Development of Electrochemical Treatment Technologies for PFOA, PFOS and 1,4-Dioxane in New Jersey Drinking Water and Regional Wastewater Treatment Plants

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Final Report

NJDEP Project #SR22-017

Development of electrochemical treatment technologies for PFAS, PFOS and 1,4-Dioxane in New Jersey Drinking Water and Regional Wastewater Treatment Plants

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2.0 Number of students supported:

Undergraduates: 1, Masters' students: 0, Ph.D. students: 2, Postdoctoral Associates: 1

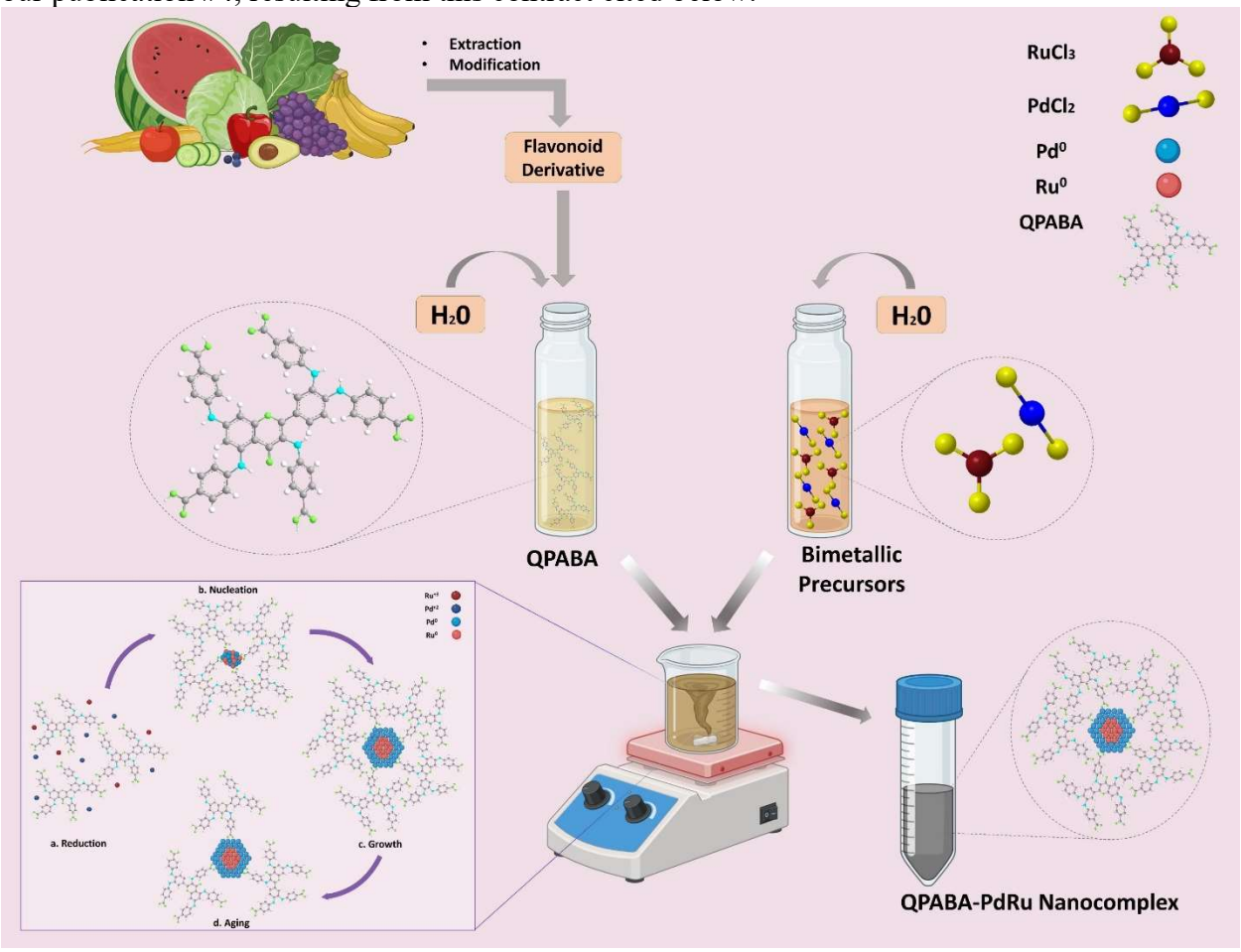
Short-term Deliverables Achieved

- We have developed a new class of polymer-embedded bimetallic nanocatalyst material and tested these for the degradation of selected PFAS. We have called this technology **IMPACT**-**I**nnovative (nano)**M**aterials and **P**rocesses for **A**dvanced **C**atalytic **T**echnologies to degrade PFOA in water. At the center of IMPACT are bimetallic Pd-Ru nano-catalysts, Quercetin Pentaparaamino Benzoic Acid ligands (Scheme 1), and specialized electrodes that use electrochemistry to detect and degrade PFOA. Control experiments did not show any degradation of PFOA in the absence of the catalysts. It has been tested for simulated wastewater within 3 hours with an efficiency of 98.5%, demonstrating its high effectiveness. IMPACT can be used as a treatment technology in a point source system to identify the source of pollution from which PFAS and 1,4-Dioxane are discharged, making it a valuable tool for environmental monitoring. When these polymer-embedded bimetallic nanocatalysts are incorporated into a prototype electrochemical system, the device could serve as a Point of Entry Technology or POET and be placed in industrial, solid, and waste management facilities. Any industry facilities that produce or process PFAS or use PFAS in manufacturing, such as electroplating, leather processing, landfills, and firefighting sites, can use this technology. Please see our publication #s 1 and 2, resulting from this contract cited below.
