From waste to resource: Computing-based optimization of used water filter for sustainable industrial effluent treatment

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Abstract

The widespread adoption of household water filters has improved access to clean drinking water but has also created an emerging solid waste challenge. Although discarded after domestic use, these filters retain functional components such as activated carbon and membranes that may be repurposed for secondary treatment applications. The reused filters achieved a 92 % chemical oxygen demand (COD) removal and a 100 % total suspended solids removal from rubber effluent when integrated with immobilised iron-copper nanoparticle treatment. However, experimental chemical engineering datasets are often limited, making optimisation of used water filters (UWFs) for reuse challenging. This study evaluates the reuse of UWFs as a sustainable pre-treatment medium for rubber wastewater and explores large language models (LLMs) for empirical equation generation under data-scarce conditions. Across five independent runs for each LLM, 12 of 15 runs generated the same empirical equation, with R^2 values of approximately 0.77 and a potential optimum condition of 1.0 L and 200 mL min^{-1}, corresponding to an estimated COD removal of 94.9 %. Although these equations remain exploratory and require further validation, the findings demonstrate the potential of LLM-assisted equation generation to support preliminary process optimisation while advancing circular economy principles and sustainable industrial water management.

Keywords: Chemical oxygen demand; solid waste valorisation; large language model; wastewater treatment; circular economy; sustainability.

Available on-line at the Journal web address: http://www.ache.org.rs/HI/

TECHNICAL PAPER

UDC 62-73:632.153:628.312.4

Hem. Ind. **80(0)** 000-000 (2026)

1. INTRODUCTION

Water pollution remains one of the most pressing environmental challenges of the modern era, with industrial effluents ranking among the primary contributors. These effluents not only threaten aquatic ecosystems but also pose serious risks to human health. According to the latest reports by the World Health Organization (WHO), 1 in 4 people globally still lack access to clean drinking water [1]. This growing awareness of water quality has led to a sharp rise in the use of household water filtration systems.

Thus, the global production and consumption of household water filters have increased dramatically over the past two decades, with tens of millions of units now manufactured and disposed of annually. In China, for instance, the water purifier market is among the fastest growing in the world, driven by a large population, rapid urbanization, and sustained economic growth. The market is projected to grow at a compound annual growth rate (CAGR) of 11.4 % between 2023 and 2030, rising from USD 9.3 billion in 2022 to an estimated USD 22 billion by 2030 [2]. Over the last twenty years, the adoption of residential water filtration systems has surged from 0.14 % in 2007 to 17.82 % in 2022, while annual sales revenue increased from 1.27 billion to 18.5 billion Chinese Yuan, corresponding to a CAGR of 18.22 % [3]. Similarly, the commercial water purifier market in China expanded from USD 0.91 billion in 2018 to USD 1.55 billion in 2022, growing

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Paper received: 3 February 2026; Paper accepted: 18 November 2026; Paper published: 24 November 2026.
https://doi.org/10.2298/HEMIND260203009H

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at a rate of 15.0 % [4]. These trends reflect a global shift from traditional purification methods, such as boiling, toward convenient point-of-use filtration technologies.

While beneficial for public health, the increased dependence on household water filters has also resulted in a mounting solid waste problem. The majority of used water filters (UWF) are disposed of in landfills, contributing to plastic pollution, activated carbon waste, and potential leachate formation. The plastic components of these filters are a significant source of microplastics, persistent pollutants that have been detected in air, water, and even the human body. Limited recycling and reuse options further add to environmental stress, endangering ecosystems and public health. Given these challenges, there is an urgent need to develop innovative reuse strategies and valorisation pathways for UWFs, which are often discarded despite retaining functional potential for secondary applications.

The increasing volume and complexity of solid waste generated by modern societies have become a critical environmental challenge, threatening both ecosystems and human health. The deterioration of bio-physical systems, driven by pollution, resource depletion, and greenhouse gas emissions, highlights the need for sustainable resource management frameworks. In this context, the circular economy (CE) has emerged as a promising approach to bridge the idealism of the sustainable development goals (SDGs) with practical, low-carbon, and low-waste industrial practices. The CE framework emphasizes waste prevention, reuse, and material recovery, transforming the traditional linear model of "produce-use-dispose" into a regenerative cycle that minimizes environmental burden. A circular alternative, illustrated in Figure 1, incorporates a repurposing stage that extends filter lifespan, retains material value, and lessens reliance on fresh resources, all while diverting waste from landfills. However, global progress toward circularity remains modest, with less than 10 % of material flows currently managed within circular systems [5].

