15th Quarterly Report
October-December 2023
AESF Research Project #R-121

Development of a Sustainability Metrics System and a Technical Solution Method for Sustainable Metal Finishing

by
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Editor's Note: *This NASF-AESF Foundation research project report covers the 15th quarter of project work (October-December 2023) at Wayne State University in Detroit. A printable PDF version of this report is available by clicking **HERE**. A listing of previous reports to date is provided at the end of this report.*

Overview

It is widely recognized in many industries that sustainability is a key driver of innovation. Numerous companies, especially large ones who made sustainability as a goal, are achieving clearly more competitive advantages. The metal finishing industry, however, is clearly behind others in response to the challenging needs for sustainable development.

This research project aims to:

1. Create a metal-finishing-specific sustainability metrics system, which will contain sets of indicators for measuring economic, environmental and social sustainability,
2. Develop a general and effective method for systematic sustainability assessment of any metal finishing facility that could have multiple production lines, and for estimating the capacities of technologies for sustainability performance improvement,
3. Develop a sustainability-oriented strategy analysis method that can be used to analyze sustainability assessment results, identify and rank weaknesses in the economic, environmental, and social categories, and then evaluate technical options for performance improvement and profitability assurance in plants, and
4. Introduce the sustainability metrics system and methods for sustainability assessment and strategic analysis to the industry.

This will help metal finishing facilities to conduct a self-managed sustainability assessment as well as identify technical solutions for sustainability performance improvement.

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Progress Report (Quarter 15)

1. Student participation

Mahboubeh Moghadasi, a PhD student in the PI's group, conducted research in this reporting period. She is financially supported by the University as a Graduate Teaching Assistant (GTA) due to a need for course assistance for the academic year of 2023-24. She has continuously worked on this AESF research project under the PI's supervision.

2. Summary of project activities

In this quarter, our work has focused on the development of a set of Digital Twins (DTs) using the Physics-Informed Neural Network (PINN) technology with application on parts rinsing simulation.

2.1. Integrated rinsing model development

An electroplating line usually has several rinsing systems, each of which may contain one or more rinsing units. The dirt and/or chemical residues on the ~~parts~~ surface are rinsed off in the rinse systems. Each rinse unit has two operating modes: the rinse mode and the idle mode. To characterize the rinse operation, we need to have two types of dynamic models.

(2.1.1) Fundamental model for characterizing the removal of the dirt/chemical residues on a part surface:

$$A_p \frac{dW_{Pr}(t)}{dt} = -r_{Pr}(t) \tag{1}$$

$$r_{Pr}(t) = k_r r_c(t_c^e)(\theta W_{Pr}(t) - x_r(t)) \tag{2}$$

where W_{Pr} is the amount of dirt on parts when the barrel is in a rinse tank (g/cm^2); r_{Pr} is the dirt removal rate in the rinse tank (g/min); k_r is the mass transfer coefficient (gal-chem·gal-water/gal-soln ·cm^2); $r_c(t_c^e)$ is the looseness of dirt on parts when leaving a cleaning tank at the time t_c^e (cm^2·gal-soln/gal-chem·min); θ is the unit conversion factor (cm^2/gal-water) and x_r is the pollutant composition in rinse water (g/gal-water).

(2.1.2) Fundamental model to reveal the dynamic change of the pollutants in a rinse unit.
The amount of pollutants in the rinse water is related to the rinsing efficiency, water flow rate, the initial dirtiness of parts and the cleanness of the influent rinse water. In a rinse unit, there are two operational modes: the rinse mode, in which the parts are submerged in the tank, and the idle mode, in which the parts are withdrawn while the rinse water still continuously flows through the tank. The following model is derived for both the rinse and the idle modes.

$$V_r \frac{dx_r(t)}{dt} = F_r(t)\big(Z_r(t) - x_r(t)\big) + (H(t) - H(t - t_r^e))r_{Pr}(t) \tag{3}$$

where V_r is the rinse tank capacity (gal-water); F_r is the rinse water flow rate (gal-water/min) and Z_r is the pollutant concentration in the influent rinse water (g/gal-water). The operational mode switch is described by a pulse function (see the second term on the right of the equation, which is expressed by two Heaviside functions appeared at two different time instants.

