Recent Research Activities of the Computational Environmental Fluid Dynamics Research Group at USF and Future Plans

Introduction: We are computational fluid dynamicists led by Dr. Tejada-Martinez with expertise in mathematical modeling of fluid flow problems, in particular turbulent flows, and numerical approximations of model equations. We pursue work focusing on applications of these methodologies to environmental flows. Currently, part of our research consists of highly resolved numerical simulations of turbulent vertical mixing driven by winds, tides, Earth's rotation (Coriolis forcing), surface waves, and surface buoyancy fluxes in the upper-ocean (Figure 1) with the ultimate goal of providing closures or parameterizations of the turbulence and its impact on physical, chemical and biological processes. These parameterizations should be suitable for inclusion in coarse-scale ocean circulation models and thus climate models. A second principal component of our research has involved numerical simulations of flows in drinking water and wastewater treatment systems in order to (1) assess the hydraulic/disinfection efficiency of these systems, (2) present improved designs capable of offering greater efficiency and (2) model the transport of chemical species within these systems. *Overall*, *we work to ensure that our computations are closely coupled with field or laboratory experiments yielding results that are far stronger than each component taken individually. It is this close connection between experiments and computations that we wish to keep pursuing in the future in order to tackle emerging fluid mechanics applications related to environmental hazards in coastal regions (e.g. accidental pollutant releases) and pathways to sustainability of drinking water and wastewater infrastructure. Thus we often seek collaborations with engineers and experimentalists.*

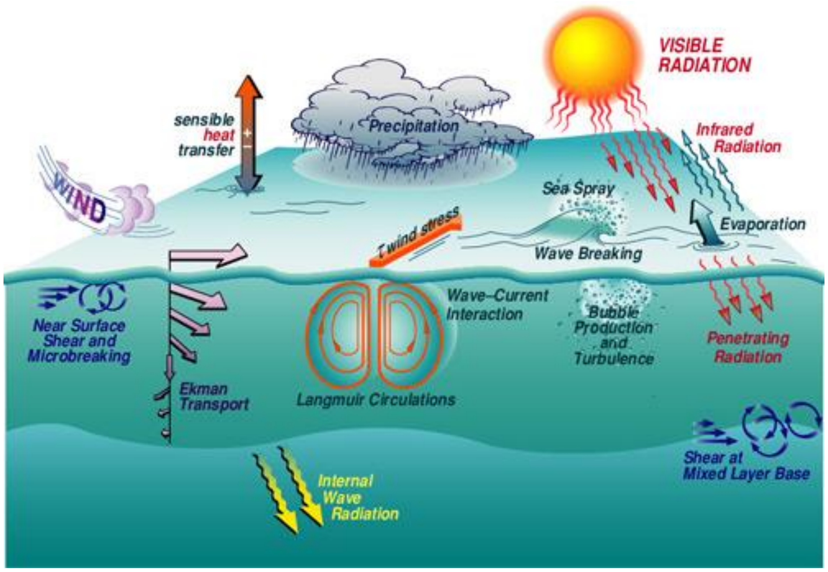

Figure 1: Sketch (summary) of mechanisms that contribute towards either the generation or suppression of vertical turbulent mixing in the upper ocean. From Edson et al. (2007), *Bulletin of the American Meteorological Society*, 88(3), 341–356.

The highly resolved simulations of upper-ocean turbulent vertical mixing consist of large-eddy simulations (LES) and direct numerical simulations (DNS). In DNS all of the scales of the turbulence are resolved while in LES all but the finest scales are resolved. The benefit of DNS and LES is that they allow for fundamental studies of the physics of turbulence, but both can be computationally expensive due to the wide range of length and time scales characterizing the turbulence. Meanwhile simulations of drinking water and wastewater treatment systems have consisted of LES and RANS. RANS is a simulation strategy based on the Reynolds-averaged Navier-Stokes equations solving for the mean component of the flow which is less computationally expensive than LES and DNS as it does not explicitly compute the turbulent flow scales. Thus RANS simulations are often used to predict global characteristics of fluid flow systems important for engineering design purposes.

