

Article

A Hybrid Physics-Informed Neural Network (PINN) for the Electro-Oxidation of 2-Chlorophenol on BDD Electrodes in a Flow-By Reactor Under Batch Recirculation

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Abstract

The electro-oxidation of persistent organic pollutants such as 2-chlorophenol (2-CPh) using boron-doped diamond (BDD) electrodes offers a promising wastewater treatment route, yet conventional mechanistic models (e.g., CFD) suffer from prohibitive computational costs. This study develops a hybrid physics-informed neural network (PINN) to model the electro-oxidation of 2-CPh in a flow-by reactor coupled with a continuous stirred tank under batch recirculation mode. The PINN integrates a diffusion–convection partial differential equation with a lumped-parameter ordinary differential equation for the tank, embedding physical constraints directly into the loss function. The model was trained on simulated data generated from a previously validated parametric model and optimized using a systematic hyperparameter grid search. The PINN achieved excellent agreement with experimental data, yielding a coefficient of determination (R^2) of 0.9927, a mean square error of 0.0009, and a root mean square error of 0.0294—outperforming both the CFD and parametric models in accuracy. Sensitivity analysis revealed that the apparent kinetic constant is the most influential parameter (normalized sensitivity of 14.20). While the CFD model required 42 days and the parametric model 8 s, the PINN achieved a balanced trade-off with a runtime of 7.36 h. We conclude that the PINN provides a highly accurate, computationally feasible surrogate model suitable for integration into digital twins and real-time control frameworks for electrochemical wastewater treatment.

Keywords: 2-chlorophenol; BDD electrodes; electro-oxidation; physics-informed neural network (PINN); flow-by reactor; batch recirculation mode



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1. Introduction

Electro-oxidation is a powerful tool for the destruction of persistent organic contaminants [1], such as chlorophenols (e.g., 2-chlorophenol). 2-chlorophenol (2-CPh) stands out among the 65 substances identified by the EPA as a significant threat to air and water due to its harmful effects [2]. The oxidation of 2-CPh has been successfully achieved in numerous literature works [1,3–7] employing diverse anodes (e.g., Nb/BDD, Ti/BDD, carbon fiber, poly-NiTSPc-modified glassy carbon electrodes, Pt/Ti, Ti/PbO₂, Ti/SnO₂, and CNTs/AG/ITO). Among these used electrodes, the BDD anode stands out in its performance in water due to the high generation of hydroxyl radicals ($\bullet\text{OH}$) on the anode surface, as indicated by Equation (1) [8].



Research efforts for the scale-up of electro-oxidation processes include the use of deterministic models based on partial differential equations (PDEs) and ordinary differential equations (ODEs) systems that accommodate hydrodynamics, mass transport, electrode kinetics, and current and potential distribution. While these equations typically represent two ideal flow conditions—plug flow and perfect mixing—real-world applications often involve some degree of dispersion that deviates from these ideal patterns, which can be analyzed using residence time distribution (RTD) analysis [9–11].

In our previous work [12], a CFD mathematical model of the electro-oxidation of 2-CPh in a flow-by reactor operating under batch recirculation mode was developed and solved using a coupled simulation approach. In this approach, COMSOL Multiphysics® 5.3 solved the continuity and Navier–Stokes equations in a laminar regime, along with the diffusion–convection equation with a reaction term, while MATLAB solved the continuous stirred-tank (CST) model via LiveLink™ for MATLAB. The main results indicated that this model provided an excellent fit to the experimental data, with a determination coefficient of 0.9917 and a root-mean-square error of 0.4041, but with an execution time of 42 days. This execution time is exceptionally long for a standard CFD-electrochemical coupling simulation, representing a major computational limitation that demands special attention.

To address this, Regalado et al. [13] developed a physics-based parametric model coupling axial dispersion with a CST and solved it using COMSOL Multiphysics® 5.3 to describe the electro-oxidation of 2-CPh in a flow-by reactor operating under batch recirculation mode. The solution was achieved by coupling an internal diluted mass transport module with the global ODE and DAE functions. The main results indicate that the model provides a very good fit to the experimental data, with a determination coefficient of 0.9831 and a root-mean-square error of 0.1754, and—crucially—an execution time of only 8 s. This model thus successfully overcame the computational bottleneck of the earlier CFD approach. However, while this physics-based model [13] is fast and accurate, it still relies on solving a system of coupled PDEs and ODEs. Although 8 s per simulation is perfectly acceptable for a single run, this structure becomes less practical when the model needs to be embedded within larger frameworks—for instance, in real-time control systems or digital twins that may require thousands of evaluations in rapid succession. Moreover, such models often require recalibration when operational conditions shift, which can limit their adaptability in dynamic environments.

To capture the complex relationships inherent in sequential data and temporal dynamics, the use of surrogate models has emerged as a contemporary approach to chemical reactor modeling, particularly for electrochemical processes [14]. These surrogate models—commonly termed black-box models—learn input–output relationships directly from data, thereby eliminating the need for explicit mechanistic descriptions [15]. Deep neural networks have increasingly been adopted as indispensable black-box predictive

tools for electro-oxidation modeling in recent years [16–20]. Within chemical reactor engineering, a prevalent methodology integrates first-principles mechanistic knowledge with data-driven learning algorithms, an approach formally designated as physics-informed neural networks (PINNs) [21]. In this paradigm, the deep neural network constitutes the sole predictive architecture. However, its training regime is constrained by governing physical laws through the incorporation of additional penalty terms within the loss function, as shown in Equation (2) [22],

$$L(\theta) = L_{data}(\theta) + \lambda L_{physics}(\theta) \quad (2)$$

Here, L_{data} quantifies the discrepancy between the neural network's predictions and the available data (whether experimental or simulated), while $L_{physics}$ penalizes deviations from the governing physical equations. θ denotes a vector that contains the parameters of the ML and physics components. The hyperparameter λ balances the relative contribution of the physics-based constraint during training.

Beyond PINNs, gray-box models represent an alternative hybrid architecture that can operate in either series or parallel configurations, offering a generalized framework for fusing physics-based and data-driven components in the realization of digital twins for chemical process systems [23]. However, unlike gray-box models, which explicitly embed mechanistic equations alongside neural network components, PINNs offer a more compact formulation by encoding physical laws directly into the loss function. This makes them particularly attractive for problems where the governing equations are well-understood but traditional solvers are cumbersome to integrate into larger workflows [22], such as electro-oxidation processes in a flow-by reactor [24–27].

In this work, we introduce a physics-informed neural network (PINN) that incorporates existing mechanistic understanding of the electro-oxidation process in conjunction with data-driven learning. More specifically, we combine a diffusion–convection equation (including a reaction term) with a continuous stirred-tank (CST) model. The coupling of first principles with simulated data—generated from the validated physics-based model [13]—provides the basis for designing a PINN to model the system dynamics accurately.

