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JECE guidelines – 2023

The editorial team of the Journal of Environmental Chemical Engineering (JECE) aims at delivering to our readers articles of the highest scientific quality. Towards this aim, the editorial team applies a strict pre-screening process. The manuscripts are examined and assessed on the grounds of relevance to the journal, novelty, impact, interest to a broad readership, and overall quality of presentation including figures, tables, and language. Therefore, at times, manuscripts are returned to authors without peer review. On this basis, authors should consider, amongst others, the following points before submitting a manuscript to JECE.

1. General criteria for regular manuscripts

- When the goal is to assess the treatment efficacy/efficiency of a given technology, research using ultrapure/demineralized water with a single target contaminant and/or a concentration of several orders of magnitude higher than in the real environment masks the applicability of the experimental data to real applications. Therefore, it is recommended to complement the work with experimental data using real matrices and/or environmentally relevant contaminants' concentrations.
- 2. Papers must demonstrate high scientific rigor, including clearly described experimental setup, reactor design, replicate samples, treatment groups and controls, analytical quality assurance/quality control, and robust statistical treatment of data.
- 3. The use of UV-Vis spectrophotometric methods to quantify a target organic molecule and obtain its kinetic profile should be analyzed carefully, especially when dealing with real matrices and/or oxidation/reduction processes. It is possible to have spectral interferences by transformation intermediates and matrix components, which may absorb radiation at the wavelength of the target organic pollutant absorption maximum. Therefore, **it is recommended** using chromatographic methods for the quantification of target organic molecules, or deconvolution of the peaks, or comprehensive controls that adequately prove the quality of the spectrum-[contaminant] correlation.
- 4. Manuscripts that are very similar to previous publications, with changed target substrates and employed materials do not fit JECE standards.
- 5. Manuscripts dealing with case studies of specific locations or facilities without presenting new insights that can be applied to a broader context do not fit JECE standards.
- 6. Manuscripts dealing with chemical engineering processes with little or no environmental relevance such as metal corrosion in chemical and power plants do not fit JECE standards.

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Available online 28 March 2023 2213-3437/© 2023 Published by Elsevier Ltd. Manuscripts focusing on environmental management and economic assessment without scientific or engineering insights do not match the JECE scope and aims.

2. General criteria for review manuscripts

- A review manuscript is expected to present a critical overview of the state of the art of a topic, with critically selected examples, to introduce the reader to trends and likely future developments and to provide a selection of important references of the current literature.
- 2. It is recommended that the authors include the following information in the Cover Letter: (1) a clear indication of the novelty and urgency of such a review paper at this time; (2) a brief description of the authors' expertise in the research areas; (3) a list of all authors' publications related to the review article topic; and (4) a brief summary on related reviews published on the topic and how their manuscript provides relevant new insights and perspective beyond the available reviews.

3. Specific guidance on selected processes/categories

3.1. Redox processes

3.1.1. Photocatalysis

 The use of dyes as model compounds for the evaluation of photocatalytic activity of novel photocatalysts claimed to operate under visible light is considered problematic, especially when the total oxidation (mineralization) of the dye is not proved. Therefore, manuscripts dealing with this subject will not be considered in JECE, with the exception of studies employing advanced tools and methods to identify the reactive oxygen species (ROS) and/or photocatalytic mechanism.

3.1.2. Oxidation/reduction processes

1. Papers dealing with oxidation/reduction processes for the removal of inorganic species, such as Cr(VI), As(III), As(V) among others, should evaluate at least one of the individual species and the total concentration. For example, Cr(VI) removal using carbon based materials normally integrates a reduction step to its trivalent form, and further binding of Cr(III) species into the sorption sites present on the surface of the solid material. At the same time, the surface of the solid material is oxidized, changing the type of binding groups and possible increase of dissolved organic carbon in the solution. Under these

circumstances, **it is recommended** to analyze the total chromium and the hexavalent chromium concentration.