2.2. Architecture of physics-informed neural networks (PINN)

In the last report (July-September 2023, 14th quarter), we described a PINN structure where an integrated cleaning model was integrated, which is shown in Fig. 1. The same structure is used for accommodating the integrated rinsing model described above in the Physics Layer in the figure.

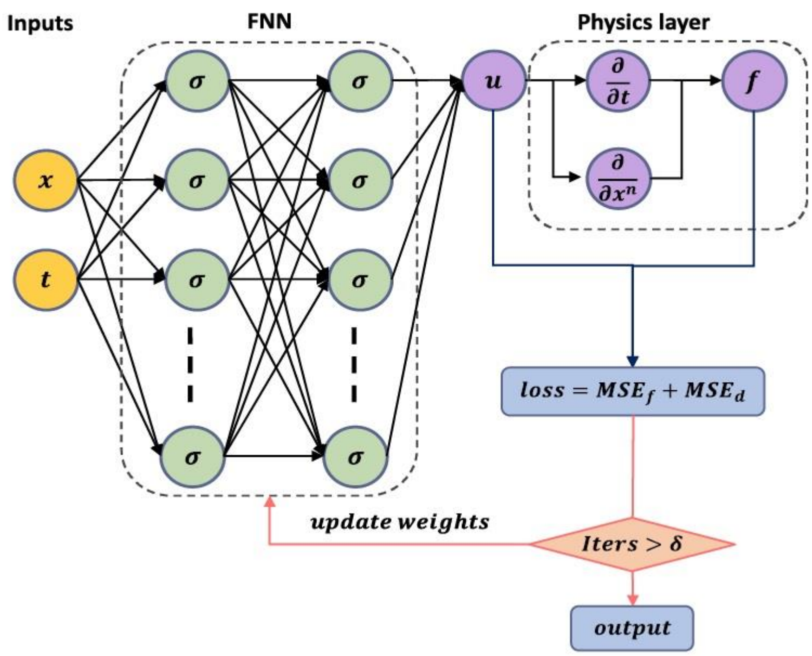

Figure 1 - PINN as the last layer of a feedforward neural network (FNN).

2.3. Rinse operation simulation

We have conducted an extensive PINN-based simulation. Table 1 shows the parameters used in the model as well as the operating condition setting used for simulation. As the first step, we simulated the rinsing of one barrel of parts. There were two scenarios for simulation study.

Table 1 – Operating condition setting and model parameters in the case study.

Rinsing time ($t_e^r - t_0^r$ (min)	0.5
V_r (gal)	220
$x_r\left(t = t_0^r\right)$ (g/L-water)	0.2
z_r (g/gal-water)	0
F_r (gal-water/min)	6.5
k_r (gal-chem·gal-water/gal-soln·cm^2)	0.0008
θ (cm^2/gal-water)	936.36

In the first scenario, the PINN was exposed to a synthesized clean dataset to assure optimal conditions for model prediction and facilitate a baseline against which the efficacy of the model could be evaluated. The simulation result of the first scenario for the amount of dirt on parts (W_{Pr}) and pollutant concentration (x_r) in the rinse tank (RT) are shown in Figures 2 and 3, respectively.

In the second scenario, the model was navigated using a synthesized noisy dataset, which reflected a real operating condition (with disturbances and some other uncertainties appeared in production). The simulation result of the second scenario for amount of dirt on parts (W_{Pr}) and pollutant concentration (x_r) in the rinsing tank (RT) are shown in Figures 4 and 5, respectively.

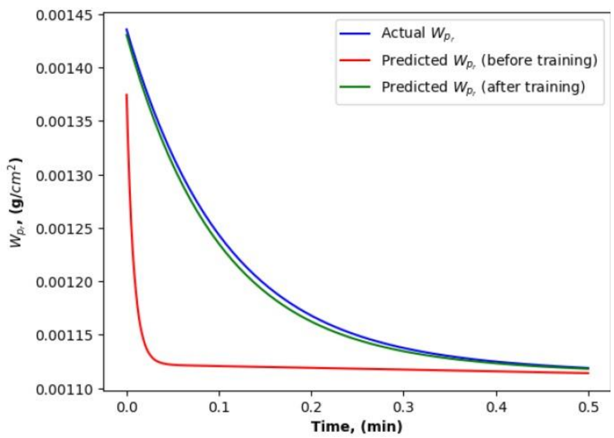

Figure 2 - Dirt/chemical removal dynamics on part (W_{Pr}) in the rinse tank.