2. Mathematical and Physics-Informed Neural Network (PINN) Dynamic Modeling of 2-Chlorophenol Electro-Oxidation

2.1. Problem Statement and Governing Equations

The case study consists of the electro-oxidation of 2-chlorophenol (2-CPh), which is carried out in a batch recirculation system coupling a flow-by reactor (FBR) with a continuous stirred tank (CST), as shown in Figure 1. In this configuration, the CST serves as the main reservoir where the contaminated solution is continuously stirred to maintain homogeneity. A magnetic pump drives the recirculation of the solution from the CST through a flow meter, which precisely regulates the flow rate before the stream enters the FBR.

Within this reactor, conductive particles are fluidized by the upward liquid flow, creating a high-surface-area electrode where electro-oxidation of 2-CPh occurs under the influence of an external power supply. Although the term “flow-by” typically describes a reactor with a stationary electrode, here it refers to the hydraulic configuration—the electrolyte passes once through the reactor in each cycle—while the working electrode itself is a fluidized bed, which enhances mass transfer and provides a large active surface area.

Upon exiting the FBR, the treated solution is returned to the CST, completing the recirculation loop; this cycle continues throughout the batch run, ensuring progressive pollutant degradation while maintaining a constant liquid volume.

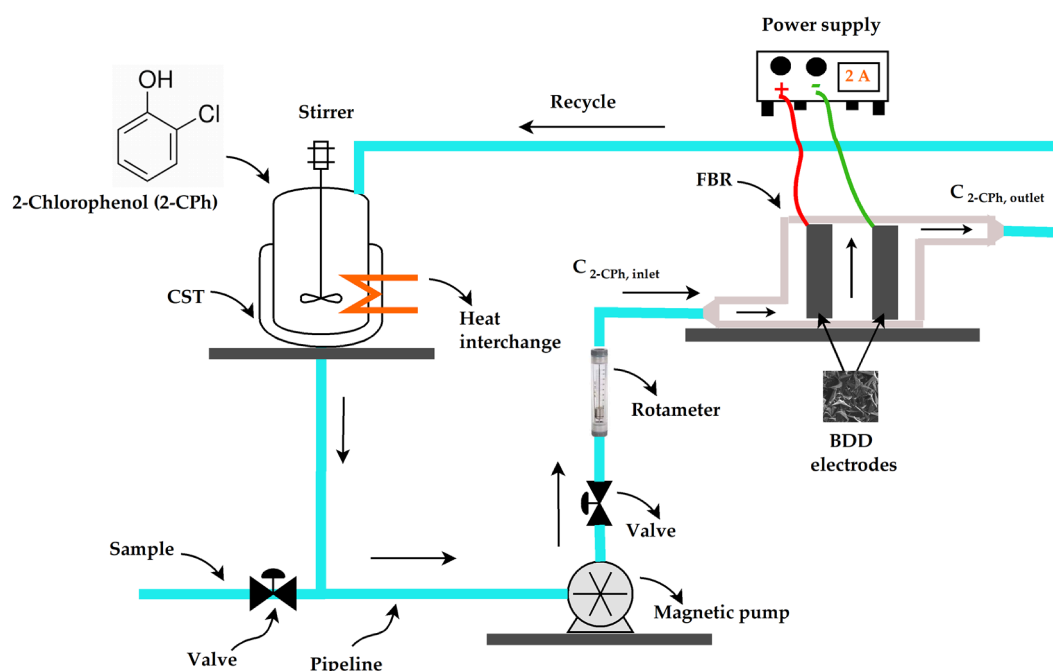


Figure 1. Batch recirculation electrochemical reaction system.

2.1.1. Mathematical Model for the Flow-By Reactor (FBR)

The mathematical model for the FBR is a typical convection–diffusion equation with a pseudo-first-order kinetic reaction (see Equation (3)) that takes place at the electrode surface, as previously reported [4,28]. The boundary conditions are of the Danckwerts type, in accordance with reference [13].

The inlet boundary condition specifies that the curvature (second spatial derivative) of the concentration profile at the inlet is constant and proportional to the feed concentration C_0 . In a FBR: (1) The inlet is the region where the fluid enters the system and initiates its flow along the reactive surface. (2) Instead of fixing the concentration itself ($C(x, t) = C_0$) or the total flux, this condition fixes the rate of change in the dispersive flux gradient at the boundary. (3) Physically, this means the dispersion mechanism at the inlet is balanced against the convective input of species at concentration C_0 . The curvature remains constant over time, meaning the shape of the concentration profile near the inlet is constrained by the feed conditions, regardless of how the interior of the reactor evolves. (4) This could represent a scenario where the inlet region is dominated by a fixed dispersive mixing pattern imposed by the flow distributor or the entrance geometry of the flow-by configuration.

The outlet boundary condition specifies that the concentration profile has zero curvature at the outlet and in a FBR:

(1) The outlet is where fluid exits the reactive zone. (2) Zero curvature means the concentration profile becomes linear at the exit. (3) Physically, this indicates that the dispersive flux is no longer changing with distance at the outlet. The system has reached a state where axial dispersion no longer introduces curvature, and any further change in concentration along x occurs at a constant gradient. (4) This is consistent with a “fully developed” concentration profile at the exit, where the influence of upstream dispersion has stabilized, and the species exits without further mixing-induced changes.

The initial condition specifies that the reactor initially contains the species uniformly at concentration C_0 throughout its entire length and in an FBR:

(1) this represents a pre-filled condition where the fluid phase is initially saturated with the species at the same concentration as the feed; (2) physically, this could correspond to a start-up scenario where the reactor is filled with feed solution before flow begins, or

a situation where recirculation establishes a uniform initial state; and (3) this condition simplifies the transient analysis by providing a spatially uniform initial field from which the concentration evolves under convection, dispersion, and reaction.

Moreover, for the initial condition, we assume that $0 < x < \ell$. This indicates the reactor is initially filled with concentration C_0 . If the inlet concentration is also C_0 , then without reaction, the system would already be at a steady state. With reaction ($k_{app} > 0$), the steady state will have a concentration profile that decreases along the reactor; thus, starting from a uniform C_0 is physically acceptable—though it is not a steady state if $k_{app} > 0$.

$$\begin{aligned} \frac{\partial C_{FBR}(x,t)}{\partial t} &= D_{ax} \frac{\partial^2 C_{FBR}(x,t)}{\partial x^2} - u \frac{\partial C_{FBR}(x,t)}{\partial x} - k_{app} C_{FBR}(x,t) \\ \text{At } x=0 \quad D_{ax} \frac{\partial^2 C_{FBR}(x=0,t)}{\partial x^2} &= u \bullet (C_{FBR}(x=0,t) - C_{CST}(t)) \quad \forall t > 0 \\ \text{At } x=\ell \quad -D_{ax} \frac{\partial^2 C_{FBR}(x=\ell,t)}{\partial x^2} &= 0 \quad \forall t > 0 \\ \text{At } t=0 \quad C_{FBR}(x, t=0) &= C_0 \quad \forall 0 < x < \ell \end{aligned} \quad (3)$$

where C_{FBR} is the concentration of 2-CPh in the FBR; C_0 is the initial concentration of 2-CPh, 1 mol/m^3 ; t is the reaction time, 4 h; ℓ is the reactor length, 0.2 m; u is the linear velocity, 0.0947 m/s [29]; D_{ax} is the axial dispersion coefficient, $0.0005 \text{ m}^2/\text{s}$ [29]; and k_{app} is the kinetic apparent constant, $1.2241/\text{h}$ [12].

