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Charge-Transfer-Resistance-Informed Kinetic Simulation of Pollutant Degradation Using Functionalized Graphene Electrodes in an Electrochemical Batch Reactor: A Dynamic Modelling Framework for Electrode Screening in Water Treatment

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ABSTRACT

Electrochemical advanced oxidation processes (EAOPs) are increasingly recognised as effective technologies for the degradation of persistent organic pollutants in water, with electrode material selection critically determining treatment performance. Functionalised graphene electrodes including graphene oxide (GO), reduced graphene oxide (rGO), and nitrogen-doped graphene oxide (N-GO) offer tunable surface chemistry and charge-transfer properties relevant to electrochemical pollutant degradation. However, the relationship between electrode electrochemical impedance characteristics and pollutant removal kinetics has not been evaluated through dynamic systems modelling. In this study, a charge-transfer-resistance-informed pseudo-first-order kinetic model was implemented in OpenModelica to simulate pollutant concentration decay and removal efficiency in an electrochemical batch reactor over a 180-minute treatment period. Electrode charge-transfer resistance values were used to derive effective degradation rate constants through an Rct-scaling relationship, enabling direct linkage between electrochemical characterisation data and kinetic performance prediction. The model predicted pollutant concentration, cumulative removal efficiency, and kinetic rate constants for GO, N-GO, and rGO electrodes. Results demonstrated that rGO achieved the highest simulated removal efficiency of 94.39% at 180 minutes, with an effective rate constant of 0.0160 min^{-1} a 3.2-fold improvement over GO (0.0050 min^{-1}, 59.34% removal). N-GO exhibited intermediate performance (0.0089 min^{-1}, 79.81% removal). Sensitivity analysis confirmed that charge-transfer resistance is the dominant kinetic parameter governing electrode performance, with removal efficiency decreasing sharply as Rct increases from 10 to 120 Ω. A time-to-threshold analysis further demonstrated that rGO achieves 50% pollutant removal 3.2 times faster than GO and is the only electrode to achieve 90% removal within the 180-minute window. The framework provides a low-cost dynamic screening tool for electrode material selection in electrochemical water treatment system design.

Keywords: Electrochemical water treatment, Graphene oxide, Reduced graphene oxide, Nitrogen-doped graphene oxide, Pseudo-first-order kinetic, Charge transfer resistance, Open Modelica, Pollutant degradation, Dynamic simulation

INTRODUCTION

Access to clean water remains one of the most pressing global challenges, with over two billion people lacking access to safely managed drinking water and industrial effluents continuing to introduce persistent organic pollutants (POPs), pharmaceuticals, and emerging contaminants into water bodies at rates that exceed conventional treatment capacity (United Nations, 2023). Electrochemical advanced oxidation processes (EAOPs) have attracted increasing attention as a versatile and scalable technology for water treatment because they can generate highly reactive oxidising species in situ including hydroxyl radicals (•OH), ozone, and persulfate without requiring chemical addition, and can be powered by renewable energy sources (Martínez-Huitle et al., 2015).

The electrode material is the central determinant of EAOP performance. An effective electrode must combine high electrical conductivity, large active surface area, chemical stability, and favourable charge-transfer kinetics to sustain efficient radical generation and pollutant oxidation at the electrode surface (Brillas et al., 2009). Carbon-based electrode materials, and graphene derivatives in particular, have emerged as promising candidates for electrochemical water treatment owing to their exceptional surface area, tunable surface chemistry, and electrochemical properties (Duan et al., 2018). Graphene oxide (GO), produced by chemical oxidation of graphite, provides abundant oxygen-containing functional groups that can interact with pollutant molecules but suffers from reduced electrical conductivity due to disruption of the sp^2 carbon network (Dreyer et al., 2010). Reduction of GO to produce rGO partially restores the conductive graphitic lattice, lowering charge-transfer resistance and improving electrocatalytic performance (Pei & Cheng, 2012). Nitrogen doping of GO to produce N-GO introduces additional active sites and improves electron-transfer kinetics at the electrode–electrolyte interface, potentially offering a balance between surface functionality and conductivity (Wang et al., 2012).