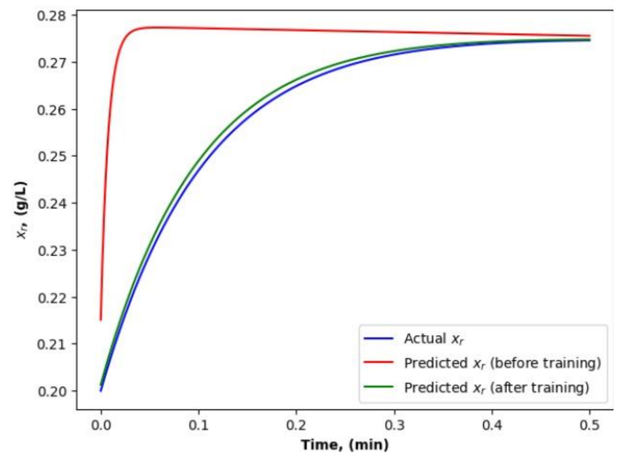

Figure 3 - Dynamic change of pollutant concentration change (x_r) in the rinse tank.

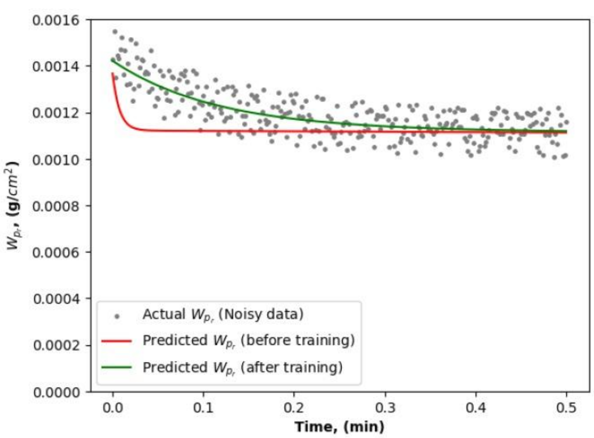

Figure 4 - Dirt/chemical removal dynamics on part (W_{Pr}) using noisy data.

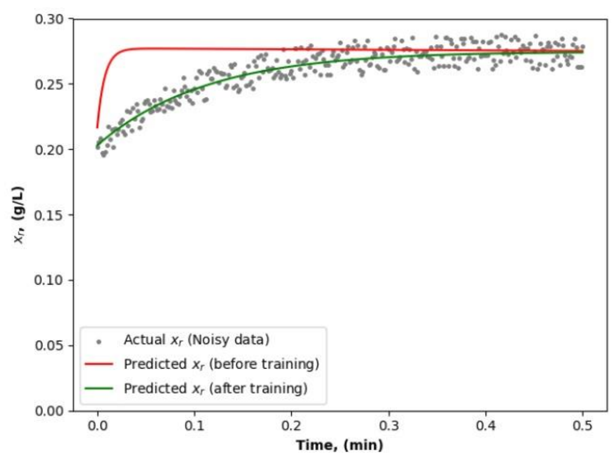

Figure 5 - Dynamic change of pollutant concentration change (x_r) using noisy data.

In the idle mode, owing to the inherent simplicity of the governing nonlinear differential equation, commendable prediction accuracy is attained even without model training. Figure 6 shows the pollutant concentration dynamics in the rinse unit in both the rinse and the idle modes. Given the elementary nature of the equation, it can be swiftly and effectively solved within the computational cell, ensuring immediate and reliable predictions. This allows for efficient system modeling and operational planning even in the absence of a thoroughly trained model, underscoring the utility and applicability of the approach in scenarios dictated by simpler differential equations. This observation further supports the versatility of the model, being adept not only in more computationally intensive scenarios but also in straightforward, analytical contexts, enhancing its practicality across a diverse array of operational

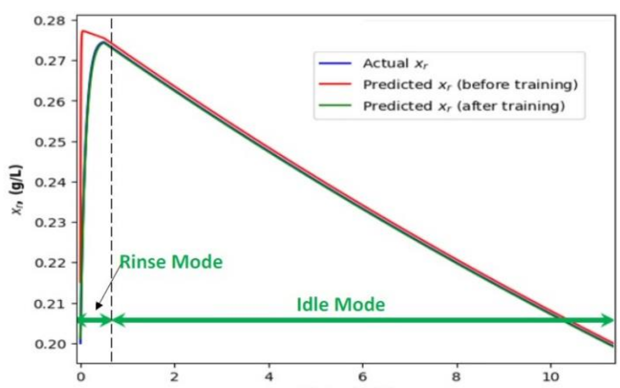

Figure 6 - Pollutant concentration change (x_r) in the rinse tank.

circumstances. These are reflected in Table 2, which shows a comparison of the operation of the rinse unit using different datasets.