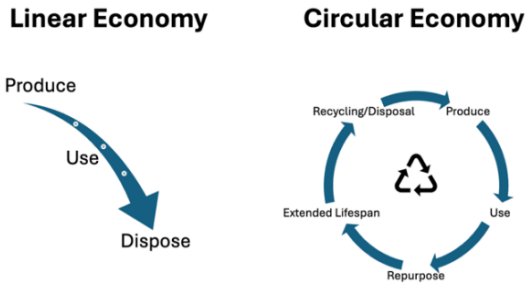


Figure 1. *Life Cycle Assessment (Linear vs Circular)*

In China, a number of waste repurposing initiatives have been carried out to demonstrate the effort to transform the discarded materials into valuable resources. For example, Beijing has paved stretches of road using rubber asphalt made from used tires; this application consumed millions of waste tires and has yielded increased pavement durability and reductions in both standard coal consumption and carbon dioxide emissions [6]. Moreover, industrial by-products like fly ash and calcined coal gangue are increasingly being used in Chinese construction materials as partial substitutes for cement. These substitutions mitigate the environmental footprint of concrete production by lowering both carbon emissions and the use of virgin raw materials, while maintaining acceptable material performance [7]. In the electronics sector e-waste recycling is also expanding rapidly. China has become one of the largest domestic generators of e-waste globally, with formal recycling efforts gradually catching up, reclaiming precious metals and rare earths from appliances and electronic components [8].

From a life cycle standpoint, household water filters typically follow a linear "use-and-dispose" model, resulting in material loss and mounting waste volumes. To demonstrate the solid waste management potential of UWF, a proof-of-concept study was conducted in which discarded household filters were repurposed as a pre-treatment medium for rubber wastewater (RWW) [9]. Most UWFs comprise layered components such as sediment filters, activated carbon, and thin-film composite membranes. While their efficiency for household purification declines over time, these materials often retain significant residual functionality, particularly in adsorption capacity and particulate removal. Thus, it is important to identify optimal conditions for reuse of UWFs.

Large language models (LLMs) are sophisticated systems developed using deep learning techniques and trained on broad contextual knowledge across multiple domains [10]. They capture semantic and syntactic patterns from large-scale pretraining and have demonstrated potential to assist with scientific reasoning, equation generation, and data

interpretation across a range of domains [11,12]. On the other hand, traditional machine-learning approaches such as artificial neural networks (ANNs) may be prone to overfitting when applied to very small datasets [13]. This issue is particularly relevant to experimental chemical engineering research, where data availability is often constrained by the costs of reagents, materials, instrumentation, and analytical procedures. Thus, exploring the use of LLMs as exploratory tools for empirical equation generation may provide an alternative approach for extracting useful relationships from data-scarce experimental systems.

This study explores the feasibility of using LLMs to assist in generating empirical response surface equations from a limited experimental dataset for estimating pollutant removal and identifying potential optimal operating conditions for reusing UWFs as a pre-treatment medium for RWW. The objective is to evaluate the potential of LLM-assisted equation generation as an exploratory decision-support tool for process optimisation under data-scarce experimental conditions. The proposed strategy not only diverts waste from landfills but also offers a cost-effective and environmentally friendly solution for wastewater treatment, aligning with the broader principles of circular economy and sustainable resource management.

2. EXPERIMENTAL

2. 1. Large language models-assisted empirical equation generation

The data used for LLM-assisted empirical equation generation were collected from an integrated UWF and immobilised iron-copper nanoparticle (UWF-iFeCu) system, which was developed to treat RWW [8]. The RWW was highly loaded with ammonia and organic matter [14]. The UWF units (INTRIX Group, Malaysia; filter cartridge manufactured in Korea) were collected by the salesperson responsible for the annual servicing of the water filtration system and delivered to SEGi University for reuse purposes. The iFeCu nanoparticles were synthesized according to the method published in a previous work [9]. The flowrate (Q) of RWW into the UWF was varied from 200 to 1000 mL min^{-1}, with each batch treating a fixed RWW volume (V) of 1 to 3 L. The samples were collected before and after the UWF to evaluate its capacity to remove total suspended solids (TSS), chemical oxygen demand (COD) and ammonia from the RWW. The UWF-treated RWW was subsequently directed to the iFeCu unit to complete the treatment process.