Despite considerable experimental progress in evaluating graphene-based electrodes for water treatment, the systematic relationship between electrode electrochemical impedance

characteristics — specifically charge-transfer resistance (Rct) derived from electrochemical impedance spectroscopy (EIS) — and macroscopic pollutant removal kinetics has not been evaluated through dynamic simulation. This gap limits the ability to predict electrode performance from impedance characterisation data alone, increasing the cost and time required for electrode screening. Pseudo-first-order kinetic models are well-established frameworks for describing pollutant concentration decay in batch electrochemical reactors and are widely used in experimental water treatment studies (Panizza & Cerisola, 2009). Linking the pseudo-first-order rate constant directly to electrode Rct would create a physics-informed screening tool that translates impedance measurements directly into removal performance predictions. OpenModelica is a free, open-source, equation-based simulation environment built on the Modelica modelling language that is well suited for implementing dynamic kinetic models of chemical and electrochemical processes (Fritzson, 2014). Its accessibility and equation-based structure make it a practical platform for developing electrode screening tools that can be deployed without specialised commercial simulation software.

In this study, a charge-transfer-resistance-informed pseudo-first-order kinetic model was implemented in OpenModelica to simulate pollutant degradation in a batch electrochemical reactor using GO, N-GO, and rGO electrodes. The model derived effective rate constants from electrode Rct values and predicted pollutant concentration decay, cumulative removal efficiency, time-to-threshold performance, and sensitivity of removal to Rct across a practically relevant range. The study contributes a dynamic modelling framework for electrode material screening in electrochemical water treatment and demonstrates the quantitative link between impedance-derived electrode properties and pollutant removal kinetics.

MATERIALS AND METHODS

Electrochemical Reactor Model

The electrochemical reactor was modelled as a well-mixed batch system in which pollutant degradation follows pseudo-first-order kinetics with respect to pollutant concentration. The governing equation for pollutant concentration C (mg/L) as a function of time t (min) is:

$$dC/dt = -k_{eff} \times C$$

which yields the analytical solution:

$$C(t) = C_0 \times \exp(-k_{eff} \times t)$$

Cumulative removal efficiency η was computed as:

$$\eta(t) = [(C_0 - C(t)) / C_0] \times 100\%$$

Charge-Transfer-Resistance-Informed Rate Constant

The effective degradation rate constant k_eff was linked to electrode charge-transfer resistance through a scaling relationship derived from the inverse proportionality between Rct and charge-transfer kinetics established in electrochemical theory (Bard & Faulkner, 2001):

$$k_{eff} = k_0 \times (Rct_{ref} / Rct)$$

where $k_0 = 0.005$ min^{-1} is the base rate constant for the GO reference electrode, Rct_ref = 80 Ω is the reference charge-transfer resistance for GO, and Rct is the electrode-specific charge-transfer resistance. This formulation ensures that electrodes with lower Rct — corresponding to faster interfacial charge transfer produce higher effective degradation rate constants and therefore faster pollutant removal.

Rct values for GO (80 Ω), N-GO (45 Ω), and rGO (25 Ω) were assigned based on the established electrochemical behaviour of these materials. GO exhibits the highest Rct due to its disrupted sp² network. N-GO has intermediate Rct reflecting improved charge transfer from nitrogen-induced active sites. rGO has the lowest Rct due to partial restoration of the conductive graphitic domain through reduction (Pei & Cheng, 2012; Wang et al., 2012).

Model Assumptions

The following assumptions apply: (1) the reactor is perfectly mixed with uniform pollutant concentration throughout; (2) degradation follows pseudo-first-order kinetics with a constant rate coefficient; (3) temperature, pH, applied voltage, electrode area, and electrolyte composition are invariant; (4) mass-transfer limitations, electrode fouling, intermediate product formation, and competitive reactions are neglected; (5) the model evaluates comparative electrode performance trends rather than predicting absolute removal of a specific pollutant under real conditions.

Simulation Setup and Parameters

All simulations were executed in OpenModelica (OMEdit) from t = 0 to t = 180 min with an initial pollutant concentration of C_0 = 100 mg/L and 500 output intervals. Table 1 summarises the model parameters for all three electrode conditions.