2.1.2. Mathematical Model for the Continuous Stirred Tank (CST)

The mathematical model for the CST (see Equation (4)) is a lumped-parameter model for a well-mixed tank or compartment ($C_{CST}(t)$) that receives inflow from a separate system (e.g., Flow-by reactor). We assume that the tank outlet concentration equals the tank's uniform concentration (well-mixed assumption). Since only one concentration difference term appears, the model assumes the tank has one inflow (from the upstream unit $C_{FBR}(x = \ell, t)$) and one outflow ($C_{CST}(t)$), and both flows have the same volumetric flow rate Q .

The initial condition in the CST means the tank initially contains a uniform concentration C_0 , likely from a previous steady state or initial filling.

$$\begin{aligned} \frac{dC_{CST}(t)}{dt} &= \frac{Q}{V_T} (C_{FBR}(x = \ell, t) - C_{CST}(t)) \\ \text{At } t=0 \quad C_{CST}(0) &= C_0 \end{aligned} \quad (4)$$

where C_{CST} is the concentration of 2-CPh in the CST; Q is the volumetric flow rate, 1 L/min [29]; and V_T is the treated volume, 2.5 L .

2.2. Hybrid PINN-Based Dynamic Process Modeling

Before presenting the PINN formulation, it is important to note that conventional, non-physics-informed neural networks often underperform in highly dynamic industrial chemical applications for three main reasons. First, they require large volumes of training data that comprehensively cover all operating conditions; in practical industrial settings, such data are often unavailable, costly to obtain, or unsafe to generate. Second, these models lack inherent knowledge of physical laws like mass conservation. Consequently, they may produce physically implausible predictions—such as negative concentrations, especially when extrapolating beyond the training domain. Third, they do not generalize well under process drift, including gradual changes like catalyst deactivation or fouling, which means they require frequent retraining to maintain accuracy.

The proposed PINN overcomes these limitations by embedding the convection–diffusion–reaction equation directly into the loss function, following the methodology of Raissi et al. [30]. This integration enforces physical consistency and ensures that predictions remain physically plausible, even in scenarios with limited experimental data.

The PINN approximates the solution using neural networks, as follows:

$$\begin{aligned}\hat{C}_{FBR}(x, t; \theta) &\approx C_{FBR}(x, t) \\ \hat{C}_{CST}(t; \phi) &\approx C_{CST}(t)\end{aligned}\quad (5)$$

The total loss function combines physics constraints and experimental data, as is shown in Equation (6). The PDE residual loss is estimated by Equation (7), and the ODE residual loss is estimated by Equation (8).

$$L = \lambda_{PDE} L_{PDE} + \lambda_{ODE} L_{ODE} + \lambda_{BC} L_{BC} + \lambda_{IC} L_{IC} + \lambda_{Data} L_{Data} \quad (6)$$

$$L_{PDE} = \frac{1}{N_{colloc}} \sum_{j=1}^{N_{colloc}} \left[\frac{\partial \hat{C}_{FBR}}{\partial t} - D_{ax} \frac{\partial^2 \hat{C}_{FBR}}{\partial x^2} + u \frac{\partial \hat{C}_{FBR}}{\partial x} + k_{app} \hat{C}_{FBR} \right]_{(x_i, t_i)}^2 \quad (7)$$

$$L_{ODE} = \frac{1}{N_{colloc}} \sum_{i=1}^{N_{colloc}} \left[\frac{d \hat{C}_{CST}}{dt} - \frac{Q}{V_T} (\hat{C}_{FBR}(x = \ell, t_i) - \hat{C}_{CST}(t_i)) \right]^2 \quad (8)$$

The loss functions for the boundary conditions (L_{BC}), initial condition (L_{IC}), and experimental data (L_{Data}) are represented by Equations (9)–(11), respectively.

$$L_{BC} = \frac{1}{N_{BC}} \sum_{i=1}^{N_{BC}} \left[D_{ax} \frac{\partial \hat{C}_{FBR}}{\partial x} - u (C_{FBR} - C_{CST}(t)) \right]_{(x=0, t_i)}^2 + \frac{1}{N_{BC}} \sum_{i=1}^{N_{BC}} \left[D_{ax} \frac{\partial \hat{C}_{FBR}}{\partial x} \right]_{(x=\ell, t_i)}^2 \quad (9)$$

$$L_{IC} = \frac{1}{N_{IC}} \sum_{i=1}^{N_{IC}} [\hat{C}_{FBR}(x_i, t=0) - C_0]^2 + \frac{1}{N_{IC}} \sum_{i=1}^{N_{IC}} [\hat{C}_{CST}(t=0) - C_0]^2 \quad (10)$$

$$L_{Data} = \frac{1}{N_{Data}} \sum_{i=1}^{N_{Data}} [\hat{C}_{FBR}(x_i, t_i) - C_{exp}(x_i, t_i)]^2 + \frac{1}{N_{Data}} \sum_{i=1}^{N_{Data}} [\hat{C}_{CST}(x_i, t_i) - C_{exp}(x_i, t_i)]^2 \quad (11)$$

The required derivatives are computed using automatic differentiation, as described by Equation (12).

$$\frac{\partial \hat{C}_{FBR}}{\partial t} = \frac{\partial N_{FBR}(x, t; \theta)}{\partial t}, \quad \frac{\partial \hat{C}_{FBR}}{\partial x} = \frac{\partial N_{FBR}(x, t; \theta)}{\partial x}, \quad \frac{\partial^2 \hat{C}_{FBR}}{\partial x^2} = \frac{\partial^2 N_{FBR}(x, t; \theta)}{\partial x^2}, \quad \frac{d \hat{C}_{CST}}{dt} = \frac{\partial N_{CST}(t; \phi)}{\partial t} \quad (12)$$

where N_{FBR} and N_{CST} denote the neural network functions for the FBR and CST, respectively.

Finally, the PINN formulation seeks to minimize the total loss, according to Equation (13).

$$\theta^*, \phi^* = \underset{\theta, \phi}{\operatorname{argmin}} [L(\theta, \phi)] \quad (13)$$

where θ and ϕ represent the trainable parameters (weights and biases) of the neural networks approximating C_{FBR} and C_{CST} , respectively.

The hyperparameters λ_{PDE} , λ_{ODE} , λ_{BC} , λ_{IC} , and λ_{Data} balance the contribution of each physical constraint and the experimental data to the total loss. Typical values can be chosen such that all loss components are of similar magnitude during training.

Finally, Figure 2 illustrates the overall PINN training workflow, showing the interaction between the neural network (NN) architecture, the physics-informed loss formulation, and the optimization process. The PINN was implemented using the *Deep Learning Toolbox* in MATLAB R2025b. Also, Table 1 displays the pseudocode for the PINN algorithm implemented with the same Toolbox from MATLAB R2025.

2.3. Accurate Performance Modeling

Neural networks (NN) come with a bunch of hyperparameters that shape both the network architecture and the learning process. The hyperparameters in the PINN structure include the activation function, the number of hidden layers, and the number of neurons in each layer. Another very important training hyperparameter is the learning rate, which controls the magnitude of the adjustment steps during training and the number of training iterations.