Gemini 2.5 Flash with Extended Thinking (Gemini) [15], DeepSeek with Deep Think (Deep Seek) [16], and GPT-5.6 Sol with High reasoning (GPT) [17] were selected as the LLMs in this study to generate empirical equations for estimating COD removal (Y) and identify the optimum operating condition when UWFs were reused as a pre-treatment medium for RWW.

Each LLM was independently evaluated in five separate new sessions (analysis date: August 2026) using the same six experimental observations and an identical standardised prompt, shown below.

Prompt 1: “Using only the experimental data provided, generate an empirical response surface equation relating COD removal, % to wastewater volume, V / L and flow rate, Q / mL min^{-1}. Use the equation to estimate COD removal at the six experimental conditions and identify the potential optimum operating condition within the experimental ranges of V = 1.0 to 3.0 L and Q = 200 to 1000 mL min^{-1}. Report the generated equation, estimated COD removal values, optimum V and Q, and the corresponding COD removal. Calculate coefficient of determination (R^2), root mean square error (RMSE) and mean absolute error (MAE) using the six experimental observations. Do not extrapolate beyond the experimental ranges. Do not introduce additional experimental data or assumptions.”

The ‘experimental data provided’ in the prompt was the experimental data listed in Table 1.

Table 1. *Experimental data used for LLM-assisted empirical equation generation*

Data set ID	V / L	Q / mL min^{-1}	COD removal, %
ID-1	1.0	600	68
ID-2	1.5	600	92
ID-3	2.0	600	43
ID-4	3.0	600	25
ID-5	1.5	200	89
ID-6	1.5	1000	80

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All generated equations and outputs were retained without manual modifications or selective exclusions, and the reported metrics were checked against the six experimental observations.

3. RESULTS AND DISCUSSION

3. 1. Experimental data

The data from previous work [9] showed that 600 mL min^{-1} was the optimum flowrate as the treated RWW exhibited the highest pollutant removal. The optimum removal capacity of UWF in treating RWW is listed in Table 2. This result reveals that even after their domestic lifespan, the filters retained notable filtration capacity, removing 92 % COD and 100 % TSS. Both parameters complied with the RWW discharge standard. The UWF-treated RWW was then directed to the immobilized iron-copper nanoparticle for ammonia removal.

Table 2. *Pollutant removal capacity of UWF in treating RWW [8]*

Pollutants in RWW	Removal rate, %	Compliance with RWW discharge standard
COD	92	Meets standard
TSS	100	Meets standard
Ammonia	23	Does not meet standard

In this study, COD was selected as a critical pollutant to be removed from RWW, while UWF consistently removed 100 % of TSS, regardless of variations in V and Q. Ammonia was excluded because UWF demonstrated poor ammonia removal performance.

3. 2. Performance of large language models generated empirical equations in estimating chemical oxygen demand removal by used water filters

Table 3 summarises the descriptive goodness-of-fit and error metrics obtained from five independent runs of each LLM. GPT showed complete consistency across the five runs, with identical RMSE of 11.64, MAE of 8.15 and R^2 of 0.7752. Gemini showed relatively small run-to-run variation, while DeepSeek produced the lowest mean RMSE and MAE, together with the highest mean R^2, but also exhibited the greatest run-to-run variability (Table 3). This variability was associated with different empirical equation patterns generated across the five runs, as shown in Table 4. Therefore, the lower mean error and higher R^2 values of DeepSeek should not be interpreted as evidence of superior predictive performance. Overall, the results show that the degree of run-to-run consistency differed among the LLMs despite the use of identical experimental data and prompting conditions.

Table 3. *Descriptive goodness-of-fit and error metrics of LLM-generated empirical equations across five independent runs*

LLMs	Gemini	DeepSeek	GPT
RMSE	12.29 ± 1.45	6.98 ± 6.38	11.64 ± 0.00
MAE	9.18 ± 2.31	4.89 ± 4.46	8.15 ± 0.00
R^2	0.7467 ± 0.0637	0.8651 ± 0.1231	0.7752 ± 0.0000

Table 4. *Empirical equations and potential optimum operating conditions generated across five independent runs of each LLM*

LLMs	Empirical equations	Frequency	Estimated optimum operating condition		Estimated optimum COD removal, %
			V / L	Q / mL min^{-1}	
Gemini	$Y = 111.6205+13.4273V-10.0909V^2-0118091Q+0.00089034Q^2$	4/5	1.0	200	94.90
	$Y = 45.4691+44.430$ V$-18.7030V^2+0.0450Q-0.000046875\ Q^2$	1/5	1.2	480	82.66
DeepSeek	$Y = 111.62+13.43V-10.09V^2-0.1181Q+8.903\times10^{-5}\ Q^2$	3/5	1.0	200	94.90
	$Y = -508.125+1060.8333V-594.5V^2+99.6667V^3+0.045Q\ -0.000046875Q^2$	2/5	1.35	480	96.58
GPT	$Y = 111.6205+13.4273V-10.0909V^2-0.118091Q+8.90341\times10^{-5}\ Q^2$	5/5	1.0	200	94.90

Table 4 presents the empirical equations and potential optimum operating conditions generated across five independent runs of each LLM. The repeated-run analysis revealed different levels of consistency among the three LLMs.