- We have studied the mechanism of the detection and degradation of PFAS using **IMPACT** and discovered that, unlike other conventional methodologies such as Advanced Oxidative Processes (AOPs), granulated activated carbon (GAC), and reverse osmosis technologies that remove and concentrate PFAS, IMPACT showed total removal of PFOA and leaves no secondary contaminants. We obtained evidence for facile degradation of PFOA from mass spectrometry and simulation data. Based on high-resolution desalting paper spray mass spectrometry (DPS-MS) analysis, this work showed that the electrochemical degradation of PFOA on GCE|PdRu yielded C_2F_5COOH, C_3F_7COOH and $C_6F_{13}OH$ as degraded products. Collision-induced dissociation (CID) confirmed that their ions dissociated by losses of CF_2O or CO_2. Hence, the mechanism proceeds by deprotonation, followed by losses of an electron and then CO_2, respectively. **IMPACT** uses an efficient electrochemical degradation mechanism to destroy PFAS without producing secondary contaminants, thereby addressing the concern that this technology could lead to the formation of toxic fragments. Please see our publication # 3, resulting from this contract cited below.

- We tested **IMPACT** for applicability in leachate samples provided by NJDEP staff. The pretreatment of the leachate samples was challenging, and multiple steps were required. The preliminary results of the treatment and analysis of WWTP leachate samples offered are detailed in our Report #2, Analysis of Leachate Samples. Fenton reaction was employed to clean the samples, which allowed

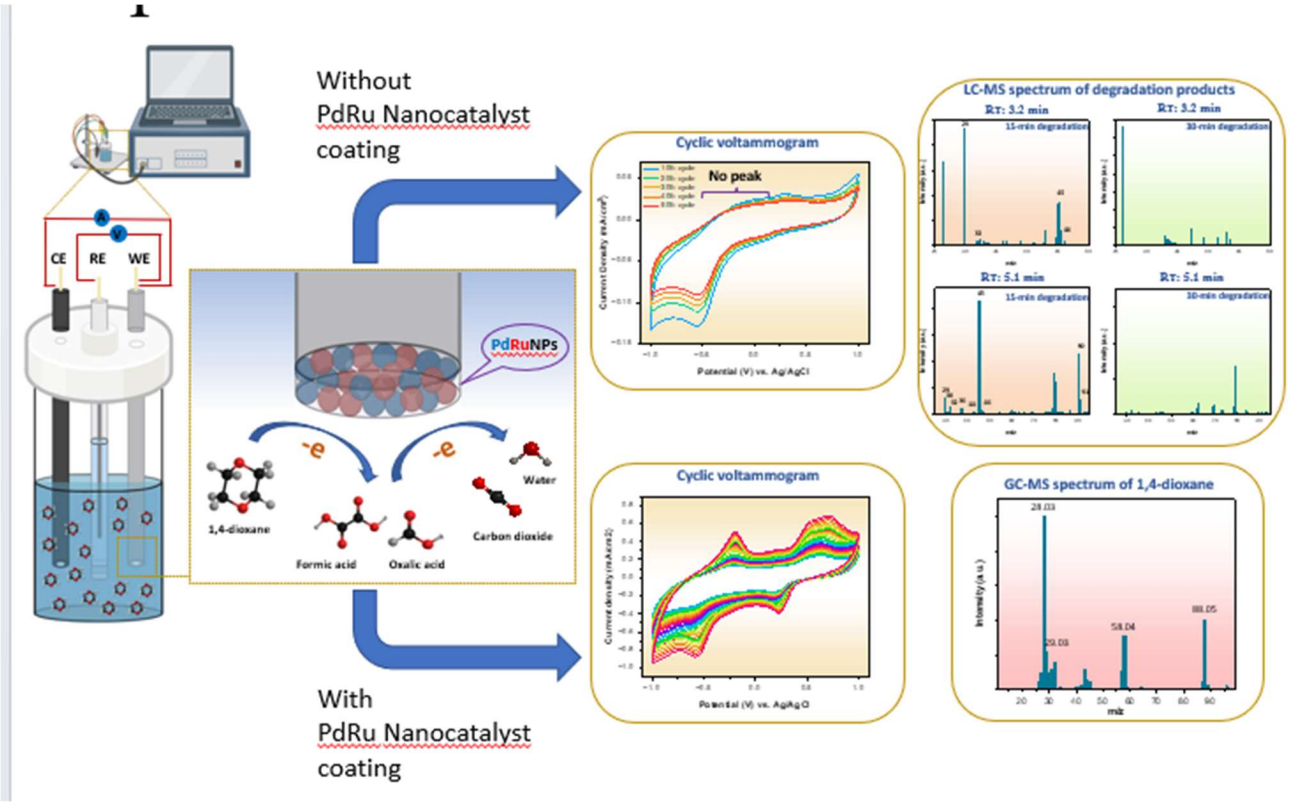
samples to clear the leachate enough to confirm the presence of multiple PFAS samples, namely perfluorooctanoic acid, perfluorooctanoic acid, and Trifluoromethanesulfonic acid using Paper Spray Mass Spectrometry. Due to blank contamination, tests for perfluorooctanoic acid, perfluorooctanoic acid, and GenX were inconclusive. While some tests have taken place for longer chain PFAS, finding perfluorooctanoic acid concentration of 12 ng/L and significantly lower levels for Perfluorononanoicacid and Perfluorooctanesulfonic acid, all being below the limit of 14ng/L in 2020. This is the preliminary work to prepare initial methods for the treatment of PFAS in leachate, which has a myriad of issues endemic to the sample type.