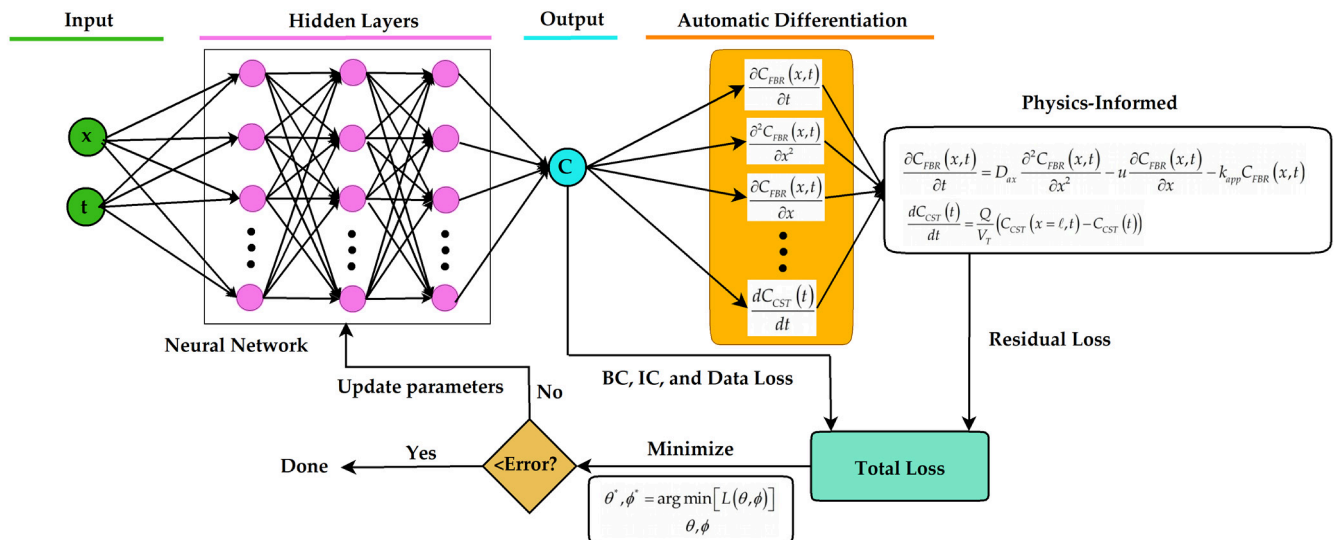


Figure 2. Physics-informed neural network (PINN) architecture and training workflow.

Table 1. Pseudocode PINN algorithm with Deep Learning Toolbox.

Step	Description
1:	Initiation and parameters $C_0 \leftarrow$, $u \leftarrow$, $Q \leftarrow$, $L \leftarrow$ $k_{app} \leftarrow$, $D_{ax} \leftarrow$ $V_T \leftarrow$, $t_Total \leftarrow$, Experimental data (t , C_{2-CPh})
2:	Neural Network architecture FBR Network: Predicts $C_{FBR}(x, t)$: Input: 2 (x, t), Hidden layers: # layers with # neurons each, Tanh activation function, and Output: 1 (C_{FBR}) Create network net for FBR CST Network: Predicts $C_{CST}(t)$: Input: 1 (t), Hidden layers: # layers with # neurons each, Tanh activation function, Output: 1 (C_{CST}) Create network net_CST with structure Initialize networks with random seed 42
3:	Training points generation: $N_x \leftarrow$ #, $N_t \leftarrow$ #, $x \leftarrow$ linspace (0, L, N_x), $t \leftarrow$ linspace (0, t_total , N_t), Collocation points $[X, T] \leftarrow$ meshgrid (x, t), $x_colloc \leftarrow$ flatten(X), $t_colloc \leftarrow$ flatten (T) FBR initial condition points ($t = 0$, all x), CST initial condition points, Boundary condition points, CST training points, and Convert all points to darray format for deep learning
4:	Loss weights: $\lambda_{pde} \leftarrow$, $\lambda_{bc} \leftarrow$, $\lambda_{ic} \leftarrow$, $\lambda_{cst} \leftarrow$, $\lambda_{cst0} \leftarrow$, $\lambda_{exp} \leftarrow$
5:	Training Loop numEpochs $\leftarrow$ #, learnRate $\leftarrow$ Initialize Adam optimizer states for both networks Initialize loss_history array For epoch = 1 to numEpochs Call [$loss_total$, gradients_FBR, gradients_CST, monitoring_vals] $\leftarrow$ Update networks using Adam optimizer loss_history [epoch, 1] $\leftarrow$ loss_total loss_history [epoch, 2:9] $\leftarrow$ monitoring_vals Display progress every 1000 epochs End
6:	Data saving: Generate high-resolution time vector $t_save \leftarrow$ linspace (0, t_total , 1000), $t_save \leftarrow$ C_CST_save , $C_FBR_out_save$ For $i = 0$ to length (t_save) Predict C_{CST} at t_save [i] Predict C_{FBR} at $x = L$ and t_save [i] Store results Update progress bar every 100 points End Save data to CSV file

Table 1. Cont.

Step	Description
7:	Visualization: Create Plot Concentration vs time Create Plot FBR spatial profiles Create Plot loss_total vs epoch
8:	Loss function subroutine (net_FBR, net_CST, x_colloc, t_colloc, x_ic, t_ic, x0, t0, xL, tL, t_cst, t0_cst, t_exp, C_exp, u, D, k, C0, Q, V_cst, L, lambda_pde, lambda_bc, lambda_ic, lambda_cstr, lambda_cstr0, lambda_exp) Forward predictions Compute derivatives using automatic differentiation Compute residuals Compute individual losses (mean squared error) Total weighted loss Compute gradients for both networks Monitoring values

Because many hyperparameters significantly impact the performance of a physics-informed neural network (PINN), a systematic approach is necessary to identify the optimal hyperparameter set. First, the hyperparameter space was discretized into a grid, all possible combinations were systematically evaluated, and model performance was assessed using metrics such as the agreement between experimental and predicted concentrations. Second, the accuracy of the PINN model was assessed using the index coefficient of determination (R^2), mean square error (MSE), and root mean square error (RMSE), as shown in Equations (14)–(16) [31]. High R^2 values (close to 1), along with low mean square error (MSE) and root mean square error (RMSE), indicate that the predictions align well with reality [23].

$$R^2 = \frac{\sum_{i=1}^n (C_{i, \text{exp}} - C_{i, \text{model}})^2}{\sum_{i=1}^n (C_{i, \text{exp}} - C_{\text{exp_average}})^2} \quad (14)$$

$$MSE = \frac{\sum_{i=1}^n (C_{i, \text{exp}} - C_{i, \text{model}})^2}{n} \quad (15)$$

$$RMSE = \sqrt{\frac{\sum_{i=1}^n (C_{i, \text{exp}} - C_{i, \text{model}})^2}{n}} \quad (16)$$