Table 1: Model Parameters for GO, N-GO, and rGO Electrode Simulations

Electrode	Rct (Ω)	Rct_ref (Ω)	k_0 (min^{-1})	k_eff (min^{-1})	C_0 (mg/L)
GO	80	80	0.0050	0.0050	100
N-GO	45	80	0.0050	0.0089	100
rGO	25	80	0.0050	0.0160	100

Sensitivity Analysis

A sensitivity analysis was conducted by varying Rct from 10 to 120 Ω and computing the simulated removal efficiency at t = 180 min for each value. This range encompasses practically achievable Rct values for carbon-based electrodes reported in the literature and provides a generalised performance envelope beyond the three specific electrode conditions modelled.

RESULTS AND DISCUSSION

Pollutant Concentration Decay

Figure 1 shows the simulated pollutant concentration as a function of treatment time for all three electrodes. All three profiles exhibit the characteristic exponential decay of pseudo-first-order kinetics, with the rate of decay directly reflecting the electrode-specific effective rate constant. rGO produced the most rapid concentration decline, reducing pollutant concentration from 100 mg/L to 5.61 mg/L at 180 minutes. N-GO achieved a final concentration of 20.19 mg/L, while GO reduced concentration only to 40.66 mg/L more than seven times higher than the rGO final concentration.

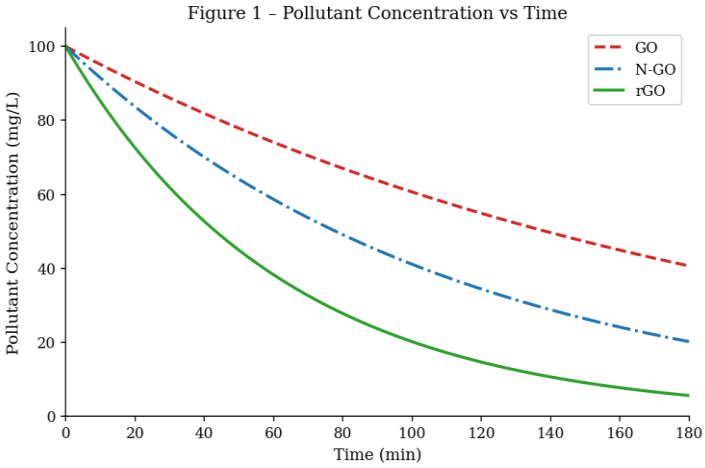

Figure 1: Simulated Pollutant CONCENTRATION versus Treatment Time for GO, N-GO, and rGO Electrodes in the Electrochemical Batch Reactor

The concentration separation between electrodes widens progressively with time, reflecting the compounding effect of the rate constant difference. At t = 60 min, the rGO concentration (38.0 mg/L) is already 36% lower than the GO concentration (74.1 mg/L). By t = 180 min this gap has grown to 35.05 mg/L absolute difference, corresponding to a 6.2-fold difference in remaining pollutant concentration. This progressive divergence underscores the practical importance of electrode selection for long-duration batch treatment processes.

Removal Efficiency

Figure 2 shows cumulative removal efficiency as a function of treatment time. rGO crossed the 80% removal threshold at approximately 100.8 minutes and reached 94.39% at 180 minutes the highest removal efficiency of the three electrodes and the only one to approach 95% within the simulation window. N-GO reached 79.81% removal at 180 minutes, falling just short of the 80% target threshold commonly cited for electrochemical water treatment performance benchmarking (Martínez-Huitle et al., 2015). GO reached only 59.34% removal at 180 minutes, indicating that its high charge-transfer resistance substantially limits degradation kinetics under the modelled conditions.