3.1.3. Disinfection

- 1. In a similar manner to dyes as model compounds, in disinfection studies the use of model microorganisms (e.g. lab strains of *Escherichia coli*) could be acceptable in the development of a new process where the bacteria are used only as a metric for efficacy evaluation. Cultivability is the minimum requirement, while additional measurements (viability, microscopy, enzymatic activity or degradation) are welcome. Complementary studies related to the context (e.g. total coliforms/total heterotrophic bacteria for natural waters or wastewater) or case-specific strains (e.g. *Staphylococcus* spp. and/or *Legionella* spp. for hospital acquired infections, *Pseudomonas spp.* for biofilms, ARB/MDR bacteria for works on antibiotic resistance) are highly encouraged.
- 2. Papers dealing with disinfection of air, water and soil or inactivation of pathogens in different substrates, such as *Eschericia coli, Salmonella, Pseudomonas,* among others, **it is recommended** to evaluate at least, one model pathogen as recognized in the standards in the field under investigation, and/or a wild or naturally occurring pathogen species with justification of its environmental concern, at environmentally relevant concentrations of pathogens. It is recommended to follow the standards for evaluation (including replicated samples or tests, and errors evaluation) and presentation of results of microbiological contamination in environment (e.g. logarithmic graphs in water disinfection, or log reduction units for drinking water) in comparison with threshold values and from relevant guidelines.
- 3. In disinfection studies, with frequently presented fitting models, i.e. Chick model, log-linear model, two-phases linear, etc., **it is recommended** that these models are used and discussed with adequate biological, physic-chemical, photo-chemical, and/or photobiological interpretation of the model parameters and clear justification of the hypothesis of the model. It is expected also that a residual sum of squares, uncertainty of model parameters and others statistical parameters should be carefully analysed.

3.2. Physico-chemical & biological processes

3.2.1. Adsorption/ion-exchange/biosorption

- 1. It is recommended that adsorption/ion-exchange/biosorption processes are modeled on the basis of phenomenological principles (e.g., conservation, equilibrium and transport kinetic equations) and not through short-cut approaches, such as pseudo-first order, pseudosecond order models and similar expressions (e.g., Elovich's equation, Intraparticle diffusion model, etc.).
- 2. Adsorption/ion-exchange/biosorption processes comprise the following steps: i) chemical and physical characterization (e.g. type and amount of functional groups, surface charge, surface area and porosity, etc.) of sorbent material; ii) equilibrium and kinetic studies at batch system, to obtain the total sorption/ion-exchange capacity of material and also to determine the selectivity and mass transfer coefficients; iii) elution and regeneration studies to define the best eluant and regenerant and respective concentrations; iv) continuous mode experiments (e.g., packed bed columns) to obtain the shape of the breakthrough curve according to the bed depth, bed diameter, feed flow rate, etc.; this allows to establish the optimal engineering parameters for the process scale-up, in order to achieve the "shortest" mass transfer zone - MTZ; v) consecutive saturation, elution and regeneration cycles are also crucial to evaluate the process applicability and cost analysis; vi) mechanistic models for full scale design and optimization. Papers dealing with at least four of those points are welcome.

- 3. Equilibrium between the solid and liquid phases have been widely represented by Langmuir, Freundlich and Dubinin–Radushkevich (D–R) models, which are able to represent experimental trends but without any interpretative intent. On the other hand, mechanistic models are theoretically derived assuming a set of reactions between the ionic/non-ionic species in solution and sorbent active sites. These models can represent, interpret, and predict the effect of the most influencing factors on equilibrium sorbate distribution and therefore are very welcome. Moreover, adsorption/ion-exchange/biosorption is strongly affected by the solution pH, and therefore, it is extremely important to use equilibrium models that include the effect of solution pH.
- 4. The units of the equilibrium constant of the Freundlich model ($q_{eq} = K \times C_e^{1/n}; q_{eq} \equiv mg g^{-1} \text{ or mmol } g^{-1}; C_{eq} \equiv mg L^{-1} \text{ or mmol } L^{-1}$) are $mg^{1-1/n} L^{1/n} g_{sorbent}^{-1}$ or $mmol^{1-1/n} L^{1/n} g_{sorbent}^{-1}$;

3.2.2. Biological processes

- 1. Manuscripts developed based on biological processes should clarify engineering application and implications. Batch studies dealing with limited substrates will not be considered unless new processes/kinetics pathways/models are demonstrated. Case studies need to address novel process/configuration and/or biological understanding.
- 2. Biological treatment processes in both natural and engineered environments that are applicable to the circular economy, reduced energy and carbon footprints, and improved social and environmental benefits are welcome.
- 3. Various molecular approaches (including omics) to understand microbiological processes and performance are encouraged. Sequences and microarray data should be deposited to appropriate database, with accession numbers acknowledged in the submitted manuscript.