2.4. Sensibility Analysis

In this work, the One-at-a-Time (OAT) variation method was used to perform a sensitivity analysis of the PINN model for the electro-oxidation of 2-CPh. OAT provides a clear and easy-to-interpret view of how each individual parameter affects the FBR coupled CST behavior—specifically, the final concentration of 2-CPh. For this purpose, the key parameters varied in the sensitivity analysis include the kinetic apparent constant (k_{app}), axial dispersion coefficient (D_{ax}), linear velocity (u), and volumetric flow rate (Q). The normalized sensibility (S_i^{norm}) was determined using Equation (17) [32]. When $S_i^{norm} > 1$ means high sensitivity—the output is very responsive to that parameter. When $S_i^{norm} < 0.2$, sensitivity is low, so that parameter has a negligible influence [33]. This analysis enables the identification of the parameters that most significantly affect the PINN model performance and, consequently, those that must be accurately measured or carefully controlled.

$$S_i^{norm} = \frac{\Delta C_{2-\text{CPh}} / C_{2-\text{CPh, baseline}}}{\Delta x_i / x_{i, \text{baseline}}} \quad (17)$$

$i = k_{app}, D_{ax}, u, Q$

where ΔC_{2-CPh} is the absolute change in output 2-CPh concentration; $\Delta C_{2-CPh, baseline}$ is the baseline output value of 2-CPh concentration, 0.0026 mol/m^3 ; $\Delta x_{i, baseline}$ is the baseline value of the input parameter i ; and Δx_i is the absolute change in the input parameter i .

Table 2 shows the variations in the key factors used in the sensitivity analysis of the PINN model for the electro-oxidation of 2-CPh in an FBR on BDD electrodes under batch recirculation mode.

Table 2. Sensitivity analysis of the key factors of the PINN model for the electro-oxidation of 2-CPh.

Values	Factor	k_{app} (1/h)		D_{ax} (m ² /s)		u (m/s)		Q (L/min)	
1		0.979	(−20%)	1×10^{-4}	(−80%)	0.0500	(−47%)	0.50	(−50%)
2		1.224	Baseline	3×10^{-4}	(−40%)	0.0700	(−26%)	0.75	(−25%)
3		1.469	(+20%)	5×10^{-4}	Baseline	0.0947	Baseline	1.00	Baseline
4		1.714	(+40%)	7×10^{-4}	(+40%)	0.1200	(+27%)	1.25	(+25%)
5		1.958	(+60%)	1×10^{-3}	(100%)	0.1500	(+58%)	1.50	(+50%)

The percentages were picked for practical reasons. For the apparent kinetic constant (k_{app}), a variation range of 20–60% was selected, as this parameter typically exhibits significant uncertainty in practical systems, often in the order of $\pm 50\%$ [34]. The axial dispersion coefficient (D_{ax}) was varied between 80 and 100% since it can change a lot depending on how the fluid behaves [35]. For the linear velocity (u), typical flow velocities in industrial reactors fall right into the 47–58% range. Finally, the volumetric flow rate (Q) was set at $\pm 50\%$ [36], as it is easy to control but can still vary slightly during normal operation [37].

3. Simulation Results and Analysis

3.1. Results of the Hybrid PINN Modeling

To perform the PINN model, the *tanh* activation function and Adam optimizer were selected a priori in the optimization study. Table 3 summarizes the optimal hyperparameters of the PINN model. These include the neural network requirements, the number of layers, the number of neurons per layer, and the learning rate. Additional details on hyperparameter tuning and the search procedure are provided in Table S2 of the supporting information.

Regarding data partitioning, all six experimental data points (see Table S1) were used exclusively for training, as the inductive bias introduced by the governing PDEs within the PINN framework compensates for the limited availability of experimental data.

To mitigate potential optimization instabilities associated with the Danckwerts boundary conditions (i.e., fixed curvature at the boundary), three strategies were implemented: (i) a soft constraint formulation incorporated into the loss function rather than strict enforcement; (ii) balanced loss weighting ($\lambda_{BC} = 1 \times 10^4$, positioned between $\lambda_{PDE} = 1.0$ and $\lambda_{IC} = 1 \times 10^6$); and (iii) the use of tanh activation functions to ensure smooth and continuous derivatives. These strategies resulted in stable training with no observed numerical instabilities. Also, all loss weights (λ values) were held constant throughout training and were determined through systematic trial and error to bring each loss component to a comparable order of magnitude. The final set of weights is reported in Table 3. Although adaptive weighting approaches (e.g., Self-Adaptive PINNs or Soft Attention methods) [38,39] were not implemented in the present study, they represent a promising direction for future work.

Figure 3a successfully captures the dynamic startup behavior of the coupled PDE-ODE electrochemical system. The PINN seems to handle the sharp concentration gradients reasonably well. Because the color bar maxes out at 1.0 mol/m^3 , this suggests that once the system nears the steady state, the CST is feeding the FBR at roughly the feed concentration,

which makes physical sense given the parameters. Figure 3a also clearly shows that the FBR effectively reduces the 2-CPh concentration, both along the reactor length and over the hours of operation. For example, at $x = 0.2$ m and $t = 4$ h, the 2-CPh concentration drops to nearly zero (0.00268 mol/m^3).

Table 3. Optimized hyperparameter values for the PINN.

Parameters	PDE ($C_{2\text{-CPh, FBR}}$)	ODE ($C_{2\text{-CPh, CST}}$)
Inputs	2 (x, t)	1 (t)
Output	1 ($C_{2\text{-CPh, FBR}}$)	1 ($C_{2\text{-CPh, CST}}$)
Hidden Layer	4	4
Neurons per Layer	60	50
Activation function	$\tanh$	$\tanh$
Final Smooth Function	Linear	Linear
	Global hypermeters	
Initial Learning Rate	1×10^{-3}	
Learning Rate	5×10^{-5}	
Epochs Training	20,000	
Optimizer	Adam	
PDE collocation points	200,000	ODE collocation points
BCs collocation points	400	ICs collocation points
ICs collocation points	50,000	400
Loss weights		2000
λ_{PDE}	1	λ_{ODE}
$\lambda_{PDE, BC}$	1×10^4	$\lambda_{ODE, IC}$
$\lambda_{PDE, IC}$	1×10^6	λ_{Data}
		1×10^4
		1×10^7
		1×10^7