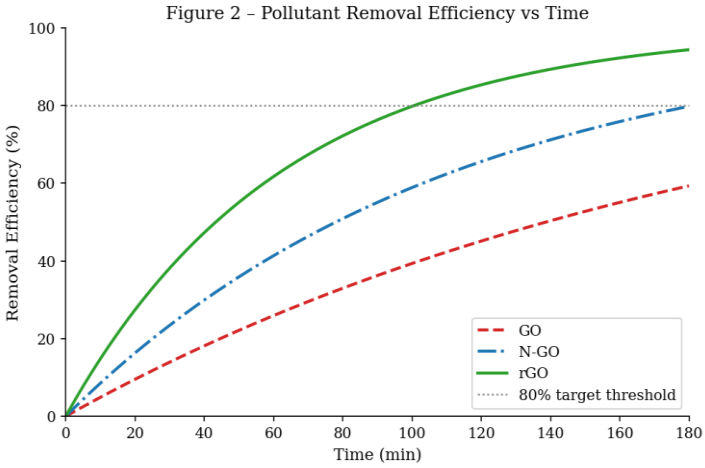

Figure 2: Simulated Removal Efficiency Versus Treatment Time for all Three Electrodes. The Dashed Line Indicates the 80% Removal Target Threshold

Effective Rate Constants

Figure 3 presents the effective degradation rate constants derived for each electrode through the Rct-scaling relationship. rGO has the highest k_eff of 0.0160 min^{-1}, compared to 0.0089 min^{-1} for N-GO and 0.0050 min^{-1} for GO. The rGO rate constant is 3.2 times higher than GO and 1.8 times higher than N-GO. These ratios are directly proportional to the inverse Rct ratios (80/25 = 3.2 and 80/45 = 1.78), confirming that the Rct-scaling framework produces internally consistent and physically interpretable rate constant predictions.

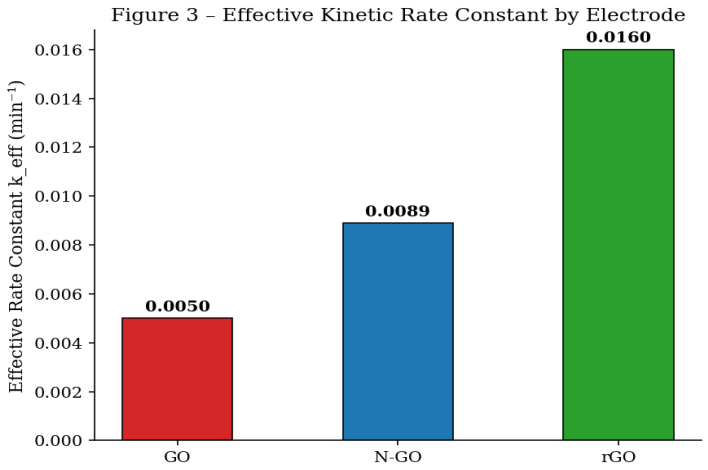

Figure 3: Effective Kinetic Rate Constants for GO, N-GO, and rGO Electrodes Derived from the Rct-scaling Relationship

The physical basis for the rate constant differences is well established in the electrochemical literature. In GO, the dense population of epoxide, hydroxyl, and carboxyl groups disrupts the sp^2 carbon network, reducing electrical conductivity and increasing Rct. This limits the rate at which electrons can be transferred from pollutant molecules to the electrode, reducing the generation of reactive oxidising species and slowing degradation (Dreyer et al., 2010). In rGO, partial reduction restores a proportion of the graphitic lattice, lowering Rct and enabling faster electron transfer. In N-GO, nitrogen incorporation introduces pyridinic-N, pyrrolic-N, and graphitic-N sites that act as electron donors, improving electrode wettability and facilitating faster charge transfer at the electrode–electrolyte interface (Wang et al., 2012).

Time-to-Threshold Analysis

Figure 4 shows the time required for each electrode to reach removal thresholds of 50%, 70%, 80%, and 90%. rGO is the only electrode to reach all four thresholds within the 180-minute simulation. It achieves 50% removal at 43.56 minutes, compared to 78.12 minutes for N-GO and 138.96 minutes for GO. At the 70% threshold, only rGO (75.60 min) and N-GO (135.72 min) succeed within the window; GO does not reach 70% within 180 minutes. Neither GO nor N-GO achieves 80% or 90% removal within the simulation period, while rGO reaches 80% at 100.8 minutes and 90% at 144.0 minutes.