Details of each run are available in Supplementary Material Table S1. GPT produced identical outputs across all five independent runs, including the estimated COD removal values, and suggested optimum operating conditions. Gemini showed high consistency, with four of the five runs generating identical results. One run produced a different empirical equation and corresponding estimated COD removal and optimum operating condition. Greater run-to-run variability was observed for DeepSeek, where three runs generated similar results, whereas two runs produced equations that exactly fitted the six experimental observations with R^2 = 1.000, as shown in Supplementary material, Table S1.

These results indicate that LLM-generated empirical equations may exhibit run-to-run variability despite identical input data and prompting conditions, although the extent of variation differed among the tested LLMs. Nevertheless, 12 of the 15 independent runs generated the same empirical equation and identified the same potential optimum operating condition of 1.0 L and 200 mL min^{-1}, with an estimated COD removal of 94.9 %. This high level of consistency suggests that LLM-assisted equation generation can provide a reasonably consistent empirical description of COD removal from the available experimental observations, even under data-scarce conditions. This is particularly beneficial to water and wastewater research, where experimental work is often constrained by the high cost of chemicals and reagents, long sampling durations, and limited laboratory operating time. The ability to derive consistent empirical relationships and potential operating conditions from limited experimental observations highlights the potential of LLM-assisted equation generation as a complementary exploratory decision-support tool for early-stage process evaluation, screening of operating conditions, and planning of subsequent experimental or pilot-scale studies.

Although experimental verification of the suggested optimum condition was beyond the scope of this study, the estimated optimum at V = 1.0 L and Q = 200 mL min^{-1}, corresponding to 94.9 % COD removal, can be interpreted in relation to contact time and wastewater volume. At lower Q, the contact time between the UWF and RWW increases, which may favour COD removal. A similar trend was reported in the literature [18], where increasing the contact time from 5 to 120 min improved COD and ammoniacal nitrogen removal from leachate, using pulverized paper waste sludge as the treatment agent, reaching 48 and 42 % removal, respectively. In addition, at lower wastewater volumes, the UWF adsorption capacity is less likely to be reached, resulting in greater availability of adsorption sites and a faster COD removal process. The influence of adsorbent availability on COD removal was also demonstrated in a study [19], in which rice husk ash, corncob ash, and sugarcane bagasse fly ash were investigated for treating real textile wastewater. An optimum adsorbent dosage of 6 g L^{-1} was reported, with COD removal reaching approximately 70-75% for the better-performing adsorbents. These findings support the importance of available adsorption capacity in COD removal and provide a plausible explanation for the high estimated COD removal at the lower wastewater volume of V = 1.0 L.

Identification of a potential optimum operating condition using LLM-assisted equation generation may support practical reuse of UWFs, maintain pollutant removal performance and thereby extend the useful life of household filter materials in industrial effluent applications. A similar attempt was made by Bote *et al.* [20], where the optimum performance of used carbon from exhausted water filter cartridges was investigated for methylene blue adsorption. This further demonstrates the practical potential of waste-to-resource applications. The remaining functional potential of UWFs demonstrates their value as secondary resources, capable of contributing to sustainable wastewater management. When redirected from household use to serve as pre-treatment media for industrial effluents, UWFs can effectively reduce suspended solids and partially remove organic pollutants, offering a low-cost and environmentally responsible alternative to conventional pre-treatment systems. Furthermore, they lessen the burden on primary treatment methods being applied in industries.

This outcome is significant not only from a treatment performance standpoint but also from a solid waste valorisation perspective. It confirms that UWF can serve a secondary functional life in industrial wastewater management rather than being disposed of as non-recyclable waste. Such reuse aligns with circular economy principles by extending the material's lifespan, reducing the volume of waste directed to landfills, and lessening the demand for fresh filtration materials such as new activated carbon and membranes for industrial wastewater treatments. In essence, the repurposing of UWF transforms a domestic waste product into a resource with added environmental value.