- As proposed in our initial contract, we tested the **IMPACT** for 1,4-Dioxane. To achieve this, we formulated another variant of the nanocatalysts and tested these for 1,4-Dioxane. We repeated the synthesis of the bimetallic PdRu nanoparticles (PdRuNPs) and demonstrated scalable variants and their application in water and wastewater. Similar to the PFOA study, Quercetin-para aminobenzoic acid (QPABA) served as both the reduction and support ligand for the preparation of the nanoparticles (Scheme 1). We studied the effect of ligand concentration and volumetric ratio of Pd: Ru metals systematically. We followed these with a computational study based on DFT B3LYP to determine the sites of QPABA's interaction with Pd and Ru ions. The findings showed that the most stable PdRuNPs are formed through the interaction of Pd and Ru ions at the OH site of the carboxyl group attached to the G-and F-rings, respectively (Scheme 2). Please see our publication #4, resulting from this contract cited below.



Scheme 1: Green fabrication of the Eco-friendly QPABA-mediated core-shell PdRuNPs.

- In addition, as proposed in our original contract, we explored the development of IMPACT for 1,4-Dioxane. We employed the PdRu nanoparticle catalysts to develop a sensitive and scalable electrochemical system for detecting and degrading 1,4-dioxane in water samples. The LOD was determined to be 0.034 ppb, which is below the USEPA advisory range of 0.35 to 35 ppb in water. A method combining liquid-liquid extraction with GC-MS was also employed for the detection of 1,4-dioxane, registering an MDL of 0.033 ppb in actual wastewater samples, also below the USEPA advisory range. wastewater design utilized bulk electrolysis with an electrode surface area of 230.79 cm^2 at 2 liters, tested with wastewater from a WWTP containing 1,4-dioxane in the range of 90 to 300 ppm, which was 100% removed within 30 minutes. Also, the time for complete removal of COD for these three samples, which ranged from 260 to 895 mg/L, were within 42 minutes (Scheme 2). This removal rate is significantly higher than other catalyzed and noncatalyzed electrolytic reactors. Finally, LC-MS analysis confirmed the reduction of 1,4-dioxane to carbon dioxide and water. Please see our publication #3, resulting from this contract cited below.



Scheme 2. Graphical illustration of the proposed mechanism for 1,4-dioxane oxidation.

Long-term Impact and Benefits

- Seamless integration of optimized nanocatalyst for PFAS degradation as a POET wastewater facility.
- The NJIT POET IMPACT was tested using water from private wells, wastewater, and a public water source. DEP assisted with leachate sampling and could further help with additional sources to evaluate different treatment techniques across media of high interest.
- The fundamental knowledge regarding the effectiveness and extent of degradation of the contaminants has been systematically carried out.
- Quantitative degradation efficiencies for PFAS, including PFOA and GenX, and 1,4-Dioxane,from synthetic wastewater, wastewater leachate samples, drinking water, and groundwater have been conducted.

- IMPACT is scalable as a POET and has been developed from lab scale (~ 100mL to 2 liters samples) as well as different electrode sizes (0.3 to 250 cm^2). In the future, the Reticulous Vitreous Carbon (RVC) electrode could be designed for a flow system. NJIT has an operational design team working on the POET for flow systems that should satisfy the program's needs. Figure 1 is a schematic of what this looks like for field practitioners, homeowners, and larger water systems.
- In the long term, this technology could create a dynamic, cost-effective electrochemical treatment system that integrates novel catalysts with off-the-shelf TFF modules for point-or-use treatment of PFAFs and 1,4-Dioxane in drinking and wastewater samples.

How to Develop IMPACT into a Point of Entry Benchtop Technology

As noted for the testing for 1,4-Diooxane, the IMPACT technology could be packaged, and a well-characterized electrochemical-tangential Flow Filtration (EC-TFF) prototype could be tested at NJDEP regional New Jersey wastewater facilities. Water treatment widely lacks in-situ groundwater applications that involve the spectrum of PFASs and PFAAs. Unlike IMPACT technology, the typical remediation of water and leachate uses extraction and ex-situ methods, adsorption, physical destruction, and overall separation from the liquid phase. The present status of ex-situ treatment does not chemically disassemble the PFAS or PFAA molecule itself and, therefore, does not fully degrade the contaminant.