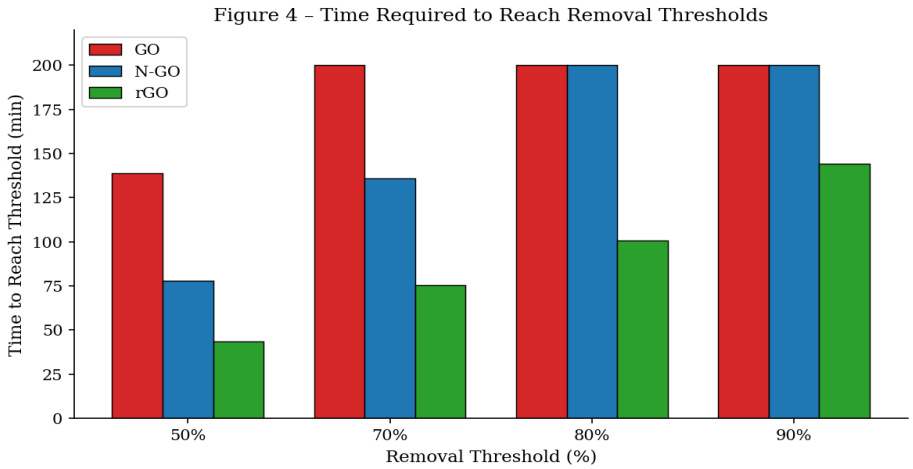

Figure 4: Time Required to Reach Removal Thresholds of 50%, 70%, 80%, and 90% for each Electrode. Bars Reaching 200 min Indicate the Threshold was not Achieved within the 180-minute Simulation Window

The time-to-threshold analysis has direct practical implications for electrochemical water treatment system design. Treatment time is a primary determinant of reactor sizing, energy consumption, and throughput capacity. The 3.2-fold reduction in time to 50% removal from GO to rGO translates directly to potential reductions in reactor residence time, treatment unit volume, and operational energy cost. For wastewater treatment applications where regulatory discharge standards define minimum removal thresholds, the model results indicate that rGO electrodes could enable compliance at substantially shorter treatment times than GO electrodes under comparable operating conditions.

Pseudo-First-Order Kinetics Confirmation

Figure 5 shows the logarithmic plot of C/C_0 versus time for all three electrodes. The linear relationship between $\ln(C/C_0)$ and time confirms that the pseudo-first-order kinetic model is internally consistent and that the simulated concentration profiles follow the expected analytical form. The slope of each line is equal to the negative effective rate constant

(−k_eff), providing a graphical verification of the rate constant values reported in Figure 3. This linearisation also provides a practical data processing method for experimentalists wishing to compare simulated kinetics against experimental concentration measurements.

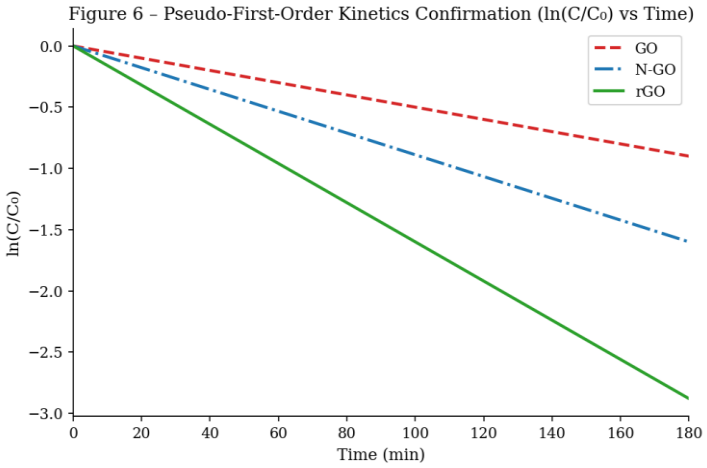

Figure 5: Pseudo-first-order Kinetics Confirmation: ln(C/C₀) Versus Time for all three Electrodes. Linear Profiles Confirm first-order behaviour; the Slope of Each Line Equals −k_eff