Over the past 10 years the group lead by Dr. Tejada-Martinez has developed a hybrid spectral/high-order LES/DNS finite difference parallel solver (code) capable of dividing large turbulent flow problems into smaller ones which are then solved concurrently on multiple processors in order to alleviate the computational constraints associated with LES and DNS. (see Tejada-Martinez and Grosch (2007) and Tejada-Martinez et al. (2009) in publications section). The code is currently being used for various projects/simulations running on computer systems at University of South Florida (USF), at supercomputing centers throughout the country through XSEDE (formerly TeraGrid), in UK through collaborators at the National Oceanography Centre and in France through collaborators at University of Lille. This code has been shown to scale well on up to ~16,000 cores while running a DNS of turbulent viscoelastic flow on ~800 million grid points (see Thais et al., 2011 in publications section).

Simulations of turbulent vertical mixing in the upper-ocean and shallow continental shelves: The previously described LES/DNS code has enabled a number of successful collaborations with scientists concerned with the vertical distribution of micro-organisms such as phytoplankton, dissolved gases, and pollutants in the upper-ocean. One of these works has been performed in collaboration with Drs. Patrick Neal and Robyn Smyth, marine biologists from Smithsonian Environmental Research Center, and Cigdem Akan, a former Ph.D. student at USF. The collaboration was supported through a research award made by the National Science Foundation (NSF) Office of Polar Programs (Antarctic Ocean and Atmospheric Sciences Program). We investigated the wave- and wind-driven turbulent mixing dependence of photosynthesis of phytoplankton in the upper-ocean mixed layer of the Antarctic Ocean. Much attention has been given to the Antarctic Ocean because increased solar ultraviolet radiation (UV) resulting from the Antarctic ozone hole has reduced primary productivity (phytoplankton) by as much as 15%. The LES simulations have allowed definition of realistic particle trajectories used in a phytoplankton photosynthesis model. Particle trajectories subject to wind and wave-driven Langmuir circulations (sketched in Figure 1) were found to reduce residence time in the photoactive zone of the water column (where maximum exposure to UV occurs) and extend residence time in the euphotic zone (below the photoactive zone where enough light is received for photosynthesis). This allows more time for the repair of phytoplankton assemblages damaged by UV exposure and enables, on average, higher photosynthetic rates in the lower euphotic zone compared to particle tracks based on deterministic circular rotations used in previous studies to account for the effect of Langmuir cells. These findings are useful for developing future representations of seasonal changes in primary productivity for inclusion in large-scale, full biogeochemical models of the Antarctic Ocean carbon flux.

In collaboration with Fabrice Veron, a physical oceanographer from University of Delaware, and current USF Ph.D. student Amine Hafsi and with support from NSF (Physical Oceanography Program), we are performing DNS (at USF) in parallel with physical laboratory experiments (at U. of Delaware) of the turbulence generated beneath wind-driven gravity-capillary surface waves in the ocean (see Hafsi et al., 2016). The goal of this project is to understand the impact of these centimeter-scale waves on the small-scale turbulence in the water-side of the air-water interface and the impact of the turbulence on gas transfer across the interface by molecular diffusion. Our simulations have shown that initiation of the waves by the wind leads to transition to turbulence on the water side which in turns leads to an increase in ocean uptake of greenhouse gases such as CO_2 by an order of magnitude for a brief period of up to 2 to 3 seconds relative to a wind-driven flow without the presence of the gravity-capillary waves and associated water-side turbulence. Given the frequency of wind gusts during normal weather conditions leading to the transition to turbulence on the water side and the previously described spike in gas transfer from the air side to the water side, we have concluded that this process must play a major role in determining long-term averages of oceanic gas uptake (Hafsi et al., 2016). Understanding such processes will result in improved parameterizations of global ocean flux uptake of greenhouse gases suitable for inclusion in climate models.

