, this modifies the meteorological conditions of air pollution by decreasing surface air temperatures and planetary boundary layer height, thus increasing surface pollution concentrations. This rural region has received non-attainment for both ozone and $PM_{2.5}$ based on the National Ambient Air Quality Standards, with high concentrations comparable to large metropolitan areas like Los Angeles. I hypothesize the persistent pollution is the result of unregulated agricultural practices which lead to high soil NO_x emissions from excessive nitrogen fertilizer use in irrigated fields, and that local meteorology exacerbates these conditions. I will be presenting preliminary analysis from the Investigating Violations Across Neighborhoods (IVAN) network, a community-led network of low-cost sensors that monitors $PM_{2.5}$ and PM_{10} in the region. Specifically, I will show how the network compares to CARB monitors and discuss how I plan to optimize this data as I aim to identify sources that amplify the region's air pollution.

11:15:00 AM – Elise Palombella

Investigating the Biological Role of Secondary Marine Aerosols (SMA) Effect on Ocean Cloud Formation

To this day, there is scientific ambiguity regarding the contribution that marine aerosols have on global atmospheric chemistry. Although the oceans cover over 70% of the earth's surface, this inconsistency regarding marine aerosols exists due to key portions of the climate remaining undersampled. Notable scientific gaps still exist between marine atmosphere field studies and laboratory studies, due to the challenge of representing a complex marine environment in the laboratory. Natural marine emissions are an important aspect of atmospheric chemistry, since oceanic gasses released are predominately reactive VOCs which influence chemical reactions, aerosol production and cloud formation. There are also unknowns surrounding the strength of marine aerosol sources and their dependence on environmental factors such as temperature, light, or biological activity. Secondary marine aerosol (SMA) is created by the oxidation of biogenic VOCs from the ocean. The physicochemical properties of SMA need to be investigated to understand their climate effects, such as their ability to scatter solar radiation in the atmosphere and their influence on clouds/precipitation. The future goal is to facilitate improvement on parameterizations of secondary aerosols in climate models that seem to be oversimplified. My research currently focuses on these marine aerosols, whether primary or secondary, and how composition (chemical property), size distribution (physical property) and ocean biological activity can affect their ability to form cloud droplets, as well as their eventual droplet size distributions.

11:30:00 AM – Stephanie Arciva

Formation and Bleaching of Light Absorbance by Phenolic Aqueous SOA by •OH and Organic Triplet Excited States

Brown carbon (BrC; light absorbing organic carbon) is an important component of biomass burning (BB) emissions that directly absorbs solar radiation and impacts Earth's radiation budget. One class of BrC precursors also emitted in BB is gaseous phenolic compounds (ArOH). ArOH react in atmospheric aqueous phases (i.e., clouds, fog drops, and aerosol liquid water) with various oxidants, including the hydroxyl radical (•OH) and the triplet excited states of organic compounds ($^3C^*$), to form secondary organic aerosol (SOA). ArOH oxidation by •OH and $^3C^*$ forms low-volatility, high molecular weight products via functionalization and oligomerization. These are important routes of SOA formation, but the light absorption characteristics of the aqueous-SOA (aqSOA) is poorly characterized.

To study this, we monitored the formation and destruction of light absorption by aqSOA formed by reactions of ArOH with •OH and $^3C^*$. We determined mass absorption coefficients (MAC) to quantify the impact of oxidation on light absorption, which demonstrates the contrast between the initial ArOH and evolving aqSOA. ArOH absorb very little tropospheric sunlight, while the aqSOA products absorb significant amounts of sunlight. We calculated the rate of aqSOA sunlight absorption (R_{abs}) by combining MAC values with modeled actinic flux. We find that •OH photobleaches aqSOA and diminishes aqSOA sunlight absorption over time. In contrast, rates of sunlight absorption by aqSOA change very little in the presence of $^3C^*$. Finally, we determined the lifetimes of sunlight absorbing aqSOA, which ranged from 140 - 1800 min during •OH oxidation, and 280 – 4100 min during $^3C^*$ oxidation.

<u>12:00:00 PM – Dr. Jasquelin Peña (New Faculty Member)</u>

Nature's most potent oxidants: Insights into manganese oxide structure-reactivity relationships

Layer-type manganese oxides (MnOx) are among the most reactive mineral nanoparticles in aquatic and soil environments. Mn oxides impact numerous biogeochemical cycles including that of carbon, metals (e.g., Co, Ni, Cu, Zn and Pb) and metalloids (e.g., Cr, As, Sb, Se). These minerals exhibit among the highest metal sorption capacities (0.1 – 0.5 mol metal mol^{-1} Mn) and oxidative properties of any natural material. Furthermore, biological precipitation is the major pathway for Mn oxide formation under most environmental conditions. Thus, biogenic Mn oxides occur as mixtures of microbial cells, extracellular polymeric substances and mineral nanoparticles.