Sensitivity of Removal Efficiency to Charge-Transfer Resistance

Figure 6 presents the sensitivity of simulated removal efficiency at t = 180 min as a function of Rct across the range 10–120 Ω. The three electrode conditions modelled in this study are marked as reference points. The sensitivity curve reveals a nonlinear, strongly decreasing relationship between Rct and removal efficiency: as Rct decreases from 80 Ω (GO) to 25 Ω (rGO), removal efficiency increases from 59.3% to 94.4%. At very low Rct values (≤ 20 Ω), the curve approaches saturation above 95%, indicating diminishing returns on further resistance reduction. At high Rct values (≥ 100 Ω), removal efficiency drops below 50%, representing practical failure of the treatment system within the 180-minute window.

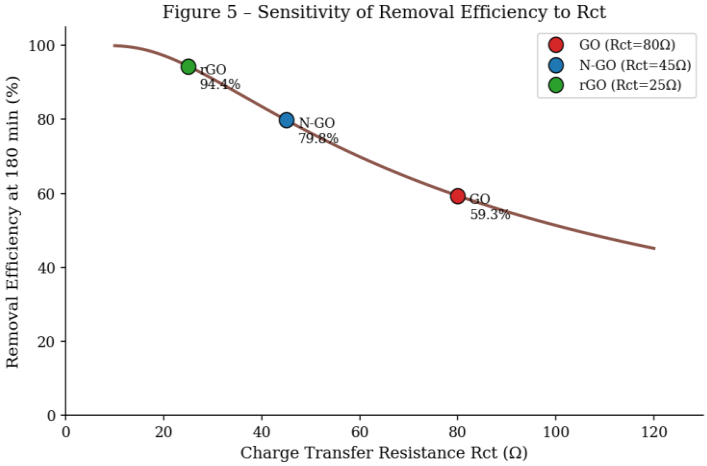

Figure 6: Sensitivity of Simulated Pollutant Removal Efficiency at 180 min to Electrode Charge-transfer Resistance. The three Modelled Electrode Conditions are Marked as Reference Points

The sensitivity analysis confirms that Rct is the dominant parameter controlling electrode degradation performance in this framework, and that the relationship is practically significant across the Rct range relevant to carbon-based electrodes. This result provides a quantitative basis for electrode development strategies: reducing Rct from 80 Ω to 45 Ω (the GO-to-N-GO improvement) yields a 20.5 percentage point gain in removal efficiency, while further reduction from 45 Ω to 25 Ω (N-GO to rGO) yields an additional 14.6 percentage point gain. The law of diminishing returns visible in the saturation region suggests that electrode engineering efforts should prioritise reducing Rct below 45 Ω rather than achieving ultra-low resistance values below 15 Ω. Figure 7 presents side-by-side comparisons of final removal efficiency and electrode Rct values, summarising the core finding of the study. Table 2 provides the complete numerical summary of simulation results.

Figure 7 - Electrode Performance and Rct Comparison

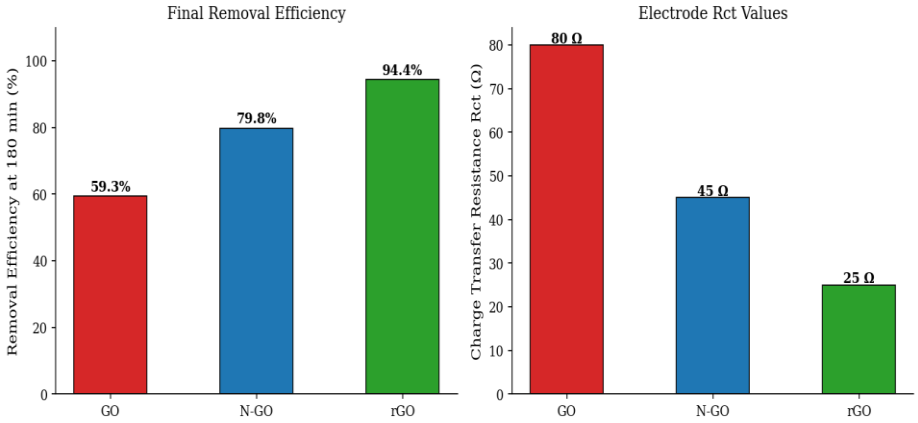

Figure 7: Summary Comparison of Final Removal Efficiency at 180 min (left) and Electrode Charge-transfer Resistance Values (right) for GO, N-GO, and rGO Electrodes

