2020 AESF Research Project (No. R-121)

15TH QUARTERLY PROGRESS REPORT
Reporting Period: 10/01/2023 – 12/31/2023

Submitted by: Yinlun Huang, Professor, Department of Chemical Engineering and Materials Science, Wayne State University, Detroit, MI 48202
Phone: 313-577-3771; Email: yhuang@wayne.edu

Students: Mahboubeh Moghadasi (PhD student of chemical engineering at Wayne State University)

Submitted to: Timothy D. Hall, Chairman, Research Board, AESF Foundation; Lab Manager, Faraday Technology, Inc., 315 Huls Drive, Englewood, OH 45315
Phone: 937-836-7749. Email: timhall@faradaytechnology.com

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

Principal Investigator: Yinlun Huang

Project Period: 04/01/2020 – 03/31/2024

A. 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.

B. SUMMARY OF PROJECT ACTIVITIES

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

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.

(1) Fundamental model for characterizing the removal of the dirt/chemical residues on parts surface:

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

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

where W_{p_r} is the amount of dirt on parts when the barrel is in a rinse tank (g/cm^2); r_{p_r} is the dirt removal rate in the rinsie tank (g/min); k_r is the mass transfer coefficient (gal-chem·gal-water/gal-soln·cm^2); $\gamma_c(t_e^c)$ 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); x_r is the pollutant composition in rinse water (g/gal-water).

(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.

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

where V_r is the rinse tank capacity (gal-water); F_r is the rinse water flow rate (gal-water/min); 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.

Architecture of Physics-Informed Neural Networks (PINN)

In the last report, 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.

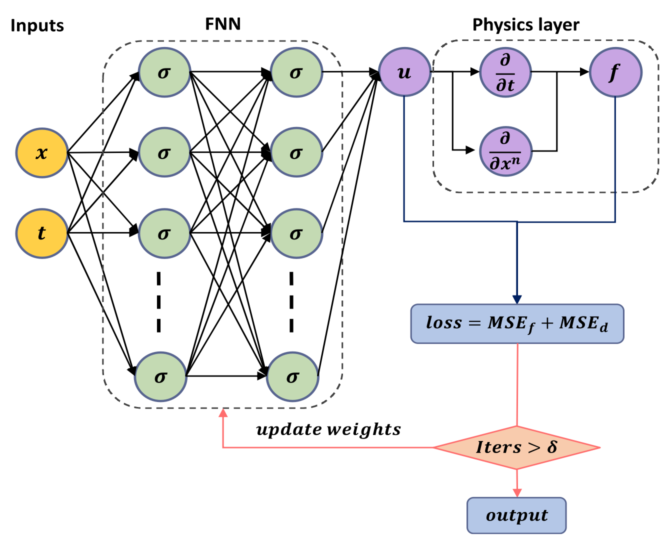

Fig. 1. PINN as the last layer of a feedforward neural network (FNN).

Rinse Operation Simulation

We have conducted an extensive PINN-based simulation. Table 1 shows the parameters used in the model as well as 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.

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 first scenario for amount of dirt on parts (W_{Pr}) and pollutant concentration (x_r) in the rinsing tank (RT) are shown in Fig's. 2 and 3, respectively.

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 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 Fig's. 4 and 5, respectively.

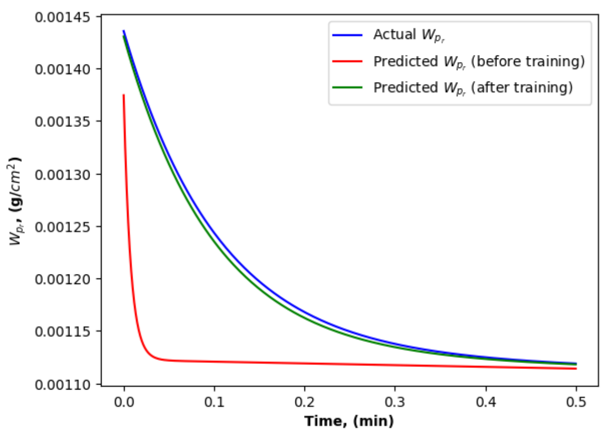

Fig. 1. Dirt/chemical removal dynamics on part (W_{P_r}) in the rinse tank.

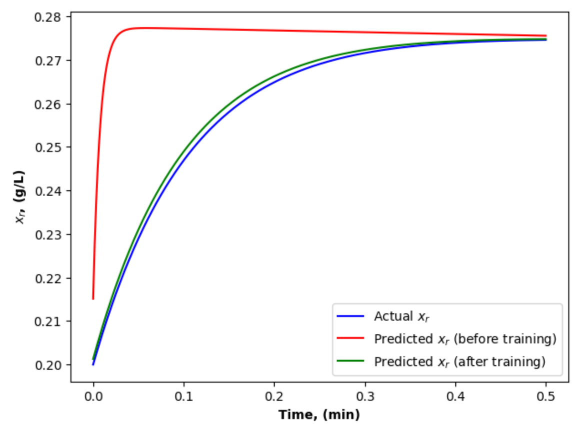

Fig. 3. Dynamic change of pollutant concentration change (x_r) in the rinsing tank.