Table 2 - Comparison of the rinse unit operation using different datasets.

Parameters \ Run	Initial guess	Clean dataset	Noisy Dataset	Actual value
Mass Transfer Coefficient (k)	0.01	0.00085	0.00085	0.0008
Dirt Removal %	-	21.85%	21.29%	Clean dataset: 22.07% Noisy Dataset: 18.63%
Pollutant conc. rise in rinse mode	-	0.07	0.07	Clean dataset: 0.07 Noisy Dataset: 0.08

In addition to the single-step rinse simulation, we also simulated two-step rinsing using the PINN. Our focus was on the estimation of crucial parameters, such as the mass transfer coefficient, k_r. The PINN framework integrates these parameters with an NN model, trained on both available data and the governing physical laws of the system. This dual reliance on empirical data and theoretical principles ensures a more robust and accurate simulation. Table 3 lists process and parameter settings used in the simulation study.

Table 3 - Process setting and process parameters for simulating a two-step rinsing system.

Cleaning operation		Rinsing operation, tank 1		Rinsing operation, tank 2	
Cleaning time $t_e^c - t_0^c$ (min)	4.16	Rinsing time $t_e^r - t_0^r$ (min)	0.5	Rinsing time $t_e^r - t_0^r$ (min)	0.5
		Idle time (min)	4.16	Idle time (min)	4.16
V_c (gal)	320	V_r (gal)	220	V_r (gal)	220
$W_{p_c}(t=0)$ (g/cm²)	0.0035	$x_r\left(t=t_0^r\right)$ (g/L-water)	0.07	$x_r\left(t=t_0^r\right)$ (g/L-water)	0.06
$C_a(t=0)$ (gal-chem/gal-soln)	7.6%	z_c (g/gal-water)	$x_r(t=t_e^{r2})$	z_c (g/gal-water)	0.06
γ_0 (cm²·gal-soln/gal-chem·min)	1.3×10^6	F_r (gal-water/min)	7	F_r (gal-water/min)	7
α	20	k_r (gal-chem·gal-water/gal-soln·cm²)	0.0008	k_r (gal-chem·gal-water/gal-soln·cm²)	0.0008
η (g-dirt/gal-chem)	3,031.6	θ (cm²/gal-water)	936.36	θ (cm²/gal-water)	936.36

The simulation results for the two-step rinsing system using PINN indicate a high degree of accuracy in predicting the dynamics of dirt removal and pollutant concentration within the tanks. The PINN based predictions closely follow the actual data trends. In Fig. 7, the prediction of dirt removal over time is very close to the actual measurements. Similarly, Fig. 8 captures the changes in pollutant concentration, which is very satisfactory. The consistency between the predicted and the actual values validates the PINN approach, offering promising avenues for reducing environmental impact through improved process efficiency.

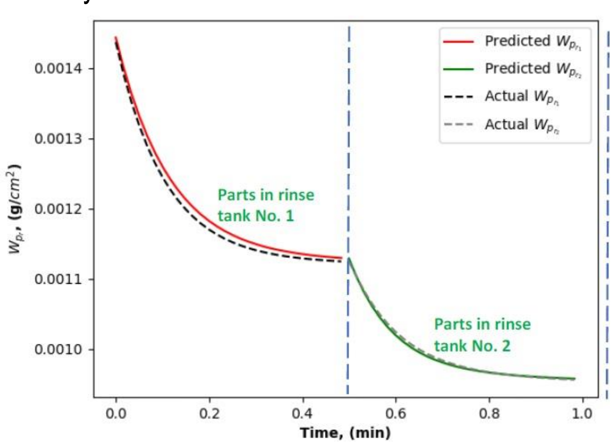

Figure 7 - Dirt removal from parts surface in the two-step rinsing system.