A limitation of the present study is the small experimental dataset (n = 6) and the absence of cross-validation, including leave-one-out analysis, or independent validation. Accordingly, the LLM-generated equations and associated

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goodness-of-fit and error metrics should be interpreted as exploratory and descriptive of the available experimental observations rather than as evidence of generalisable predictive performance. Further studies using larger independent experimental datasets and appropriate validation procedures are required to establish the predictive capability and generalisability of the generated equations.

4. CONCLUSION

The reuse of UWFs as a pre-treatment medium for RWW presents a technically feasible, low-cost, and sustainable solution for industrial effluent management. The integrated UWF and immobilized iron-copper nanoparticle system achieved 92 % COD and 100 % TSS removal at the optimal operating flow rate of 600 mL min^{-1}, meeting the regulatory discharge standards stipulated in the Malaysian Rubber Wastewater Guideline. The LLM-generated empirical response surface equations suggested a potential optimum operating condition of V = 1.0 L and Q= 200 mL min^{-1}. The results demonstrate that UWFs retain significant adsorption and filtration capacity beyond their domestic service life, providing an effective means to reduce suspended solids and organic load prior to advanced treatment. This integration not only minimizes solid waste generation and the demand for virgin filter media but also contributes to Sustainable Development Goals through improved resource utilization, reduced carbon footprint, and enhanced process circularity. Although operational challenges such as filter heterogeneity, potential contamination, and regulatory limitations persist, these can be addressed through standardized quality control, pilot-scale validation, extended producer responsibility (EPR) mechanisms and circular business models. Overall, UWF reuse establishes a technically robust waste-to-resource framework, coupling solid waste valorisation with sustainable industrial wastewater treatment toward achieving resilient, circular water management.

Acknowledgements: This research was funded by SEGi University, grant number SEGiIRF/2022-Q1/FOEBEIT/004. Special thanks to Intrix Lifestyle Sdn. Bhd. for providing us with the used water filters.

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Od otpada do resursa: Računarska optimizacija ponovne upotrebe korišćenih filtera za vodu u održivom prečišćavanju industrijskih otpadnih voda

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(Stručni rad)

Izvod

Široka primena kućnih filtera za vodu doprinela je poboljšanju dostupnosti čiste vode za piće, ali je istovremeno dovela do pojave novog izazova u upravljanju čvrstim otpadom. Iako se nakon upotrebe u domaćinstvima odbacuju, ovi filteri zadržavaju funkcionalne komponente, poput aktivnog uglja i membrana, koje se mogu ponovo koristiti u sekundarnim postupcima prečišćavanja. Ponovo upotrebljeni filteri omogućili su smanjenje hemijske potrošnje kiseonika za 92 % i potpuno uklanjanje ukupnih suspendovanih materija (100 %) iz otpadnih voda industrije gume, kada su primenjeni u kombinaciji sa tretmanom imobilisanim nanočesticama gvožđa i bakra. Međutim, eksperimentalni skupovi podataka u hemijskom inženjerstvu često su ograničenog obima, što otežava optimizaciju ponovne upotrebe korišćenih filtera za vodu. U ovom istraživanju ispituje se mogućnost ponovne upotrebe korišćenih filtera za vodu kao održivog sredstva za pred-tretman otpadnih voda industrije gume, kao i primena velikih jezičkih modela za generisanje empirijskih jednačina u uslovima ograničene dostupnosti podataka. U pet nezavisnih ponavljanja za svaki od primenjenih velikih jezičkih modela, u 12 od ukupno 15 pokušaja generisana je ista empirijska jednačina, sa vrednostima koeficijenta determinacije (R^2) od približno 0,77. Kao potencijalno optimalni uslovi identifikovani su zapremina od 1,0 L i protok od 200 mL min^{-1}, pri čemu je procenjeno smanjenje HPK iznosilo 94,9 %. Iako su dobijene jednačine preliminarnog karaktera i zahtevaju dodatnu validaciju, rezultati ukazuju na potencijal primene velikih jezičkih modela za generisanje empirijskih jednačina kao podrške početnoj optimizaciji procesa, uz istovremeno unapređenje principa cirkularne ekonomije i održivog upravljanja industrijskim otpadnim vodama.

Ključne reči: Hemijska potrošnja kiseonika; valorizacija čvrstog otpada; veliki jezički modeli; prečišćavanje otpadnih voda; cirkularna ekonomija; održivost