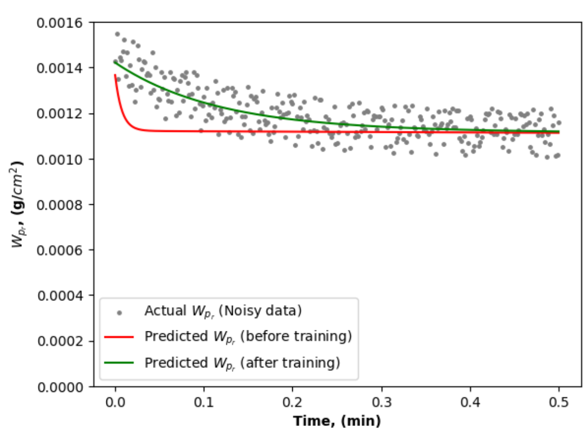

Fig.4. Dirt/chemical removal dynamics on part (W_{P_r}) using noisy data.

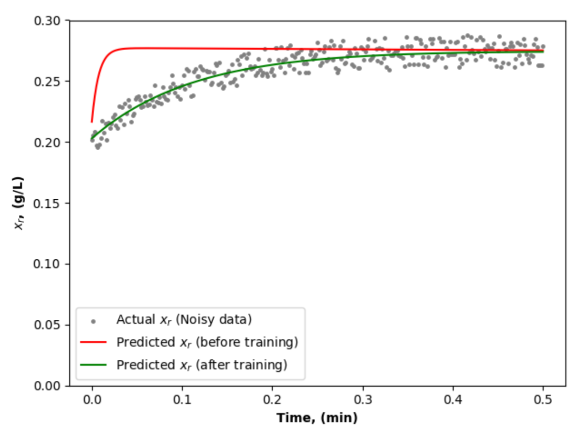

Fig. 5. Dynamic change of pollutant concentration (x_r) using noisy data.

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

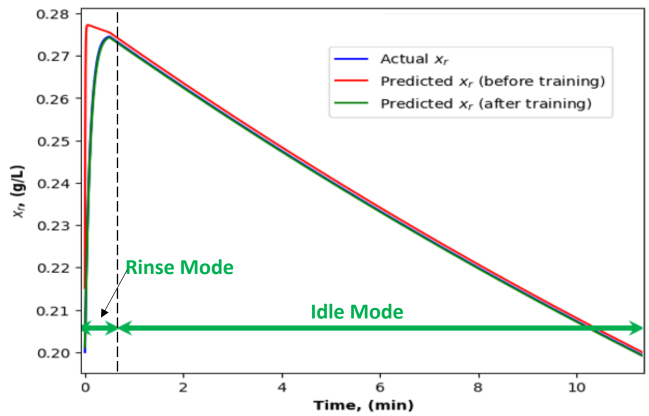

Fig. 6. Pollutant Concentration change (x_r) in the rinse tank.

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 setting 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/cm^2)	0.0035	$x_r(t=t_0^r)$ (g/L-water)	0.07	$x_r(t=t_0^r)$ (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 (cm^2·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·cm^2)	0.0008	k_r (gal-chem·gal-water/gal-soln·cm^2)	0.0008
η (g-dirt/gal-chem)	3,031.6	θ (cm^2/gal-water)	936.36	θ (cm^2/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.

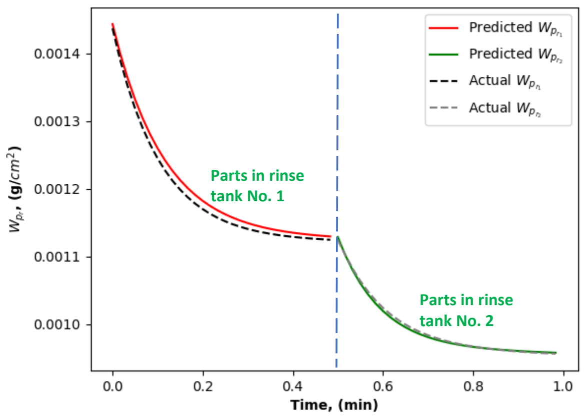

Fig. 7. Dirt removal from parts surface in the two-step rinsing system.

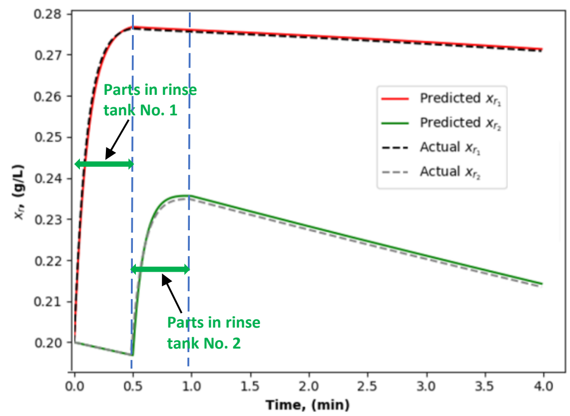

Fig. 8. Pollutant concentration change in two rinse tanks.

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 be used to simulate an entire electroplating plant eventually.

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.

Attachment

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 online accessible (https://link.springer.com/article/10.1007/s10098-023-02696-9). The hard copy of the paper is attached to this report. 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 the National Science Foundation.