Response to Reviewer-1

This article contributes to the field on an important topic of water treatment. In this work, Indian Gooseberry Seed Powder was used for the sequestration of Cr(VI) from aqueous solution. As I read this paper, I found that the paper has some issues that prevent it from being published in its current state. The manuscript needs to be revised extensively before it can be published. As such, the authors should seriously consider all of the following comments:

Author Response: The authors would like to thank the Editor and Reviewers for the time they spent reviewing our manuscript. The suggestions provided were constructive to enhance the quality of the manuscript. We have tried to answer all your questions/remarks/suggestions to the best of our knowledge. We hope you find the answers satisfactory and the manuscript of better quality.

Reviewer #1 Concern #1: The paper should be checked for subscripts and superscripts.

Author Response: Thank you for your suggestions. As suggested by the reviewer, we have checked for typo errors of subscripts and superscripts.

Author Action: The below are identified as typo errors in subscripts and superscripts. All these are corrected and the same is highlighted in blue colour in update manuscript.

Typo Errors in superscript and subscript	Corrected
Cr2O72	$Cr_2O_7^{2-}$
K2Cr2O7	$K_2Cr_2O_7$
Percentage removal of Cr(VI)=a * Initial concentration of Cr(VI) + b * pH + c * Adsorbent dosage (g/L)	Percentage removal of Cr (VI)=(a*IC) +(b*pH) + (c*AD)
$Z = \frac{f_i - \mu_{f_i}}{f_{\sigma_i}}$ (where $1 \le i \le N$, mean $\mu_{f_i} = \frac{1}{N}\sum_{i=1}^{N}$ and standard deviation $f_{\sigma_i} = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(f_i - \mu_{f_i}\right)^2}$)	$Z = \frac{f_i - \mu_{f_i}}{f_{\sigma_i}}$ where $1 \le i \le N$ mean $\mu_{f_i} = \frac{1}{N}\sum_{i=1}^{N}$ and standard deviation $f_{\sigma_i} = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(f_i - \mu_{f_i}\right)^2}$
$Removal\%of Cr(VI) = \frac{I_c r - F_c r}{I_c r} \times 100$	$\text{Percentage Removal of Cr(VI)} = \frac{I_{Cr} - F_{Cr}}{I_{Cr}} \times 100$
R2-score	R^2-score

Reviewer #1 Concern #2: Avoid unnecessary paragraphs.

Response: Thank you for your suggestions. As suggested by reviewer, we have reduced unnecessary paragraphs and same is reflected in revised manuscript.

Reviewer #1 Concern #3: Many acronyms are introduced directly. First give the full form and then follow the acronym throughout the paper.

Response: Thank you for your suggestions. As suggested by the reviewer, we have checked all the acronyms used in this manuscript and corrected wherever necessary and reflected in revised manuscript.

Reviewer #1 Concern #4: Give a novelty statement.

Response: Thank you for your suggestions. The novelty of this work is presented in the revised paper in the introduction section of this manuscript.

The introduction section sub-divided as Motivation section, Literature review section, Research gap section, Major contribution section; and organisation section along with novelty section. Hence, it was highlighted with blue color in the revised manuscript.

Reviewer #1 Concern #5: For Cr(VI) adsorption on plant, here are the references to cite: Removal of Cr (VI) from aqueous solution on seeds of Artimisia absinthium (novel plant material); Removal of Cr(VI) from electroplating wastewater using fruit peel of Leechi (Litchi chinensis).

Response: As suggested by reviewer, we felt that the suggested references were appropriate and cited in revised manuscript with reference numbers 29 and 30.

Reviewer #1 Concern #6: For BBD and ANN, here is a reference to cite: The artificial neural network and Box-Behnken design for Cu2+ removal by the pottery sludge from water samples: Equilibrium, kinetic and thermodynamic studies.

Response: As suggested by reviewer, we felt that the suggested reference was appropriate and cited in revised manuscript with reference number 23.

Reviewer #1 Concern #7: Section 2.1. "desired particle sizes". Mention the number.

Response: As suggested by the reviewer, we have included size of particles and updated in revised manuscript.

Author Action: Desired particle sizes of 63 µm, 89 µm, and 125 µm.

Reviewer #1 Concern #8: As the experimental study was conducted, optimization should be used to confirm its results. Hence, the results of experimental studies should also be presented and discussed.

Response:

The suggestion from the reviewer to utilize optimization for validating the experimental results and to thoroughly present and discuss these findings is highly valued. We concur that optimization is essential for confirming the experimental outcomes and guaranteeing the reliability of our results. Consequently, we have updated our manuscript to incorporate a detailed analysis of the optimization results and their correlation with our experimental data.

Revisions Made:

The results obtained from ETR-Nelder-Mead optimization were validated through experimentation as reported in Table 7. The results shows that the experimental outcome for optimal parameters such as optimal-Initial-concentration of Cr(VI) with 99.25, optimal pH with 4.97, and optimal Adsorbent dosage (g/L) (9.62) strongly aligns with experimentation results with an 6.56% of error rate.

Optimal Initial concentration of Cr(VI)	Optimal pH	Optimal Adsorbent dosage (g/L)	Optimal Cr(VI) removal %	Obtained Cr(VI) removal %	% Error
99.25	4.97	9.62	85.11	79.75	6.72

Reviewer #1 Concern #9: The study seems incomplete without characterization analysis.

