



GUJARAT TECHNOLOGICAL UNIVERSITY

(Established by Government of Gujarat under Gujarat Act No. : 20 of 2007)

ગુજરાત ટેકનોલોજીકલ યુનિવર્સિટી

(ગુજરાત સરકારના ગુજરાત અધિનિયમ ક્રમાંક : ૨૦/૨૦૦૭ દ્વારા સ્થાપિત)

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Abstract of the Thesis



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Faculty : ENGINEERING

Discipline/Branch : CHEMICAL

Title of the Thesis : A Combined Computational and Experimental

Approach for Electrochemical Oxidation of Reactive Black 5 in

Wastewater

Abstract

The discharge of dye containing industrial effluents continues to pose a significant challenge to wastewater management because many reactive azo dyes exhibit high chemical stability and resist conventional biological treatment. Electrochemical oxidation has emerged as an effective alternative owing to its ability to mineralize persistent organic pollutants without the addition of external oxidizing chemicals. Despite considerable experimental research, the development of computational models capable of reliably predicting reactor behaviour under varying operating conditions and supporting process scale-up remains limited. Most reported investigations either emphasize experimental observations or employ simplified modelling approaches that do not adequately account for the interaction between reaction kinetics, thermal effects, and reactor configuration. This research presents an integrated computational and experimental framework for the electrochemical oxidation of Reactive Black 5 using titanium supported mixed metal oxide ($\text{Ti/TiO}_2\text{IrO}_2\text{RuO}_2$) anodes. The electrodes were fabricated using the standard thermal decomposition technique and characterized through scanning electron microscopy, energy-dispersive X-ray spectroscopy, and X-ray diffraction to establish their structural and compositional characteristics. Electrochemical oxidation experiments were subsequently performed under controlled operating conditions using both synthetic dye solutions and industrial wastewater. Since



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chemical oxygen demand (COD) reflects the extent of organic mineralization more effectively than colour removal, it was adopted as the principal performance indicator throughout the investigation. Experimental observations were combined with computational modelling to establish a predictive framework for the electrochemical process. A non-spatial COMSOL Multiphysics® model was developed using experimentally derived kinetic parameters and progressively refined to account for temperature dependent reaction behaviour and concentration-dependent effects. The influence of thermal evolution during electrooxidation was examined through Arrhenius based kinetic analysis, leading to a thermally coupled model that more accurately represented the experimentally observed degradation characteristics than an isothermal formulation. Model performance was assessed through comparison with experimental observations and published data, providing a systematic evaluation of its predictive capability over a range of operating conditions. To investigate reactor scalability beyond laboratory batch operation, a continuous three tanks in series reactor was designed, fabricated, and experimentally validated. The study further developed a dynamic framework for evaluating specific energy consumption, enabling the influence of operating voltage and current efficiency on process energetics to be examined under both batch and continuous configurations. Integration of experimental measurements with computational simulation provided a unified methodology for analysing degradation behaviour, reactor performance, and energy requirements within a common modelling framework. The outcomes of this investigation demonstrate that coupling experimentally validated electrochemical kinetics with computational modelling provides a practical approach for interpreting electrooxidation behaviour and supporting reactor design. The developed framework establishes a methodology for predicting COD removal, evaluating reactor performance, and assessing energy consumption while reducing dependence on extensive experimental trials. The incorporation of thermally coupled kinetics and validation of both batch and continuous reactor configurations extend the applicability of electrochemical oxidation modelling and provide a foundation for the optimization and scale-up of electrochemical treatment systems for dye containing industrial wastewater.

Keywords: Electrochemical oxidation; Reactive Black 5; Chemical oxygen demand (COD); Mixed metal oxide (MMO) electrode; COMSOL Multiphysics®; Computational modelling; Specific energy consumption; Three tanks in series reactor

This PhD Thesis will help in

The development of a systematic, computationally supported approach for treating dye-containing industrial wastewater through electrochemical oxidation. The developed framework can enable researchers and process engineers to predict COD reduction, understand the influence of operating conditions and thermal effects on degradation kinetics, and evaluate the energy requirements of electrochemical treatment. The comparative investigation of batch and continuous three-tank-in-series reactor configurations provides insights into reactor selection, process intensification, and



the transition from laboratory-scale experiments towards larger treatment systems. Furthermore, integrating experimental findings with COMSOL Multiphysics® modelling can reduce dependence on extensive experimental trials during preliminary process evaluation and support the identification of appropriate operating conditions. The dynamic assessment of specific energy consumption also provides a basis for examining the relationship between treatment performance and electrical energy demand. Overall, this research offers a methodological foundation for developing predictable, energy-conscious, and scalable electrochemical treatment strategies for persistent dye pollutants. The framework may also be extended to other industrial wastewater streams, subject to appropriate kinetic parameter estimation and experimental validation.

List of Publication(s):

JOURNAL PAPERS

I. FIRST AUTHOR

- 1) Nair, G., Soni, B., & Shah, M. (2023). A comprehensive review on electro-oxidation and its types for wastewater treatment. Groundwater for Sustainable Development, 23, 100980. [10.1016/j.gsd.2023.100980](https://doi.org/10.1016/j.gsd.2023.100980) (IMPACT FACTOR: 6.61)
- 2) Nair, G., & Soni, B. (2025). Parametric simulation of voltage and current efficiency effects on specific energy consumption in electrooxidation systems. International Journal of All Research Education & Scientific Methods, 13(11), 1076–1084. <https://doi.org/10.56025/IJARESM.2025.1311251076> (IMPACT FACTOR: 9.175)
- 3) Nair G, Soni B (2026) Thermally Coupled Modelling and Experimental Investigation of Electrooxidation for Reactive Black 5 Degradation. Indian Journal of Science and Technology 19(18): 1182-1193. <https://doi.org/10.17485/IJST/v19i18.550> (IMPACT FACTOR: 0.4)

II. CORRESPONDING/CO-AUTHOR

- 1) Soni, B. D., Ruparelia, J. P., & Nair, G. (2025). Electrochemical remediation of Reactive Black 5 (RB5) dye: A novel approach with Tanks in a series (TIS) model with dimensionally stable anodes (DSA) and boron doped diamond (BDD) anodes. Results in Engineering, 107384. <https://doi.org/10.1016/j.rineng.2025.107384> (IMPACT FACTOR: 7.9)
- 2) Patel, D., Nair, G., Patel, F., & Soni, B. (2024). Electrochemical degradation of reactive dyes mixture over DSA electrodes: A sustainable approach. Materials Today: Proceedings, 111, 111–120. [10.1016/j.matpr.2023.11.148](https://doi.org/10.1016/j.matpr.2023.11.148) (IMPACT FACTOR: 2.84)



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SUBMITTED PAPERS

I. CONFERENCE PAPER

- 1) Nair, G., Soni, B., Shah A. (2026). "Comparative Energy Analysis of Batch and Continuous Electrooxidation Reactors Using COMSOL-Based Modelling" Special Issue -Environmental Science and Pollution Control Research (ESPR), May 2026 (IMPACT FACTOR: 5.59) (under review)

II. BOOK CHAPTER

- 1) Nair, G., Soni, B., Shah A. (2026). "Modelling of Energy Consumption in Non-spatial Electro-oxidation model of Reactive Black 5 Using COMSOL Multiphysics", Elsevier book volume -CHEMCON 2025 (under review).