The significant advantage of this technology is the tunable chemistry of the nanocatalyst, which enables both broad applicability and specific applications. Furthermore, the IMPACT technology is scalable and eco-friendly because of the QPABA, which is a naturally derived material for synthesis. Given the fact that the fundamental efficiency of the catalyst has been established, it may be equipped with TFF to create the EC-TFF. Figure 3A shows the EC-TFF concept. We envision that the catalyst could be sequestered into polymeric membranes with a Tangential Flow Filtration device (TFF) to create an innovative Electrochemical EC-TFF system for drinking water cleanup. (a) establish

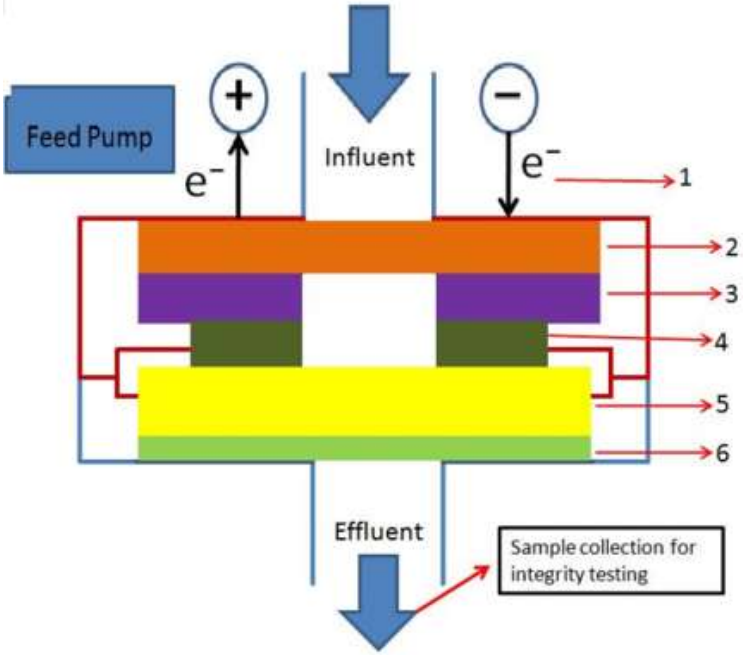


Figure 1: *Design of the EC-TFF device consisting of (1) applied potential, 2) perforated stainless steel cathode, (3) an insulating silicone rubber separator and seal, 4) a titanium anodic ring that is pressed onto the bimetallic nanocatalyst RVC, 5) IMPACT Membrane anodic filter supported by a gold mesh substrate (6).*

important filtration performance such as TFF feed rates, flux, contaminant concentration, run time, integrity & permeability testing, and removal efficiency; (b) Conduct demonstration (batch) TFF experiments with the nanoporous polymers synthesized. Ultimately, it should be possible to determine the degradation time, contaminant concentration, surface morphology, regeneration, and material stability. In that respect, the EC-TFF experiment could utilize the benchtop Minim II (Pall Corporation, NY), equipped with control pumps, stirrer speed, and display pressure to control the temperature effectively. This system can process sample volumes of 20 liters and higher while efficiently concentrating samples to as little as 5 mL.

To begin the contaminant and degradation process, we will plug a "Minimate" capsule equipped with an IMPACT membrane into a TFF device. Drinking water samples could be added, and the pump turned on. The

water could then be filtered over the IMPACT catalyst at a specified pressure and room temperature as the voltage is applied. The feed solution (laboratory water samples or well water from regional NJ sites), permeate (2 batches of each), and retentate will be collected and analyzed for MCL of organic contaminants using EPA Method 537.1 and the electrochemical degradation device available in the EC-TFF. By flowing a large volume of aqueous samples through the filter, all PFAF and any organics at low concentrations can be accumulated on the surface of the membrane. Finally, the targeted PFAFs can be captured and degraded upon applying electrical potential, while the Pd-Ru will catalyze the degradation as proposed on various membranes. The performance of the EC-TFF will be assessed in terms of filtration time, degradation efficiency, concentration, and type of water matrix. The best-performing catalyst will be selected for pilot-scale testing at the water facility. Additionally, the development and running of scaled-up and continuous systems controlled by the monitoring system is feasible due to their potential for automation.

Results

Determination of 1,4-Dioxane in WWTP effluent by liquid-liquid extraction and GC-MS

Fig. 2c illustrates the percentage of COD degradation to explore the effect of initial COD values on COD removal rate. The COD removal profiles for samples 1-3 exhibit a pattern like that observed for dioxane removal in **Fig. 2b**. Significant reductions in COD were noticed for all three samples following the electrochemical treatment by use of the scaled-up setup containing $PdRuNP_3$ catalyst-modified RVC as working electrode. The complete COD degradation was achieved within 25 minutes for sample 1 with a COD of 260 mg/L and approximately 38 and 42 minutes for samples 2 and 3 with COD of 560 and 895 mg/L, respectively, demonstrating efficient removal of COD under designed experimental conditions. The achieved COD removal rates exceed those documented in the literature.

