Přírodovědecká fakulta
Faculty of Science

Jihočeská univerzita v Českých Budějovicích
University of South Bohemia in České Budějovice

OPPONENT'S REVIEW ON BACHELOR THESIS

Name of the student: **Ivan Khodonovych**

Thesis title: Computational study of greenhouse gas adsorption on biochar
Supervisor: Dr. Babak Minofar, Ph.D.

Referee: Dr. David Řeha, Ph.D.
Referee`s affiliation: University of South Bohemia, Institute of Chemistry

	Point scale[1]	Points
(1) FORMAL REQUIREMENTS		
Extent of the thesis (for bachelor theses min. 18 pages, for masters theses min. 25 pages), **balanced length of the thesis parts** (recommended length of the theoretical part is max. 1/3 of the total length), **logical structure of the thesis**	0-3	2
Quality of the theoretical part (review) (number and relevancy of the references, recency of the references)	0-3	1
Accuracy in citing of the references (presence of uncited sources, uniform style of the references, use of correct journal titles and abbreviations)	0-3	2
Graphic layout of the text and of the figures/tables	0-3	1
Quality of the annotation	0-3	2
Language and stylistics, complying with the valid terminology	0-3	0
Accuracy and completeness of figures/tables legends (clarity without reading the rest of the text, explanation of the symbols and labeling, indication of the units)	0-3	2
Formal requirements – points in total		10
(2) PRACTICAL REQUIREMENTS		
Clarity and fulfillment of the aims	0-3	2
Ability to understand the results, their interpretation, and clarity of the results, discussion, and conclusions	0-3	1
Discussion quality – interpretation of the results and their discussion with the literature (absence of discussion with the literature is not acceptable)	0-3	2
Logic in the course of the experimental work	0-3	3
Completeness of the description of the used techniques	0-3	1
Experimental difficulty of the thesis, independence in experimental work	0-3	3

[1] Mark as: 0-unsatisfactory, 1-satisfactory, 2-average, 3-excellent.

Quality of experimental data presentation	0-3	2
The use of up-to-date techniques	0-3	3
Contribution of the thesis to the knowledge in the field and possibility to publish the results (after eventual supplementary experiments)	0-3	2
Practical requirements – points in total		19
POINTS IN TOTAL (MAX/AWARDED)	**48**	**29**

Comments of the reviewer on the student and the thesis:

The author of the thesis studied adsorption of greenhouse gases on the biochar surface using method of classical Molecular Dynamics simulations. Particularly the focus of this thesis was to study the mechanism of physisorption of selected greenhouse gases (CO_2, N_2O, CH_4) to the two models of biochar (smaller and larger) with different functional groups (-OH, $-COO^-$, -COH, $-OCH_3$). As a result a different characteristic of the physisorption of studied gases on both biochar models were observed. The simulations also allowed to analyze detail binding sites of gas molecules at biochar model, leading to the conclusion, that different gases prefers to bind to different parts of biochar (flat part or side part with functional groups). These results are useful, as they can be used for prediction of biochar materials with more desirable adsorption characteristic for particular gas. This would have application in environmental chemistry for reduction of greenhouse gases.

The structure of the thesis is acceptable and the most of the stated objectives were fulfilled and addressed in Conclusions, however I have problem with the last objective *"How pyrolysis temperature and functional groups on the surface of biochar molecules can influence the adsorption of greenhouse gas? "* and the way how it was addressed in Conclusions, since there is no relation between author's computational work in the thesis and pyrolysis temperature. This definitely should not have been set as one of the thesis aim, and therefore it is not valid conclusion.

The biggest problem of this thesis is the quality of language. The construction of English sentences is very poor and many sentences are completely incomprehensible. Just one example of such a poor sentence: *"All these forces are simply rated from the mechanical model will be mentioned in the previous chapter."*

The theoretical part of the Methods contain introduction to the methods used for this work (Molecular mechanism, molecular dynamics, periodic boundary conditions, etc.) and describe them quite in detail, however there were several factual mistakes, like *"The force acted on the system is calculated by applying Newton's equations of motion"*, while in reality we are calculating acceleration from forces (calculated from the forcefield) by aplying Newton's equations of motion. The chapter "Slab geometry simulations" is completely incomprehensible.

In the chapter Methodology author describe in very detail all the operations with different modules of the program and all the files used. This detailed description is almost like a short reference guided and manual and can be used as a tutorial for the students. The inclusion of such a detail description is completely fine for the Bc thesis, however in my opinion author sometimes went in too much detail, when describing how he get access in computer grid (Metacentrum) and how to submit the job in the queue. Such detailed info depends on the actual computer system used, queuing software, etc. and it is unique only for the student circumstances and should not be part of the thesis. There also omitted some information about simulations themselves, like temperature of the simulations.

The general graphical layout of the thesis is OK, but author did not follow prescribed fonts size (font size 14 is used instated of 12). This has resulted in the artificial inflation of the length of thesis by approximately 25%. Thus the length of the thesis (if the thesis would be written in the prescribed fonts size and line spacing) just slightly exceeds 20 pages, which is still more then the prescribed minimal length (18 pages).

Suggestions and questions, to which the student has to answer during the defense. Mistakes, which the students should avoid in the future:

1. What is the slab geometry, when would you use it and how it is connected to the periodic boundary conditions?
2. How would you construct the simulation box for simulation in the bulk water and how simulation box would be constructed for simulation of water - air (or vacuum) interface?
3. What type of simulation box have you used during your work (box for bulk water simulation, box for simulation of water-air interface or both type of the boxes) and why?
4. What are differences between NVT and NpT simulations and which of them you would use for which type of the simulation box (box for bulk water simulation and box for the simulation of water-air interface)?
5. Can you discuss a possible reasons why CO_2 prefers to interact with central part of biochar while N_2O would interact with the sides of the biochar (as it is observed according Figure 9)?

Conclusion:

In conclusion, I

r e c o m m e n d

the thesis for the defense and I suggest the grade **Good** .[2]

In **Ceske Budejovice** date **29.1.2020**

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signature

[2] You can suggest a grade, which can be modified during the defense based on the presentation. However, if the reviewer is not present at the defense, the grade will not be counted. Grades: excellent (1). Very good (2), Good (3), Unsatisfactory/failed (4).