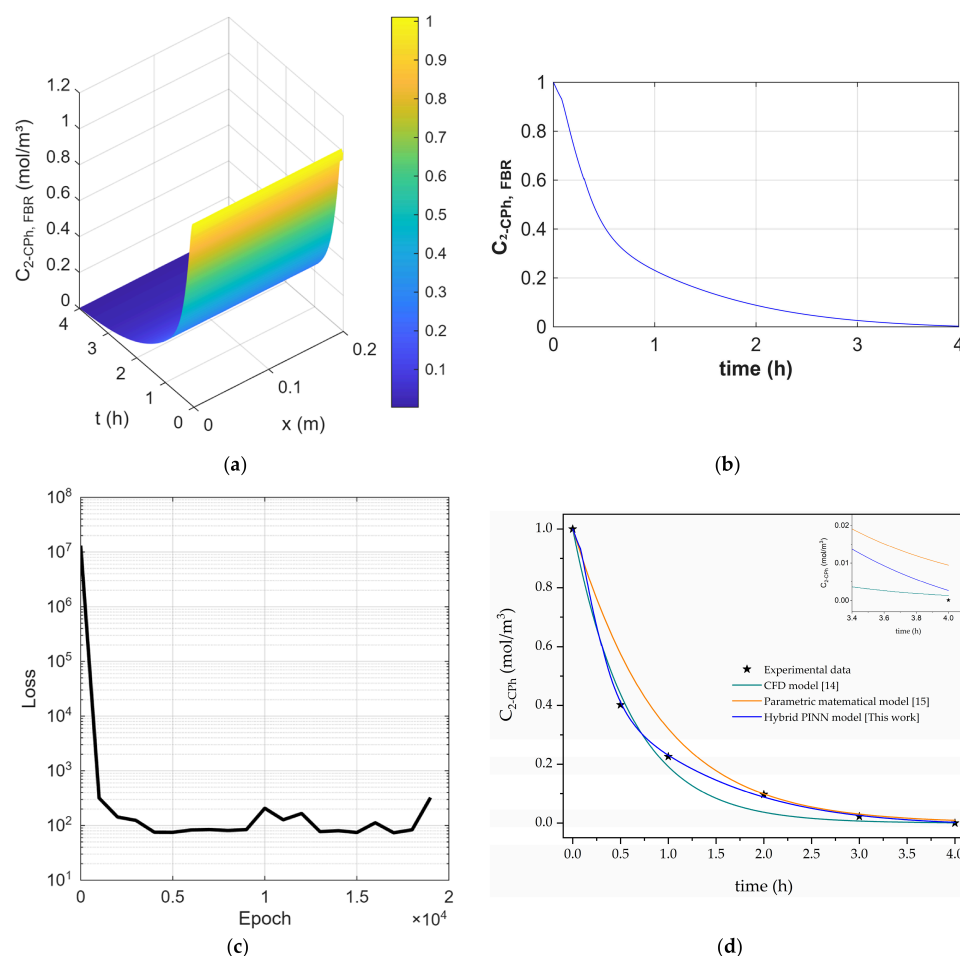


Figure 3. PINN simulation results of electro-oxidation of 2-CPh. (a) Space-time evolution of 2-CPh in the FBR; (b) time evolution of 2-CPh in the CST; (c) PINN model training loss vs. epoch training; (d) time evolution of 2-CPh concentration: hybrid PINN model vs. experimental data and literature models.

Figure 3b demonstrates successful 2-CPh concentration depletion in the coupled reactor system over the 4 h simulation window. The plot shows a smooth, convex exponential decay, implying that the PINN's prediction of 2-CPh concentration follows first-order kinetics with the given rate constant. Moreover, the smooth, noise-free PINN output indicates that the neural network has learned a stable solution without overfitting or oscillations—demonstrating good convergence behavior. The concentration is essentially fully depleted for 4 h, suggesting that the reaction time scale is well captured within the simulation domain.

Figure 3c illustrates the effect of training duration on the convergence behavior of PINN. The loss function decreases rapidly during the initial training phase. However, accurate inversion results are not obtained at 20,000 epochs, as the loss begins to increase beyond approximately 18,000 epochs. The training dynamics can be clearly divided into three stages: (1) rapid convergence over 0–1000 epochs, during which the network captures the dominant features of the solution space; (2) a quasi-stable plateau between 1000 and 18,000 epochs, characterized by minor oscillations and progressive refinement of the solution; and (3) a divergence between 18,000 and 20,000 epochs, where the loss increases again, indicating degradation in model performance. The loss attains its minimum within the range of approximately 10,000–18,000 epochs, beyond which additional training does not yield further improvements. Instead, overtraining leads to a deterioration in predictive accuracy, likely due to the imbalance among loss components or the accumulation of numerical errors during optimization. These results highlight the importance of appropriate early stopping criteria to ensure optimal model performance and stable convergence in PINN training.

Figure 3d compares three different modeling approaches for the electro-oxidation of 2-CPh. The blue line follows the black stars almost perfectly throughout the entire process. It corrects the underestimation seen in the CFD model [12] and the overestimation of the parametric model [13]. As a result, the PINN model matches the experimental data very well, showing high accuracy.

The zoomed-in section highlights the “tail” of the decay, where each simulation gives a slightly different concentration of 2-CPh. For example, at the end of the experiment, the values are 0.0001 mol/m^3 for the experimental data, 0.00130 mol/m^3 for the CFD model [12], 0.00943 mol/m^3 for the parametric model, and 0.00268 mol/m^3 for the PINN model.

Among the models evaluated, the CFD model [12] shows the closest agreement with experimental data at $t = 4 \text{ h}$ (0.00130 mol/m^3), albeit at a substantial computational cost of 42 days of computation. In contrast, the parametric model completes its computation in only 8 s, but its prediction (0.00943 mol/m^3) shows the largest deviation from the experimental value. The PINN model provides a balanced compromise between accuracy and efficiency: with a runtime of 7.36 h, it yields a concentration of 0.00268 mol/m^3 . It is worth noting that CFD is a first-principles model, whereas the PINN is a hybrid data-driven approach; therefore, a direct comparison is not strictly equivalent. Nevertheless, the PINN performs the same predictive task in 7.36 h compared to 42 days for CFD, underscoring the practical speed advantage of trained PINNs for rapid predictions.

Importantly, the reported 7.36 h for the PINN corresponds to a one-time offline training cost (implemented in MATLAB R2025b). Once trained, the PINN achieves an average inference time of 8.0 milliseconds per prediction (averaged over 1000 evaluations), making it highly suitable for real-time control frameworks and digital twin applications.

Overall, the physics-informed neural network (PINN) approach—likely combining the physical laws used in the CFD [12] and parametric [13] models with data-driven learning—offers a more robust and accurate prediction of the system's behavior than traditional modeling methods alone.

3.2. Accuracy Index Performance

Table 4 summarizes the R^2 , MSE, and RMSE values for the concentration of 2-CPh at $x = 0.2$ m and $t = 4$ h in an FBR under batch recirculation mode. The results indicate that the PINN model offers higher accuracy and robustness than the CFD [12] and parametric models [13], achieving a high R^2 score of 0.9927 and low MSE and RMSE values of 0.0009 and 0.0294, respectively.

Table 4. Performance metrics indexes (R^2 , MSE, and RMSE) of the PINN model for predicting the concentration of 2-CPh at $x = 0.2$ m and $t = 4$ h in a FBR under batch recirculation mode.

Model Type	Ref.	R^2	MSE	RMSE	Remark
PINN	[This work]	0.9927	0.0009	0.0294	Excellent model fit
CFD	[12]	0.9917	0.1633	0.4041	Very good model fit
Parametric	[13]	0.9831	0.0307	0.1754	Very good model fit

3.3. Sensitivity Analysis

To perform a sensitivity analysis for all four key factors (k_{app} , D_{ax} , u , Q), the program runs up to 8000 epochs. Table 5 summarizes the sensitivity analysis of the PINN model for predicting the concentration of 2-CPh at $x = 0.2$ m and $t = 4$ h in a FBR under batch recirculation mode.

Table 5. Sensitivity analysis summary.