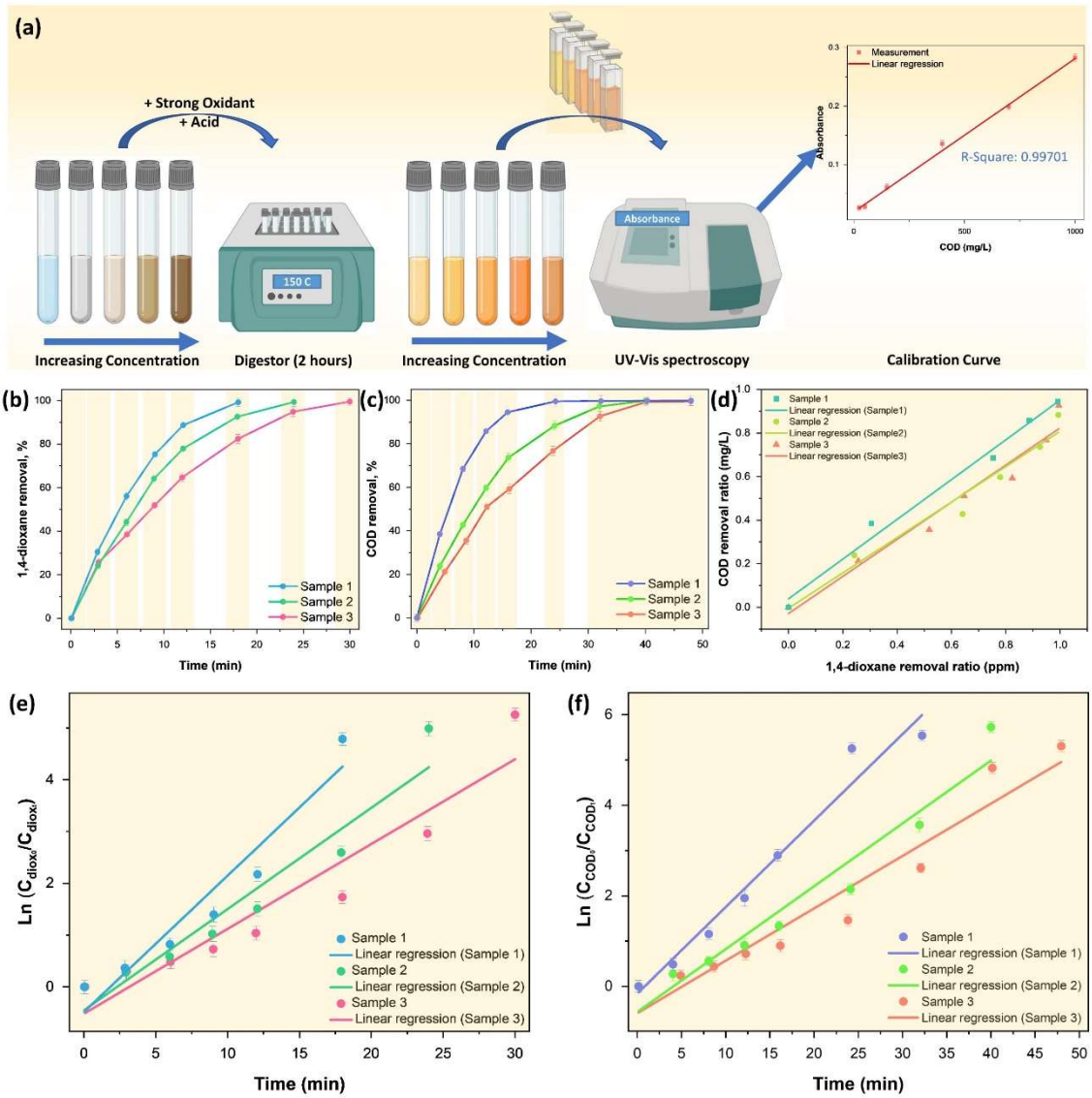


Fig. 2. (a) graphical illustration of COD measurement, (b, and c) The 1,4-dioxane and COD removal during the electrochemical oxidation of dioxane in three samples: sample 1 ($C_{dioxane}$ of 90 ppm, and COD of 260 mg/L), sample 2 ($C_{dioxane}$ of 170 ppm, and COD of 560 mg/L), and sample 3 ($C_{dioxane}$ of 300 ppm, and COD of 895 mg/L) using $PdRuNP_3$ embedded GCE, (d) The relationship between 1,4-dioxane oxidation, and COD removal for samples 1-3, (e) The first-order kinetic model for 1,4-dioxane removal at various initial 1,4-dioxane concentration over time, and (f) The first-order kinetic model for COD removal at various initial COD values over time.

The correlation between the concentration of COD removed and the rate of dioxane removal is depicted in **Fig. 2d** for three distinct samples (Sample 1-3) with a regression coefficient higher than 0.96 for all three samples. The linear regression parameters between the removal rate of COD and the 1,4-dioxane degradation rate are summarized in **Table S10**. Increasing the removed amount of 1,4-dioxane correlates linearly with a reduction in the quantity of COD in the solution. For all three samples varying from the low initial concentration of 1,4-dioxane (sample 1) to the high initial concentration (sample 3), the rate of COD removal correlates consistently

with the oxidation rate of 1,4-dioxane. This illustrates the proportional enhancement of COD degradation with 1,4-dioxane oxidation. These findings play a pivotal role in employing electrochemical oxidation for treating real water samples contaminated with 1,4-dioxane and have engineering significance. The noted linear correlation between 1,4-dioxane degradation and COD reduction for all three samples enables the estimation of COD removal rates without the necessity for long-lasting COD measurements that might take several days. The use of real WWTP samples in these examinations was vital since their composition contains natural organic substances that could notably influence both COD removal and its correlation with the 1,4-dioxane degradation [1].