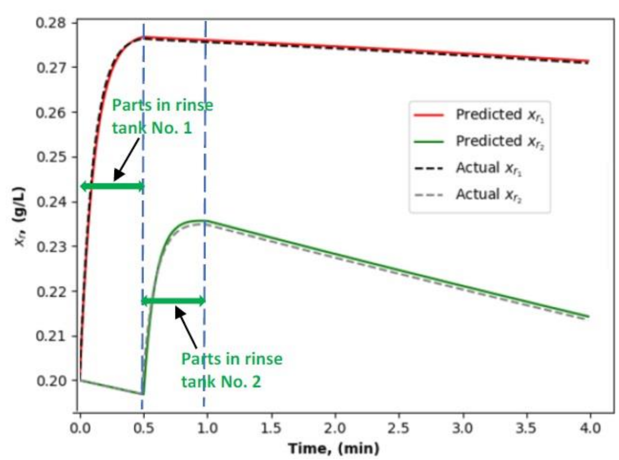

Figure 8 - Pollutant concentration change in two rinse tanks.

3. Summary and plan

In the last report, we reported our success in the development of Physics-Informed Neural Networks (PINN's) based digital twinning method for simulate cleaning processes. In this quarter, we made good progress in using the PINN technology to simulate a rinse system consisting of one or two rinsing units. We are confident that this technology can eventually be used to simulate an entire electroplating plant.

In the next project period, we will simulate the rinsing system operated for any period of time, such as for a shift, a day or multiple days. We will also start to simulate the electroplating operation. Hopefully, a plant-wide Digital Twin platform using PINN will be eventually created, which should be highly valuable for conducting dynamic sustainability assessment and decision making for significant sustainability performance improvement.

4. Published paper

The PI and his students, Abdurrafay Siddiqui (PhD student in the PI's group) and Rebecca Potoff (PhD student now at SUNY Stony Brook) has published a paper, titled "Sustainability metrics and technical solution derivation for performance improvement of electroplating facilities," in Clean Technologies and Environmental Policy. It is accessible online (https://link.springer.com/article/10.1007/s10098-023-02696-9). The paper contains a complete set of sustainability metrics developed for the metal finishing industry, and its application for sustainability performance improvement. In the acknowledgement section, AESF's financial support through Project No. R-121 is acknowledged, together with that of the National Science Foundation.

5. Past project reports

1. Quarter 1 (April-June 2020): Summary: *NASF Report* in *Products Finishing*; *NASF Surface Technology White Papers*, **84** (12), 14 (September 2020); Full paper: http://short.pfonline.com/NASF20Sep1
2. Quarter 2 (July-September 2020): Summary: *NASF Report* in *Products Finishing*; *NASF Surface Technology White Papers*, **85** (3), 13 (December 2020); Full paper: http://short.pfonline.com/NASF20Dec1
3. Quarter 3 (October-December 2020): Summary: *NASF Report* in *Products Finishing*; *NASF Surface Technology White Papers*, **85** (7), 9 (April 2021); Full paper: http://short.pfonline.com/NASF21Apr1.
4. Quarter 4 (January-March 2021): Summary: *NASF Report* in *Products Finishing*; *NASF Surface Technology White Papers*, **85** (11), 13 (August 2021); Full paper: http://short.pfonline.com/NASF21Aug1
5. Quarter 5 (April-June 2021): Summary: *NASF Report* in *Products Finishing*; *NASF Surface Technology White Papers*, **86** (1), 19 (October 2021); Full paper: http://short.pfonline.com/NASF21Oct2
6. Quarter 6 (July-September 2021): Summary: *NASF Report* in *Products Finishing*; *NASF Surface Technology White Papers*, **86** (4), 19 (January 2022); Full paper: http://short.pfonline.com/NASF22Jan3
7. Quarter 7 (October-December 2021): Summary: *NASF Report* in *Products Finishing*; *NASF Surface Technology White Papers*, **86** (7), 17 (April 2022); Full paper: http://short.pfonline.com/NASF22Apr2
8. Quarter 8 (January-March 2022): Summary: *NASF Report* in *Products Finishing*; *NASF Surface Technology White Papers*, **86** (10), 17 (July 2022); Full paper: http://short.pfonline.com/NASF22Jul2
9. Quarter 9 (April-June 2022): Summary: *NASF Report* in *Products Finishing*; *NASF Surface Technology White Papers*, **87** (1), 17 (October 2022); Full paper: http://short.pfonline.com/NASF22Oct1