3.3. Novel materials for environmental, chemical and energy applications

- Papers dealing with the development of sensors for the detection and quantification of organic/inorganic species should demonstrate their capabilities when working with real matrices and/or environmentally relevant contaminants' concentrations, as well as compare the results with more precise or established analytical methods (e.g., AAS, ICP, GC, HPLC, IC, etc.).
- 2. Papers dealing with "novel materials (e.g., catalysts, photocatalyts, electrocatalysts, adsorbents, membranes) or technology" are often described in the submission as "novel", i.e., a material or process that has not been previously reported. While complete characterization of the new material is expected, the majority of the paper should focus on the material's performance, including careful assessment at environmentally relevant conditions and a proper comparison with the accepted benchmark material to demonstrate a better performance or a higher efficiency. For example, a study of new adsorptive materials reporting multiple isotherms but without presenting benchmarking against common materials (e.g., activated carbon for adsorption, titanium dioxide for photocatalysis), or not performed at environmentally relevant concentrations, is unlikely to be sent for peer review. Similarly, a new synthesis method that is described as "greener" and more sustainable, but lacks widely accepted sustainability assessment metrics will be unlikely to be advanced beyond prescreening. New applications of materials should consider energy (carbon) and/or water footprints to support claims of "sustainability" or information on energy savings potential (e.g., kWh/m³). It is recommended to display the processes (catalytic, adsorption, membranes, etc.) and mechanisms using schematic illustrations (data visualization) to assist visual perception and representation of research hypothesis.

3.4. Machine learning and artificial intelligence

1. Manuscripts that adopt machine learning (ML) and artificial intelligence (AI) in modeling and prediction should demonstrate clear superiority of ML/AI over conventional approaches. Their application for real-world settings or complex systems with multidimensional features (e.g., field-scale systems or at least the prototypes) is preferred. The training dataset should be sufficiently large and the robustness of the methodology (including non-bias) should be clearly demonstrated.

4. Specific guidance on statistical analysis standards and formating rules

- 1. Given the potential problems associated with linearization of nonlinear equations and the availability of nonlinear regression tools, **it is recommended** that linear solutions to nonlinear equations be discarded (mainly for adsorption studies), in favor of fitting the nonlinear equation to untransformed data.
- 2. Often the validation of a model seems to consist of nothing more than quoting the coefficient of determination (R^2 or r^2). However, a high R^2 value does not guarantee that the model fits the experimental data well. The residual sum of squares, uncertainty of model parameters and others statistical parameters should be carefully analysed. For example, the adequacy of the mathematical models (equilibrium, kinetic, etc.) should be compared by using the F-test statistical parameter, and not by comparing only the coefficient of determination (R² or r²). As an example, F_{cal} is defined as $F_{cal} = S_R^2(A)/S_R^2(B)$, where $S^2_R(A)$ and $S^2_R(B)$ are respectively the model variances of model A and B. F_{α} and α are respectively, the critical value tabulated and the level of confidence. In general, the residual variance of the model expected to produce the better fitting is placed in denominator (model B). If $F_{cal} > F_{\alpha}$, the model corresponding to the denominator is statistically better than the other, according to the chosen level of significance (1- α = 0.95). If not, for a level of significance, the difference is not significant.
- 3. The use of Response Surface Methodologies (RSM) or other experimental design approaches will unavoidably include presentations of several tables. As these presentations are merely to show experimental design matrix and statistical analysis, they should be presented as Supplementary Information and only a concise table/figure should be included in the main text. The optimum configuration values of the parameters obtained by RSM should be verified to validate the proposed approach.
- Please use "k" (lowercase) for kinetic constants and "K" (CAPITAL LETTERS) for equilibrium constants.
- 5. In chemical equations it may be important to know the states, which are abbreviated as: (s) solid, (l) liquid, (g) gas or (aq) aqueous (in water).
- 6. Chemical reaction formulas show the process of how one thing becomes another. The right arrow (→) is the most common arrow in chemical reaction formulas. The direction points in the direction of the reaction. The double arrow (⇐) denotes a reversible reaction. The reactants become products and the products can become reactants again using the same process. Two arrows with single barbs (⇐) pointing in opposite direction show a reversible reaction when the reaction is at equilibrium. The single double arrow (↔) is used to show resonance between two molecules.