Factor	Range	$C_{2-CPh, final\ variation}$ (%)	Max (S)
k_{app}	0.9790 to 1.958 1/h	−556.34	14.20
D_{ax}	1×10^{-4} to 1×10^{-3} m ² /s	−85.67	3.32
u	0.05 to 0.15 m/s	−290.13	6.20
Q	0.5 to 1.5 L/min	−32.92	6.55

The parameters' sensitivity (S^{norm}) ranking is ($k_{app} > u \approx Q > D_{ax}$). These values indicate the elasticity of each factor with respect to $C_{2-CPh, final\ variation}$. Specifically, $S^{norm} = 14.20$ means that a 1% change in k_{app} leads to a 14.20% change in $C_{2-CPh, final\ variation}$. $S^{norm} = 3.32$ means that a 1% change in D_{ax} leads to a 3.32% change in $C_{2-CPh, final\ variation}$. $S^{norm} = 6.20$ means that a 1% change in u leads to a 6.20% change in $C_{2-CPh, final\ variation}$. Finally, $S^{norm} = 6.55$ means that a 1% change in Q leads to a 6.55% change in $C_{2-CPh, final\ variation}$.

The sensitivity analysis reveals that the PINN model's prediction of 2-CPh concentration is most sensitive to the k_{app} , u and Q also exert substantial influence, and D_{ax} is comparatively less critical. Accurate estimation of k_{app} is paramount for reliable model predictions. This k_{app} depends on the current intensity (I) in electro-oxidation processes. Hence, it is correct that it is the most influential factor, which agrees with reference [20].

Beyond quantifying parameter influence, the sensitivity analysis also provides insight into the robustness and stability of the network under realistic operating conditions. In this context, a PINN can be considered stable if small, bounded perturbations in input parameters lead to correspondingly small, bounded variations in the output, without inducing oscillatory behavior or physically implausible predictions. The proposed PINN guarantees stability through three key mechanisms: (i) the use of $\tanh$ activation functions ensures Lipschitz continuity of the network mappings [40], promoting smooth input–output mappings; (ii) the inclusion of PDE residual loss enforces the governing physical laws, thereby penalizing solutions that deviate from physically consistent behavior; and (iii) the computed sensitivity coefficients provide quantitative bounds on the propagation of input

uncertainties to the model outputs. From a practical perspective, for a representative pumping system experiencing $\pm 10\%$ fluctuations in flow rate (common in industrial electro-oxidation processes), the corresponding variation in the predicted 2-CPh concentration is approximately $\pm 0.62\%$ (using $S_u^{norm} = 6.20$). Likewise, a $\pm 10\%$ variation in the dispersion coefficient yields a concentration change of approximately $\pm 0.33\%$ (using $S_{D_{ax}}^{norm} = 3.32$). The relatively small magnitude of these responses indicates that the model predictions remain bounded and well-conditioned under typical operating disturbances. Collectively, these results confirm the numerical stability and robustness of the PINN, supporting its suitability for deployment in practical wastewater treatment systems.

3.4. Results Analysis

Building on this, the study confirmed that PINN modeling offers a feasible solution to the addressed problem we set out to address. Figure 4 further illustrates key aspects of the simulated electro-oxidation of 2-CPh. It is worth noting that all three modeling approaches for electro-oxidation achieved a good fit for the data. However, PINN stood out as the best overall—delivering a high R^2 score, low MSE, and a solid RMSR value, all within a moderate computing time.

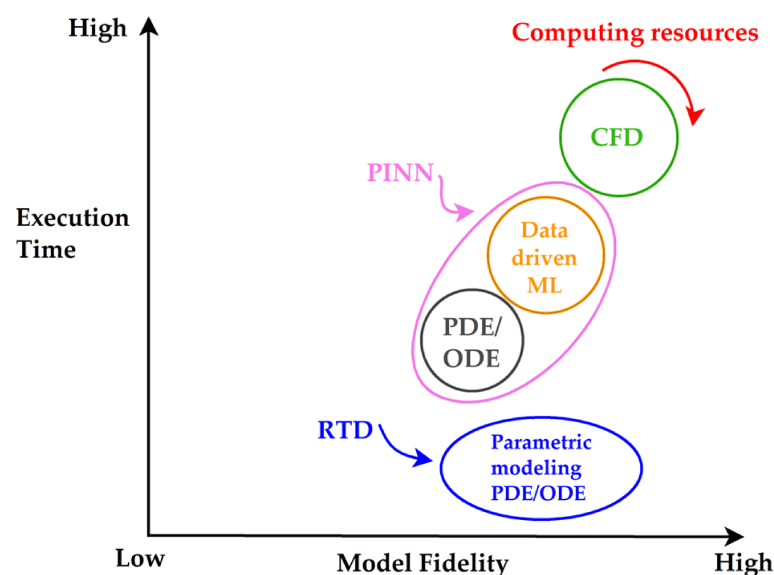


Figure 4. Various modeling techniques with their level of fidelity, execution time and computing resources.

Figure 5 presents a PINN-based sensitivity analysis for several parameters (e.g., k_{app} , D_{ax} , u , and Q). All subfigures show a 2-CPh concentration decay forming a single indistinguishable trajectory that closely matches experimental data, as expected from the model. Figure 5a indicates that as the apparent kinetic constant increases, the reaction accelerates—implying a more kinetically favorable environment over time. It also shows that mass transfer dominates the depletion of 2-CPh concentration. Figure 5b shows that a significant increase in axial dispersion leads to a flow regime that is less plug-flow-like and more mixed as the reaction progresses. Figure 5c illustrates that, in the flow-by (PDE) configuration coupled with a CST reaction, the residence time dominates; therefore, the flow velocity in the PDE section may have a minimal impact on the bulk concentration. Figure 5d shows that if CST mixing dominates and the residence time is long, variations in flow rate within this range do not significantly alter the concentration profile.