10. Quarter 10 (July-September 2022): Summary: *NASF Report* in *Products Finishing*; *NASF Surface Technology White Papers*, **87** (4), 17 (January 2023); Full paper: http://short.pfonline.com/NASF23Jan2
11. Quarter 11 (October-December 2022): Summary: *NASF Report* in *Products Finishing*; *NASF Surface Technology White Papers*, **87** (6), 19 (March 2023); Full paper: http://short.pfonline.com/NASF23Mar1
12. Quarter 12 (January-March 2023): Summary: *NASF Report* in *Products Finishing*; *NASF Surface Technology White Papers*, **87** (10), 20 (July 2023); Full paper: http://short.pfonline.com/NASF23Jul1
13. Quarter 13 (April-June 2023): Summary: *NASF Report* in *Products Finishing*; *NASF Surface Technology White Papers*, **88** (2), 19 (November 2023); Full paper: http://short.pfonline.com/NASF23Nov2
14. Quarter 14 (July-September 2023): Summary: *NASF Report* in *Products Finishing*; *NASF Surface Technology White Papers*, **88** (4), 17 (November 2023); Full paper: http://short.pfonline.com/NASF24Jan2

6. About the principal investigator (P.I.)

Dr. Yinlun Huang is a Professor at Wayne State University (Detroit, Michigan) in the Department of Chemical Engineering and Materials Science. He is Director of the Laboratory for Multiscale Complex Systems Science and Engineering, the Chemical Engineering and Materials Science Graduate Programs and the Sustainable Engineering Graduate Certificate Program, in the College of Engineering. He has ably mentored many students, both Graduate and Undergraduate, during his work at Wayne State.

He holds a Bachelor of Science degree (1982) from Zhejiang University (Hangzhou, Zhejiang Province, China), and M.S. (1988) and Ph.D. (1992) degrees from Kansas State University (Manhattan, Kansas). He then joined the University of Texas at Austin as a postdoctoral research fellow (1992). In 1993, he joined Wayne State University as Assistant Professor, eventually becoming Full Professor from 2002 to the present. He has authored or co-authored over 220 publications since 1988, a number of which have been the recipient of awards over the years.

His research interests include multiscale complex systems; sustainability science; integrated material, product and process design and manufacturing; computational multifunctional nano-material development and manufacturing; and multiscale information processing and computational methods.

He has served in many editorial capacities on various journals, as Co-Editor of the ASTM *Journal of Smart and Sustainable Manufacturing Systems*, Associate Editor of *Frontiers in Chemical Engineering*, Guest Editor or member of the Editorial Board, including the ACS *Sustainable Chemistry and Engineering*, *Chinese Journal of Chemical Engineering*, the *Journal of Clean Technologies and Environmental Policy*, the *Journal of Nano Energy and Power Research*. In particular, he was a member of the Editorial Board of the AESF-published *Journal of Applied Surface Finishing* during the years of its publication (2006-2008).

He has served the AESF and NASF in many capacities, including the AESF Board of Directors during the transition period from the AESF to the NASF. He served as Board of Directors liaison to the AESF Research Board and was a member of the AESF Research and Publications Boards, as well as the Pollution Prevention Committee. With the NASF, he served as a member of the Board of Trustees of the AESF Foundation. He has also been active in the American Chemical Society (ACS) and the American Institute of Chemical Engineers (AIChE).

He was the 2013 Recipient of the NASF William Blum Scientific Achievement Award and delivered the William Blum Memorial Lecture at SUR/FIN 2014 in Cleveland, Ohio. He was elected AIChE Fellow in 2014 and NASF Fellow in 2017. He was a Fulbright Scholar in 2008 and has been a Visiting Professor at many institutions, including the Technical University of Berlin and Tsinghua University in China. His many other awards include the AIChE Research Excellence in Sustainable Engineering Award (2010), AIChE Sustainable Engineering Education Award (2016), the Michigan Green Chemistry Governor's Award (2009) and several awards for teaching and graduate mentoring from Wayne State University, and Wayne State University's Charles H. Gershenson Distinguished Faculty Fellow Award.