The physical, chemical and biological complexity of biogenic manganese oxides has rendered the study of their surface chemistry difficult. My group has overcome these challenges by integrating chemical and spectroscopic investigations of experimental systems of varying complexity, including chemically synthesized oxides, mixtures of microbial biomass and Mn oxides, and biogenic Mn oxides produced by model Mn-oxidizing bacteria and fungi. In addition, we have implemented routine wet-chemical methods to determine the redox state of the oxides through quantification of solid-phase Mn(III) content and/or average Mn oxidation number. Kinetic analysis of both sorption processes and evolution in Mn redox state—especially solid-phase Mn(III) content--have been key in advancing our understanding of their surface chemistry.

In this talk I will present our findings on three aspects of the surface chemistry of Mn oxides: 1) environmental parameters controlling particle size, particle aggregation and redox state; 2) reactivity of particle edges and basal surfaces in the absence and presence of microbial biomass; and 3) the impact of Mn(III) on redox reactivity. This research provides a mechanistic basis to understand how manganese oxides impact the cycling of trace elements and contaminants in surface environments.

<u>2:00:00 PM – Alex Chassy (UCD Alumni)</u>

Analytical Chemistry in Industrial Biotechnology: An Amyris Case Study

Amyris is an established leader in bringing new products to market through sustainable, industrial biotechnology. For example, the high-quality skin emollient squalane was previously only accessible by harvesting it from deep-sea shark livers, which threatens shark species and endangers oceanic ecosystems. Amyris developed an alternative to shark-derived squalane that is sustainable, effective, and commercially scalable using sustainably sourced sugarcane, engineered yeast, and Amyris' fermentation technology. Amyris now produces sugarcane-derived squalane at scale for the skincare industry, led by the Amyris brand Biossance. Similarly, Rebaudioside M, the most promising zero-calorie steviol glycoside sweetener in *Stevia rebaudiana* plants, only represents <0.1% of all steviol glycosides, making it unsustainable to access and purify at scale. Amyris now produces cost-effective, high-purity Rebaudioside M at scale through fermentation, granting the food and flavor industries access to this healthy sugar replacement. While microorganism development is often viewed as the primary platform of an industrial biotechnology firm, analytical chemistry serves as the critical underpinning that supports the product development pipeline. Using Rebaudioside M as an example, the analytical methods employed to bring this product to market will illustrate the diversity of techniques utilized at Amyris and how methods are tailored to meet the demands of each step in the pipeline (strain engineering, scale-up fermentation, product purification, and final product).

<u>2:45:00 PM – Angela Encerrado</u>

The Interactions of Chemical Mixtures with P-glycoprotein in Honeybees

Honeybees are key pollinators of numerous commodity crops in the US and worldwide. Just in California, 2.4 million honeybee colonies brought during the 2020 almond bloom, pollinated 1.2 million almond acres. The steady increase in the use of crop pesticides and hive medicines often exposes bees to multiple chemicals at once. Additionally, unintended xenobiotic exposures through contaminated water are a stressor to colony health. While single pesticides and in-hive products are regularly tested for bee safety before being released into the market, the effects of environmentally relevant chemical mixtures on bee health remain understudied. Bioaccumulation of such xenobiotics is typically prevented by an evolutionarily conserved cellular defense system consisting of multi-xenobiotic efflux transporters such as P-glycoprotein. These exporters typically recognize and immediately eliminate foreign chemicals before they can enter cells to exert toxicity. However, the polyspecificity towards various chemicals can be a disadvantage when multiple xenobiotics compete and impair transporter functions. In this project, we seek to investigate how environmentally relevant levels of chemical mixtures, such as neonicotinoids, PFAS and miticides, interact with honeybee P-glycoprotein. We will test the hypothesis that mixtures of known transporter substrates and inhibitors among the chemicals can competitively inhibit P-glycoprotein and promote toxic bioaccumulation. We will clone honeybee P-glycoprotein from forager bees and subsequently express and purify the protein for structure-activity analysis. Our goal is to identify bee-safe combinations of crop pesticides and in-hive medicines that are better eliminated by honeybees P-glycoprotein and can serve as a guideline for both beekeepers and crop farmers.

3:30:00 PM – Dr. Sieglinde Snapp (Keynote Speaker)

A Soil Living Laboratory in Africa: Linking local knowledge to remote sensing

Agricultural development and sustainable soil management on smallholder farms is challenged by complexity, as well as high uncertainty and value conflicts. There is widespread interest in how local adaptation can address this challenge, through co-learning with farmers, hand-held sensors, and remote sensed data analytical approaches. We are testing approaches through a living lab on-farm platform in Central Malawi http://globalchangescience.org/eastafricanode. This was established in 2013 with soil scientists, agronomists, geographers, extension educators and agricultural economists working together with rural communities and farm families. This was supported by the USAID Feed the Future program, as part of the Africa RISING partnership in Malawi. Our soil living lab involves annual monitoring of 1000s of fields, participatory action research on integrated nutrient management and sustainable intensification, carried out with hundreds of farmers. Malawi government has released technologies such as the doubled up legume rotation for soil rehabilitation, based on this research platform. Recent findings highlight the role of crop diversification, weeds and residues in soil carbon status, conditioned by soil texture. This talk will highlight how a learning laboratory can complement traditional research and extension approaches.