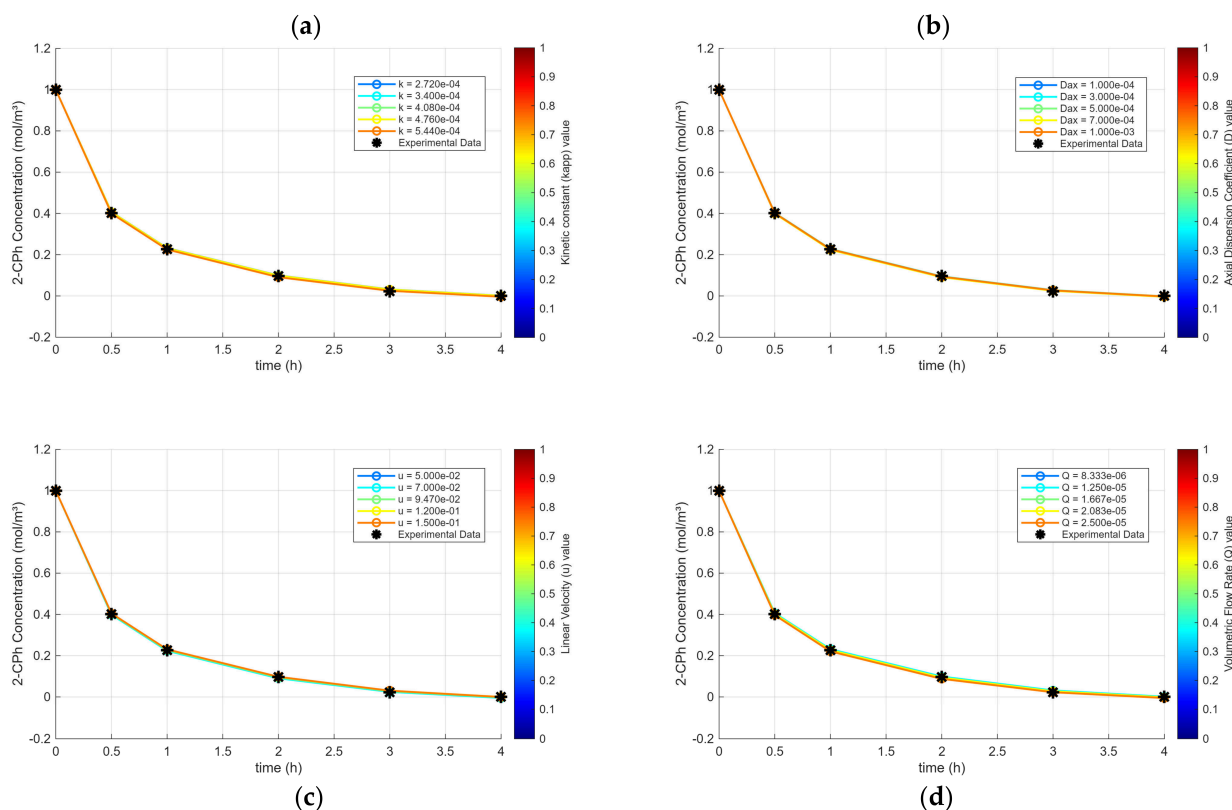


Figure 5. PINN sensitivity analysis. (a) Sensitivity to kinetic constant (k_{app}); (b) sensitivity to axial dispersion constant (D_{ax}); (c) sensitivity to linear velocity (u); (d) sensitivity to volumetric flow rate (Q).

4. Limitations and Future Works

Dynamic modeling of advanced oxidation process (AOP)-based wastewater treatment systems presents several challenges. These include process nonlinearity, complex reaction mechanisms, insufficient data from unstable reactive oxidant species (ROS), and difficulties in validation due to substantial data requirements. Furthermore, there is a need to enhance dynamic modeling strategies through the application of black-box or gray-box methods. Additional limitations pertain to process control, such as stringent effluent quality regulations, the necessity to reduce operating costs, potential shifts in environmental regulations, and a heightened risk of effluent quality fluctuations due to disturbances, particularly given the short process time delay.

Control-specific limitations include:

- Limited adjustability range of implemented control valves, pumps, and motors.
- The need for sensors with short response times to match the process's short time delay.
- The possibility of forming complex by-products due to excess reactants in the effluent.
- Sluggish response or overshoot after controller implementation.
- A high likelihood of human error in manual-based control.
- Challenges in optimal sensor placement.

Future work includes modeling the kinetic reaction of 2-chlorophenol using the Butler–Volmer equation or obtaining a pseudo-kinetic reaction in terms of the current intensity. It also includes modeling the electro-oxidation of 2-chlorophenol by a physics-informed neural network (PINN), incorporating the Butler–Volmer equation into the mass balance transport equation, as well as including the current distribution equation.

To properly assess generalization, the model should be tested against experimental data collected under different operating conditions or at different time points. Finally,

future work will explore the implementing linear and nonlinear, optimal, cascade, and/or plantwide control strategies to control the current intensity and/or volumetric flow rate.

5. Conclusions

Based on the findings of this study, the electro-oxidation of 2-chlorophenol on BDD electrodes in a flow-by reactor under batch recirculation was successfully modeled using a hybrid physics-informed neural network (PINN). The developed hybrid PINN exhibited high predicted accuracy, achieving an R^2 value of 0.9927 with low MSE and RMSE values of 0.0009 and 0.0294, respectively. These results underscore the potential of PINNs for modeling electrochemical wastewater treatment processes.

Sensitivity analysis further ranked the parameters influencing the PINN predictions of 2-Chlorophenol concentration, identifying the most critical factor whose precise estimation is essential for ensuring reliable predictions. Moreover, in comparison with computational fluid dynamics (CFD), the PINN reduced computational time from 42 days to 7.36 h—a 137-fold speedup—while maintaining excellent accuracy ($R^2 = 0.9927$).

It was also concluded that increasing the number of epochs does not inherently guarantee stable convergence; thus, incorporating early stopping criteria remains essential.

Supplementary Materials: The following supporting information can be downloaded at: <https://www.mdpi.com/article/10.3390/pr14121862/s1>, Table S1. Experimental data at best operating conditions. Table S2. Explored ranges for key hyperparameters.

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Abbreviations

AOP	Advanced oxidation process
BDD	Boron-doped diamond
COMSOL	Computational solutions
CFD	Computational fluid dynamics
CNTs	Carbon nanotubes
CST	Continuous stirred-tank
DAE	Differential-algebraic equation
FBR	Flow-by reactor
L	Loss function
MATLAB	Matrix laboratory

MSE	Mean square error
ODEs	Ordinary differential equations
PDEs	Partial differential equations
PINN	Physics-informed neural network
Pt	Platinum
RMSE	Root means square error
RTD	Residence time distribution
ROS	Reactive oxidant species
t	Time, h
Ti	Titanium
x	Flow direction in the FBR, m
Greek symbols	
λ	Balances the relative contribution of the physics-based constraint during training
θ	Weights of the neural networks approximating
ℓ	Reactor length, 0.2 m
ϕ	Biases of the neural networks approximating
Δ	Change
Nomenclature	
2-CPh	2-Chlorophenol
C	Concentration, 1 mol/m ³
$C_{2-CPh, baseline}$	Baseline output value of 2-CPh concentration, 0.0026 mol/m ³
D_{ax}	Axial dispersion coefficient, 0.0005 m ² /s
e^-	Electron
I	Current intensity, A
H^+	Hydrogen ion or proton
H_2O	Water
k	Kinetic constant, 1.224 1/h
NiTSPc	Nickel(II) tetrasulfonated phthalocyanine
N_{FBR}	Neural network functions for the FBR
N_{CST}	Neural network functions for the CST
$\bullet OH$	Hydroxyl radicals
PbO_2	Lead oxide
poly-NiTSPc	Polymerized film of NiTSPc
Q	Volumetric flow rate, 1 L/min
R^2	Coefficient of determination
S^{norm}	Normalize sensitivity
SnO_2	Tin oxide
u	Linear velocity, 0.0947 m/s
V_T	Treated volume, 2.5 L
ΔC_{2-CPh}	Absolute change in output 2-CPh concentration
$x_{i, baseline}$	Baseline value of the input parameter i
Δx_i	Absolute change in the input parameter i
Subscripts	
0	Initial
App	Apparent
BC	Boundary conditions
IC	Initial condition
i	Factor (k_{app} , D_{ax} , u , and Q)

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