Dr. Oleg Rud

Department of Physical and Macromolecular Chemistry Faculty of Science, Charles University Hlavova 8, 128 43 Prague, Czech Republic

E-mail: oleg.rud@natur.cuni.cz

Prague, September 16, 2022

Dear Dr. David Díaz-Díaz,

In response to your e-mail from 23d August 2022, we hereby submit the revised version, of our manuscript, entitled "Water desalination using polyelectrolyte hydrogel. Gibbs ensemble modeling".

We carefully considered all reviewer comments and introduced changes in the manuscript in order to address them. Below, we provide a point-by-point response to all reviewer comments, including a brief description of the modifications introduced in response to these comments. Additionally, we provide a pdf version of the manuscript with the relevant changes highlighted in colour.

Main changes in the manuscript include:

- Minor changes in title of the article.
- The rewritten abstract and introduction.
- Added the detailed explanation of model and methods used in the study.
- Minor changes in Figures.

We also attache the pdf file reflecting the difference between the current version of the manuscript and the submitted one.

We believe that, after considering the modifications in response to reviewer comments, you will find our manuscript suitable for publication in Gels.

On behalf of all authors, with best regards

Oleg V. Rud

## Reviewer 1

- 1. The main findings of your results should be highlighted in abstract We have rewritten the abstract.
- 2. Please do not separate introduction in three sections combine with problem and technology you used and challenges and your solutions.
  - We have rewritten the Introduction section. We wanted to keep the separation of the Introduction section into the respective subsections because the Introduction is relatively lengthy, so we believe that dividing it into subsections reduces its readability.
- 3. In page 4 heading 2. (How to start with and ??). Corrected.
- 4. All formula and models should be supported with reference for instant equation 3. Corrected
- 5. In page 6, please remove the footer, it is not a book to describe issues below. Corrected. Now this sentence appears in text (in brackets).
- 6. How do you think control factors in open system such as pressure and temperature In our simulation, we control the volume of the simulation box and measure the pressure using the virial theorem. The pressure value which is depicted in the Figures assumed to be a partial pressure of the gel, which is calculated as the difference between the pressure in the gel and the pressure calculated in a separate simulation box containing only ions (with no gel). Temperature assumed to be constant and equal to 300 K, which is guaranteed by applying a Langevin thermostat.

Reviewer 2 This manuscript is about creating a new model the thermodynamic equilibrium between coexisting phases of the gel and supernate aqueous solution.

- 1. Abstract needs to re-write as and please follow the IMRAD instruction.

  We have rewritten the abstract. We believe that the abstract is much more attractive now.
- 2. There is introduction in the abstract, however, it needs to write more about the aim of this work, method, result and conclusion.

  Corrected
- 3. Avoid to use word 'we' in the abstract as well as manuscript. Corrected.
- 4. line 247 in what table?
  We meant Table 1. Corrected in text.
- 5. Where is the method of this work?

  The method idea is outlined in the paragraph "Physics behind the desalination process" and described in the section "Model and methods".
- 6. It is suggested that to carefully improve this manuscript as well as the writing and grammatical error.
  - We improved the writing style of the manuscript and corrected the grammatical errors.
- 7. Please explain more detail about the process, how the process run and how the data could be explained and become more interesting for reader.

  Added corresponding paragraph in "Model and methods" section

- 1. The full stop in the title should be revised. Noted. Revised.
- 2. The abstract needs to be revised and be more attractive. The research gap, novelty and main findings should be concisely mentioned in the abstract.
  - We have rewritten the abstract. We believe that the abstract is much more attractive now.
- 3. In this current shape, the manuscript looks like a report. The authors have to revise the flow of the context to attract the readers.
  - We have revised and changed the manuscript to be more attractive for the readers.
- 4. The manuscript must be improved by checking once again in English and technical writing.
  - We improved the writing style of the manuscript and corrected the grammatical errors.
- 5. The whole manuscript must be supported by enough recent references. Revise the whole context.
  - We added more recent references.
- 6. The beginning of the introduction part must be revised to be more attractive. Corrected. We have rewritten the Introduction section.
- 7. The authors can follow the following references to generally highlight the global contamination and environmental pollution problems at the beginning of the introduction part

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https://doi.org/10.1016/j.jwpe.2022.102847;
https://doi.org/10.1016/j.ceramint.2022.05.151;
https://doi.org/10.3390/catal12050500;
https://doi.org/10.1007/s11356-022-21160-7;
https://doi.org/10.3390/ma15134547.
Then, highlight the water desalination technologies and Gibbs ensemble (https://doi.org/10.3390/nano10020293).
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Corrected. We added the citations, which are relevant to the studied problems, in their

- appropriate places.

  8. Authors should indicate a clear gap in knowledge which this study seeks to bridge, and
  - potentially contribute to knowledge.

    The purpose of our paper is to show that desalination using polyelectrolyte hydrogels is a cheap and therefore competitive alternative to reverse osmosis. We highlighted this idea in the Introduction and Conclusion sections.
- 9. L 125-126, meaningless sentence. Revise the whole context. Corrected.
- 10. All sections/subsections titles must be revised to be expressive. Corrected. We have rewritten and improved not only the Introduction, but the sections Model and Methods, Results, Conclusions as well.
- 11. Statistical physics considerations including setup and calculations should be added.

  We rewritten the section "Model and methods" and added there a detailed explanation of our methodology.
- 12. The authors should identify the limitations of this study and the recommended future studies in the conclusion part.
  - We identified the study limitations and considered the implications and future per-

spectives of the study. We added the respective paragraphs.