5. Specific guidance on technical guidelines

1. Authors are expected to carefully consider the list and order of authors before submitting their manuscript and provide the definitive list of authors at the time of the original submission. Any addition, deletion or rearrangement of author names in the authorship list should be made only before the manuscript has been accepted and only if approved by the journal Editor. To request such a change, the Editor must receive the following from the corresponding author: (a) **the reason for the change in author list**, (b) **written confirmation (institutional e-mail, formal letter) from all authors that they agree with the addition, removal or rearrangement**, and (c) **formal letter from the Faculty Dean supporting this addition, removal or rearrangement**. In the case of addition or removal of authors, this includes confirmation from the author being added or removed. Only in exceptional circumstances will the Editor consider the addition, deletion or rearrangement of authors after the manuscript has been accepted. While the Editor considers the request, publication of the manuscript will be suspended. If the manuscript has already been published in an online issue, any requests approved by the Editor will result in a corrigendum.

- 2. The authors are expected to adopt the best practices in literature citation. Unethical citation is a violation of publishing ethics which may result in retraction of the published articles. Authors should not disproportionately cite publications of any particular groups including their own or research groups from any particular country or region.
- 3. Please submit, with the manuscript, the names, addresses (including countries), and work email addresses of five potential referees who are outside the authors' institutions, and must not have conflict of interest with the authors.
- 4. This journal uses the Elsevier Article Transfer Service to find the best home for your manuscript. This means that if an editor feels your manuscript is more suitable for an alternative journal, you might be asked to consider transferring the manuscript to such a journal. The recommendation might be provided by a Journal Editor, a dedicated Scientific Managing Editor, a tool assisted recommendation, or a combination. If you agree, your manuscript will be transferred, though you will have the opportunity to make changes to the manuscript before the submission is complete. Please note that your manuscript will be independently reviewed by the new journal.
- 5. Please write your text in good English (American or British usage is accepted, but not a mixture of these). Authors who feel their manuscript requires English editing to eliminate possible grammatical/spelling errors and to conform to correct scientific English may use the English Language Editing service available from Elsevier's Author Services.
- 6. Highlights are optional yet highly encouraged for this journal, as they increase the discoverability of your article via search engines. They consist of a short collection of 3–5 bullet points that capture the novel results of your research as well as new methods that were used during the study (if any) with a maximum 85 characters, including spaces, per bullet point.
- 7. The authors should ensure that they have written entirely original works, and if the authors have used the work and/or words of others, that this has been appropriately cited or quoted and permission has been obtained where necessary. Proper acknowledgment of the work of others must always be given. Authors should cite publications that have influenced the reported work and that give the work appropriate context within the larger scholarly record. Information obtained privately, as in conversation, correspondence, or discussion with third parties, must not be used or reported without explicit, written permission from the source. Plagiarism takes many forms, from 'passing off' another's paper as the author's own paper, to copying or paraphrasing substantial parts of another's paper (without attribution), to claiming results from research conducted by others. Plagiarism in all its forms constitutes unethical behavior and is unacceptable. Editors have access to a Similarity Report obtained by iThenticate, which is a flexible document that provides a summary of matching or similar text in submitted work compared against a huge database of Internet sources, journals and previously submitted work, allowing editors to review matches between a

submitted work and the database. The use of a software for detecting potential plagiarism with already published works such as iThenticate (https://www.ithenticate.com/) or Turnitin (http://www.turnit inuk.com/) is suggested. It is highly recommended avoiding a similarity index above 25 %. Please be aware that theses (PhD, MSc) are not taken into account for the similarity index.

8. Submitting the same manuscript to more than one journal concurrently constitutes unethical behavior and is unacceptable. Elsevier duplicate submission check is able to detect manuscripts, currently under consideration, that are similar. Elsevier services notify the editors responsible by the manuscripts to verify whether the similarity is appropriate. In the case of confirmation, the manuscripts are immediately rejected.

Finally, we would like to emphasize that this Guidelines are not intended to discourage authors to submit their results for publication at JECE. To the contrary, we do indeed welcome and look forward to receiving well-prepared manuscripts from around the world.

Sincerely,

Executive Editors.

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