The electrocatalytic degradation for both 1,4-dioxane and COD removal was analyzed using a first-order kinetic model [2]:

$$r_{degradation} = -{}^{dC}/_{dt} = k_{app}C \quad (1)$$

After integration, the equation can be reformulated as:

$$ln\left({}^{C_0}/_{C_t}\right) = k_{app}\, t \quad (2)$$

For COD measurements, C_{COD_0} and C_{COD_t} denote the initial and final concentration of COD, respectively. The symbol k_{app} signifies the pseudo-first-order constant (min^{-1}), and t represents the time elapsed (min). However, for 1,4-dioxane degradation, C_{diox_0} and C_{diox_t} refer to the initial and final 1,4-dioxane concentration.

The linear correlation between the variable $ln\left({}^{C_{diox_0}}/_{C_{diox_t}}\right)$ and time (t) in our system is depicted in **Fig. 2e**. The rate constants of 0.26, 0.19, 0.16 min^{-1} for samples 1,2 and 3 were calculated respectively (**Fig. 2e**, and **Table S11**). Therefore, an elevation in the 1,4-dioxane concentration leads to a slight reduction in the degradation rate constant. As indicated in **Table S11**, an R^2 value exceeding 0.92 signifies a strong correlation with first-order kinetics. Additionally, **Fig. 2f** illustrates the linear regression between the variable $ln\left({}^{C_{COD_0}}/_{C_{COD_t}}\right)$ and degradation time (t). The slopes of linear regression give the rate constants of 0.19, 0.138, and 0.117 min^{-1} for samples 1,2, and 3, respectively with regression coefficients higher than 0.94 (**Table S12**). The obtained R^2 values indicate a significant correlation between the COD removal rate and first-order kinetics. As observed in **Tables S11** and **S12**, an increase in the concentrations of 1,4-dioxane and COD from sample 1 to sample 3 leads to a slight reduction in the rate constant. This phenomenon can be attributed to the gathering of intermediates near the electrode interface, which slightly decreases the overall degradation efficiency [1]. Consequently, for all three samples varying from the low initial concentration of 1,4-dioxane

(sample 1) to the high initial concentration (sample 3), there is a consistent correlation between the rate of COD removal and the 1,4-dioxane oxidation rate. Both processes exhibit first-order kinetics. The efficient COD and 1,4-dioxane removal are attributed to the significant surface area of PdRuNPs, which offers a considerable quantity of active sites [3]. The sample obtained after CA was analyzed by LC-MS, which served as a trace analytical technique.

Determination of degradation products using LC-MS

The sample obtained after the CA underwent further scrutiny through LC-MS studies to investigate the degradation products after 15 minutes and 30 minutes of CA, with the results depicted in **Fig. 3** (**c**, **d**, **e**, and **f**). The presence of additional peaks of varying intensities, beyond those corresponding to formic acid and oxalic acid, can be attributed to the presence of other compounds with varying compositions and concentrations in the water sample obtained from WWTPs effluents, which were subjected to CA analysis. Due to their distinct structures and molecular weights, the potential products were identified at various retention times, with formic acid detected at a lower retention time of 3.2 minutes compared to oxalic acid, which exhibited a retention time of 5.1 minutes. In **Fig. 3** (**c**, and **e**), the LC-MS spectra obtained after 15 minutes of CA are provided, which closely match the standard LC-MS spectrum provided by the National Institute of Standards and Technology (NIST) for formic acid and oxalic acid, respectively. In **Fig. 3c**, the molecular ion peaks at a mass-to-charge ratio (m/z) of 45 signify the intact molecular ion of formic acid, whereas the peaks at (m/z) of 19 and 32 denote ions fragmented from the main compound. Concerning oxalic acid, the peak at m/z of 90 signifies the intact molecular ion, whereas those around 30 and 45 are linked to fragment ions (**Fig. 3e**) [4,5]. The absence of peaks corresponding to formic and oxalic acid in the mass spectrometry obtained after 30 minutes of CA (**Fig. 3d**, and **f**), as opposed to their presence at the 15-minute mark, suggests their potential degradation or conversion into alternative products such as CO_2, and water during this extended timeframe. This phenomenon likely arises from ongoing chemical transformations or interactions within the degradation process, resulting in the alteration or breakdown of formic and oxalic acid into alternate chemical species.