Dr. Tejada-Martinez is currently a member of the Consortium for Advanced Research for Transport of Hydrocarbon in the Environment (CARTHE) (carthe.org). This consortium of physical oceanographers and modelers is funded through the Gulf of Mexico Research Initiative (gomri.org) with the overall goal of improving oil spill models predicting the transport of oil in the oceans. As part of CARTHE, we have continued work with LES simulations of wind and surface wave-driven turbulent mixing processes such as Langmuir circulations (sketched in Figure 1) and associated Langmuir turbulence occurring on shallow coastal shelves that serve to heavily influence the bottom bed boundary layer, the re-suspension and transport of sediments and thus the sedimentation of oil. Oil sedimentation refers to when oil is adsorbed on the suspended material and deposited to the bottom. We are using our simulations to derive parameterizations or closures of turbulent vertical mixing of momentum and pollutants induced by Langmuir turbulence for inclusion in oil spill tracking models. Up to date, the wind and wave-generated Langmuir turbulence has not been taken into account by oil spill tracking models which can lead to significant errors in track and concentration predictions as shown via field measurements and simulations conducted by CARTHE investigators. Prior to the support from CARTHE, this work had been funded through a NSF CAREER award. This work has formed the basis of research for three former Ph.D. students (Roozbeh Golshan, Nityanand Sinha and Rachel Walker) and two post-doctoral researchers (Mario Juha (former) and Jie Zhang (current)).

In following along the lines of our work with CARTHE, a goal over the next several years is to obtain funding in order to further the development of an LES code or model capable of resolving not only turbulent vertical mixing processes in the ocean in response to meteorological forcing, but also the interactions of these processes with the general circulation within closed or semi-enclosed regions such as ports and natural harbors. The LES code will consist of an unstructured-grid finite element method able to represent anthropogenic structures such as docks, piers and breakwaters. The planned LES code is expected to provide improved predictions of lateral and vertical transport of accidentally spilled pollutants from ships and improved estimates of flushing efficiency and water quality in ports and harbors. Such estimates are important in light of the fact that lack of water mixing and flushing can negatively impact the environment within ports and detract from tourist activities.

Simulations of drinking water and wastewater treatment systems: In addition to the previously described projects related to upper-ocean turbulence, former Ph.D. student and current post-doctoral researcher Jie Zhang, master/Ph.D. student Faissal Ouedraogo and group lead Tejada-Martinez have pursued various projects involving the numerical simulation of flows in (1) drinking water disinfection systems such as baffled ozone contactors (Figure 2) and in (2) wastewater treatment systems. These studies have been made in collaboration with environmental engineering faculty in our department at USF and engineers from local public water utilities (see the various Zhang et al. papers in the publications section as well as Oudraogo et al. (2016), Verbyla et al. (2013) and Kinyua et al. (2015)).

At a fundamental level, we have made significant contributions towards understanding how near-wall turbulence modeling in flows through baffled ozone contactors can strongly affect RANS simulation predictions of important parameters that serve to measure the hydraulic efficiency of baffled ozone contactors such as mean residence time, baffling factor and short circuiting index. Previous studies had concluded that improved prediction of these parameters could only be achieved through increased mesh resolution ultimately leading to more expensive computations involving LES. Our work demonstrated for the first time that increased mesh resolution and thus LES is not required as long as the turbulence near the baffle walls is accurately modeled or represented in the RANS simulation (Zhang et al., 2013, Journal of Environmental Engineering).