Table 2: Summary of OpenModelica Simulation Results at t = 180 min for all Three Electrode Conditions

Electrode	k_eff (min⁻¹)	Removal at 180 min (%)	C_final (mg/L)	Time to 50% removal (min)	Time to 90% removal (min)
GO	0.0050	59.34	40.66	138.96	N/A
N-GO	0.0089	79.81	20.19	78.12	N/A
rGO	0.0160	94.39	5.61	43.56	144.0

The modelling framework presented here has practical utility as an electrode screening tool in electrochemical water treatment system design. Given EIS-derived Rct values for candidate electrode materials, the framework can predict comparative pollutant removal performance without requiring full experimental batch treatment studies. This capability is particularly valuable during early-stage electrode development, where rapid screening of multiple material formulations is needed and experimental batch testing is resource-intensive. The framework can be extended to any electrode material for which Rct data is available, including metal oxide electrodes, boron-doped diamond, and composite carbon materials.

The present model is a simplified kinetic framework and does not capture the full mechanistic complexity of electrochemical pollutant degradation. The pseudo-first-order assumption does not account for competitive oxidation of reaction intermediates, electrode fouling, electrolyte depletion, pH variation, or mass-transfer limitations that become significant at higher pollutant concentrations or longer treatment durations. The Rct-to-rate-constant scaling relationship is an empirical approximation that assumes a linear inverse proportionality; real electrode kinetics may exhibit more complex dependences on overpotential, current density, and electrode geometry. The Rct values used are representative literature-informed estimates rather than cell-specific EIS measurements. The model does not simulate spatial concentration gradients, fluid dynamics, or electrode potential distribution within the reactor. Future work should validate the framework against experimental batch degradation data for specific pollutants, incorporate mass-transfer terms, and extend the Rct-scaling relationship to account for nonlinear electrode kinetics and electrode ageing.

CONCLUSION

A charge-transfer-resistance-informed pseudo-first-order kinetic model was implemented in OpenModelica to simulate pollutant degradation in a batch electrochemical reactor using GO, N-GO, and rGO graphene-based electrodes. By linking electrode Rct values directly to effective degradation rate constants through a physically motivated scaling relationship, the model translates impedance characterisation data into pollutant removal performance predictions without requiring experimental batch testing.Simulation results over a 180-minute treatment period demonstrated clear and physically consistent performance separation between the three electrodes. rGO achieved the highest removal efficiency (94.39%), the fastest rate constant (0.0160 min⁻¹), and was the only electrode to achieve 90% pollutant removal within the simulation window. N-GO reached 79.81% removal with an intermediate rate constant of 0.0089 min⁻¹. GO achieved only 59.34% removal due to its high charge-transfer resistance of 80 Ω. Time-to-threshold analysis demonstrated that rGO achieves 50% removal 3.2 times faster than GO and 1.8 times faster than N-GO, with direct practical implications for reactor sizing and energy efficiency in water treatment system design.

Sensitivity analysis confirmed that Rct is the dominant kinetic parameter governing electrode performance, with removal efficiency exhibiting a strongly nonlinear decreasing relationship as Rct increases from 10 to 120 Ω. The results support electrode development strategies focused on reducing Rct below 45 Ω as the highest-value target for improving electrochemical water treatment performance. The dynamic modelling framework presented here provides a computationally accessible and low-cost tool for electrode material screening in electrochemical water treatment and can be applied to any electrode material for which impedance characterisation data is available.

DATA AVAILABILITY

The simulation data generated in this study, including OpenModelica model code and exported CSV results files for all three electrode conditions, are available from the corresponding author upon reasonable request.

COMPETING INTERESTS

The authors declare no competing financial or non-financial interests.

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