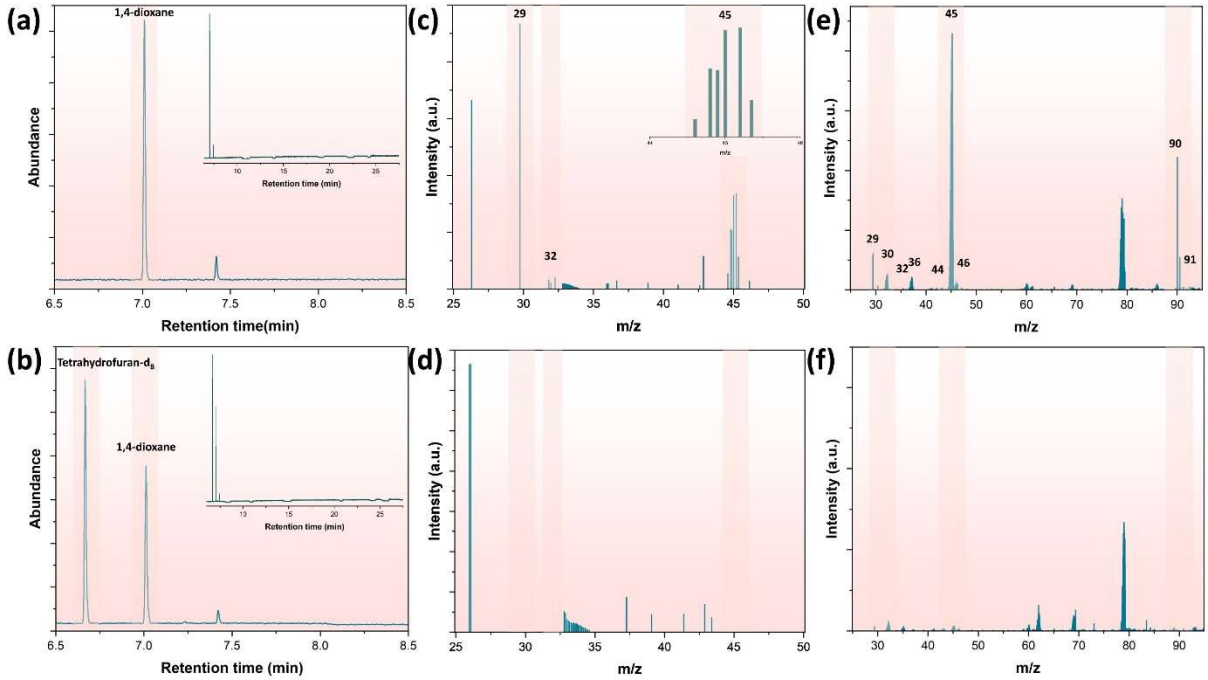


Fig. 3. The total ion chromatograms of (a) 1,4-dioxane, (b) 1,4-dioxane, and its SUR in water by LLE technique- Insets depict the identical chromatogram with extended retention time (for each of parts a and b). The LC-MS spectra of formic acid with retention time: 3.2 min after (c) 15 minutes, and (d) 30 minutes. The LC-MS spectra of oxalic acid with retention time: 5.1 min after (e) 15 minutes and (f) 30 minutes.

Significant Findings and Future Work

- The NJIT team developed the project's Quality Assurance Project Plan (QAPP), which was approved by the NJDEP management.
- We have achieved a 3-hour efficient electrochemical degradation of PFOA on Palladium-Ruthenium (PdRu) nanocatalyst materials fabricated onto Glassy Carbon Electrode (NcM/GCE) with an efficiency of 98.5 %. Simulation studies on PFOA correlated and agreed with the experimental results. The electrochemical Degradation of PFOA on PdRu/GCE yielded C_2F_4COOH, C_3F_7COOH, and $C_6F_{13}OH$ as degraded products, based on desalting paper spray mass spectrometry (DPS-MS) analysis of the degraded products. Collision-induced dissociation (CID) confirmed that their ions dissociated by losses of CF_2O or CO_2. Hence, the mechanism proceeds by deprotonation, followed by the loss of electrons and $CO_{2.}$, respectively. This work promotes the general sustainable electrochemical degradation of recalcitrant organics in water systems using PdRu core-shell nanomaterials.
- We have embarked on a selected sample collection for drinking water and WWTPs around NJ.
- We have accomplished the detection of 6 PFAS in selected WWTPS around New Jersey.
- We have determined the diffusion coefficient of PFOA for the first time and have reported these in the manuscript below.
- We have implemented IMPACT, which is the electrochemical degradation work of 1,4-dioxane.
- We have published three manuscripts in this contract.