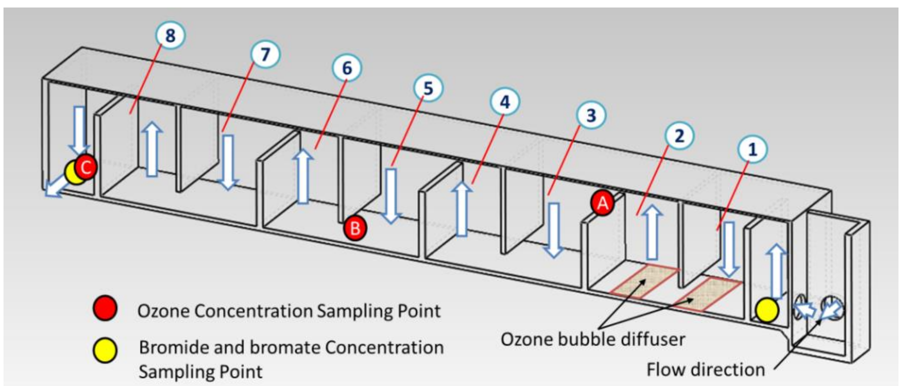

Figure 2: Sketch of the baffled ozone contactor used in the process of disinfection of drinking water at the David L. Tippin Water Treatment Facility operated by the City of Tampa Water Department. Dimensions are Length × Height × Width = 51.7 m × 7.32 m × 12.2 m. From Zhang et al. 2014, Water Research (see publications list).

In collaboration with the City of Tampa Water Department, a public water utility, our work has also focused on modeling the complex chemical processes occurring in turbulent flows within full-scale ozone contactors for the treatment of drinking water. More specifically we have developed the first RANS simulations with kinetics-based modeling for bromate within ozone contactors. Prior simulations had been limited to empirical models for bromate concentration requiring calibration of reaction rate coefficients. Note that bromate is an undesired by-product of ozone disinfection presenting a health risk. Results of our simulations are encouraging as they are consistent with ozone and bromate concentration measurements recorded at the ozone contactor managed by the City of Tampa Water Department (Figure 2) (Zhang et al., 2014, Water Research) despite uncertainties in some of the chemical reaction parameters in the physical system.

In addition to drinking water disinfection systems, we have also studied wastewater treatment systems, helping to quantify the pathogen removal capability of waste stabilization ponds and the mean residence time of suspended solids in anaerobic digestors of livestock wastewater (Verbyla et al., 2013; Kinyua et al., 2015).

In the future we plan to continue the use of numerical simulation techniques to assess the efficiency of water and wastewater treatment systems, while addressing the sustainability of these systems. For example, recently we have analyzed the sustainability of ozone contactors via RANS and have just completed a manuscript, which we believe would be the first publication in the literature detailing the application of computational fluid dynamics to sustainability of drinking water disinfection systems (Zhang et al. (2016), Water Research). In this work, we explored the environmental and economic impacts of making upgrades to the ozone contactor at the City of Tampa Water Department, for example, by changing baffle configurations. An outcome of this study has been the development of a composite indicator quantifying the sustainability of the upgrades incorporating technological, environmental and economic dimensions.

At USF we have been able to establish working relations with engineers at public water utilities such as the City of Tampa Water Department and Tampa Bay Water. The relationship with City of Tampa Water Department facilitated the Ph.D. research of former student and current post-doc Dr. Jie Zhang. The relationship with Tampa Bay Water has led to a current project serving as basis for current Ph.D. student Faissal Ouedraogo's dissertation. In this project we are making use of computational fluid dynamics to assess and improve water quality models and their coupling with the hydrodynamics in water distribution network models.

These collaborative relationships with professional engineers are expected to occur at a greater frequency through a recently established ASCE Task Committee in CFD (computational fluid dynamics) applications in water and wastewater treatment. The goal of the committee is to promote applications of CFD throughout the drinking water and wastewater industry and academia and to provide a primer on best CFD practices for these applications. The primer is currently being developed based on contributions from an impressive list of task committee members across academia and industry. I am a founding member of the committee and Jie Zhang, former Ph.D. student and current post-doc, is the current head.