Response:

We appreciate your insightful feedback and the emphasis on the significance of characterisation analysis in our research. We recognize that characterisation analysis is essential for comprehending the properties and behaviour of the materials utilized.

In our present research, our main emphasis was on improving the removal efficiency of Cr(VI) by utilizing tree-based machine learning models and Nelder-Mead optimization. Our main goal was to assess the effectiveness and enhancement of the elimination process. Nevertheless, we recognize that conducting a comprehensive analysis of the Indian Gooseberry Seed Powder could offer more profound understanding of its composition, functional groups, and adsorption mechanisms.

In our future work, we intend to conduct thorough analysis of the characteristics, which will entail utilizing methods like

1. Fourier Transform Infrared Spectroscopy (FTIR): To identify the functional groups present in IGSP.
2. Scanning Electron Microscopy (SEM): To observe the surface morphology and porosity of IGSP.
3. X-Ray Diffraction (XRD): To determine the crystalline structure of IGSP.

Reviewer #1 Concern #10: Rewrite conclusion. It is similar to the abstract.

Response: As suggested by the reviewer, we agreed with the perception of reviewer, and we have updated the previous conclusion as follows.

The previous conclusion:

A detailed batch experimental study was carried out for the removal of chromium (VI) from wastewater by Indian gooseberry seed powder. The objective of the present study was to find out the optimum process parameters, using ML models and Nelder-Mead optimization for the removal of Cr(VI) from wastewater by Indian gooseberry seed powder as adsorbent.

Among all the models, DTR, RFR, and ETR displayed exceptional performance, achieving R^2-scores of 99\%, respectively. Remarkably, all models exhibited an RRMSE of 1\%. These statistics further support the notion that these models performed exceptionally well.

Notably, the ETR approach outperformed all other models, showcasing a remarkable R^2-score. Furthermore, the MAE, MSE, and RMSE of the ETR indicated significantly lower error rates compared to the other models. Moreover, the percentage of Cr(VI) removal for Initial concentration of Cr(VI) of 99.55 mg/L, pH of 4.0, and Adsorbent dosage of 8.0 (g/L) gives highest Cr(VI) removal percentage such as 78.21\% and 78.107 respectively by DTR and RFR is as shown in Table 6. The removal efficiency of ETR model was 85.11\% for Initial concentration of Cr(VI) of 99.24284408 mg/L, pH of 4.96268861, and Adsorbent dosage of 9.61957019 (g/L). Furthermore, the optimization results presented in Table 6 reported optimized values obtained by ML based Nelder-Mead optimization approach to obtain maximum Cr(VI) removal percentage. That is, the DTR-Nelder-Mead, RFR-Nelder-Mead and ETR-Nelder-Mead optimization approaches were able to obtain maximum of 78.107\% to 85.11\% of Cr(VI) removal which reported increase in Cr(VI) removal percentage ranging from 4.66\% to 11.56\% than the Cr(VI) removal percentage of 73.55\%

obtained by experimentation for Initial concentration of Cr(VI) of 20 mg/L, pH of 2.0, and Adsorbent dosage of 8.0 (g/L).

In summary, based on the comprehensive evaluation, it is concluded that the ML models exhibited strong performance overall. ETR, in particular, stood out as the top performer, demonstrating superior accuracy with minimal error rate and obtains higher Cr(VI) removal percentage than all other models. Furthermore, The ML based Nelder-Mead optimization results indicated that the maximum of 85.11\% chromium VI removal is possible with Initial concentration of Cr(VI) of 99.24284408 mg/L, pH of 4.96268861, and Adsorbent dosage of 9.61957019 (g/L). These results indicated that the maximum Cr(VI) removal percentage by ML modeling and ML based Nelder-Mead optimization reported 11.56\% of increase in Cr(VI) removal percentage for different absorptions which were not tested during experimentation.

The Revised Conclusion:

This study examined a novel approach for percentage of Cr(VI) removal efficiency from wastewater by employing ML models combined with Nelder-Mead optimization. Especially, this combined strategy for adsorption capacity estimation using any solute or material has not been previously reported in the literature. This research not only leverages the power of ML for accurate prediction of percentage of Cr(VI) removal efficiency but also utilizes Nelder-Mead optimization to identify optimal process parameters which maximize Cr(VI) removal efficiency, ultimately achieving a significant enhancement in Cr(VI) removal efficiency compared to standalone experimentation.

In this work, particularly the ETR, achieved outstanding performance in predicting Cr(VI) removal. The ETR model exhibited a remarkable R^2-score of 99% and significantly lower error rates compared to other models. Furthermore, ML-based Nelder-Mead optimization identified optimal process parameters, leading to a maximum Cr(VI) removal efficiency of 85.11%. This represents an improvement of up to 11.56% compared to standalone experimentation.

These results demonstrate the effectiveness of the combined ML and optimization approach for maximizing Cr(VI) removal using Indian gooseberry seed powder. This research work paves the way for further exploration of ML-driven strategies in wastewater treatment applications.

Thank you again for reviewing our paper and providing valuable suggestions to improve the quality of the paper.