4.0 Publications and Presentations Resulting from this Contract

1. Yadav M., F. Osonga, O. Sadik, Unveiling Nano-empower Catalytic Mechanisms for PFAS Sensing, Removal and Destruction in Water, *Science of the Total Environment. 912:169279.* **2024**.
2. Md.Tanim-Al-Hassan, X. Chen, P. Ivan Joel FNU, F. Osonga, O. Sadik, M. Li, and H. Chen, Rapid detection of per- and polyfluoroalkyl substances using paper spray-based mass spectrometry, *J. Hazardous Materials*, 465:133366. **2024**.
3. Osonga, F., G. Eshun, S. Kurilla, A. Qamar, H. Xue, Md. Tanim-Al Hassan, H. Chen & O. Sadik, IMPACT: Innovative (nano) Materials and Process for Advanced Catalytic Technologies to Degrade PFOA in Water*, Chemosphere. 364:143057.* **2024**.
4. Milad Torabfam, Francis Osonga, Quentin Young, Omowunmi Sadik, Scalable Electrochemical Detection and Degradation of 1, 4-Dioxane in Water and Wastewater: A Core-shell Bimetallic Nanocatalyst and Simulation Study, *ES&T Water* **2025.**
5. Omowunmi Sadik, Sustainable Nanocatalysts for Degradation of Recalcitrant Environmental Pollutants (Invited Lecture), Joint School of Nanoscience & Nanoengineering, February 17, **2023**, UNC Greensboro.
6. Sadik OA., Electrochemical Methods for Detection, Measurement and Destruction of "Forever Chemicals" PFAS, ID: PC-1031 Abstract Title: Sensing and Analytical Technologies for Emerging Environmental Contaminants (Invited Abstracts: Symposium Track: Environmental Associate Your Session: Sensing and Analytical Technologies for Emerging Environmental Contaminants (Andreescu), Pittcon 2023, March 18-22, Philadelphia, PA.
7. Francis J. Osonga, & Omowunmi A. Sadik, Novel bimetallic nanoformulation for the electrochemical Degradation of PFOA and PFOS, (Invited Oral presentation) SEAC - The Student Session in Electroanalysis- Pittcon conference, March 18-22, 2023, Philadelphia, Pennsylvania, USA.
8. Sadik OA, Sustainable Nanocatalysts for Degradation of Recalcitrant Environmental Pollutants, April 14, 2023, NJIT Campus, Newark, NJ.
9. Stephen Kurilla, Gaddi Eshun, Francis J. Osonga Omowunmi A. Sadik, Palladium-Nickel Nanoparticle Catalyzed Degradation of Polyfluorooctanoic Acid, Gordon Research Seminar, Environmental Nanotechnology, Grand Summit Hotel at Sunday River, Considering all Dimensions of the Nanotechnology - Environment Interface, June 3-4, 2023, Newry, ME, United States.

5.0 Conclusions

This contract has led to the development of a novel bimetallic nanocatalyst and a POET system that can detect and degrade PFAS and 1,4-Diooxane. The IMPACT system is scalable and has been demonstrated to be effective for the organic class of pollutants. To the best of our knowledge, no comprehensive investigation has been conducted into the development of an energy-efficient and eco-friendly nanocatalyst and a scalable and sensitive electrochemical system utilizing a PdRu bimetallic nanocatalyst for the simultaneous detection and degradation of PFAS and 1,4-dioxane in synthetic water samples.

6.0 References Cited

1. J.H. Suh, M. Mohseni, A study on the relationship between biodegradability enhancement and oxidation of 1,4-dioxane using ozone and hydrogen peroxide, Water Res 38 (2004) 2596–2604. https://doi.org/10.1016/j.watres.2004.03.002.

2. N.K. Sethy, Z. Arif, P.K. Mishra, P. Kumar, Green synthesis of TiO2 nanoparticles from Syzygium cumini extract for photo-catalytic removal of lead (Pb) in explosive industrial wastewater, Green Processing and Synthesis 9 (2020) 171–181. https://doi.org/10.1515/gps-2020-0018.

3. L. Murruni, G. Leyva, M.I. Litter, Photocatalytic removal of Pb(II) over TiO2 and Pt–TiO2 powders, Catal Today 129 (2007) 127–135. https://doi.org/10.1016/j.cattod.2007.06.058.

4. W.E.W. director NIST Mass Spectrometry Data Center, NIST Standard Reference Database 69: NIST Chemistry Web Book, Formic acid, (n.d.).

5. W.E.W. director NIST Mass Spectrometry Data Center, NIST Standard Reference Database 69: NIST Chemistry WebBook, Oxalic acid, (n.d.).

Table S10. Retention times, and main peak indices in the GC-MS spectrum.

Compound	Peak index (m/z)	Retention time (min)
1,4-dioxane	30.08, 46.13, 48.16, 80.18	7.01
Tetrahydrofuran-d_8	28.03, 29.05, 58.04, 88.05	6.67

Table S11. The MDT and linearity of calibration curve for 1,4-dioxane using the LLE technique.

Method	Surrogate	The range of calibration (ppb)	Y = a X + b			MDL (ppb)
			a	b	r^2	
LLE	tetrahydrofuran-d_8	0.1-10.0	324571	465588	0.9967	0.03379

Table S12. Recovery and precision evaluation for 1,4-dioxane using the LLE method.

Target concentration (ppb)	Measured concentration Four repeats (ppb)				Mean recovery (%)	Precision (%)
0.500	0.4679	0.5309	0.4721	0.5048	98.78	5.200
10.00	10.09	9.88	10.39	9.75	100.275	2.412

Table S13. The linear regression parameters between the degradation rate of COD and the 1,4-dioxane removal rate

Sample	1	2	3
Slope	0.9122	0.8120	0.8514
R-Square	0.9867	0.96704	0.96256

Table S14. The parameters of the linear correlation between the natural logarithm of 1,4-dioxane concentration factor and time.

Sample	1	2	3
Slope	0.2633	0.1956	0.1639
R-Square	0.9332	0.9394	0.9285