Reviewer report of PhD thesis

M.Sc. Mehran Sajad:

„Production of light olefins via (oxidative) dehydrogenation of light alkanes over nontraditional heterogeneous catalysts“

PhD thesis of Mehran Sajad is focused on a detailed investigation of three catalytic systems (supported alkali chlorides, hexagonal boron nitride and encapsulated Pd nanoparticles within MFI, IPC-2 and IPC-4 zeolites) for (oxidative) dehydrogenation of light alkanes (ethane, propane) to produce light olefins. Attention is paid to the structure-activity-stability relationship and the phenomena influencing the catalytic activity. Parameters such as chemical composition, crystallinity, textural properties, reaction conditions, pretreatment/regeneration effect, stability, activity and selectivity were investigated. Topic of PhD thesis is actual since light olefins are essential feedstock for industry processes such as the production of polymers, oxygenates etc. and currently used methods are carried out at severe reaction conditions at high temperatures with significant CO_2 emission.

The PhD Thesis of Mehran Sajad is written in English and elaborated on 62 pages as commented set of published papers. It contains the original results, partly accepted by scientific community in five articles in peer-reviewed impacted journals. I would like to highlight that Mr. Mehran Sajad is the first author of four publications. Moreover, his work “Imidazolium-type ionic liquid-assisted formation of the MFI zeolite loaded with metal nanoparticles for hydrogenation reactions” was published in *Chemical Engineering Journal* which is journal with excellent ranking (1st decil in Chemical Engineering and also in Environmental Engineering, WoS) and although it was published in January 2021, it already has 10 citations. Remaining articles were published in *Catalysts* (Q2), *Applied Materials Today* (Q1) and *Scientific Papers of the University of Pardubice*. Last paper will be submitted in *Reaction Chemistry & Engineering* (Q1).

The dissertation is logically divided into subchapters with respect to the focus of thesis. Objectives of thesis are clearly and comprehensibly described similarly as the obtained results, which are thoroughly compared with literature. I liked the chapter 6.3, the procedure and the experiments performed to clarify the contribution of homogeneous and heterogeneous reactions to oxidative dehydrogenation, where boron nitride was used as a catalyst.

From a formally point of view, dissertation is written in a good English. Overall, I would characterize the work as very successful.

The following remarks are formulated as the topics for discussion during the thesis defense:

- The alkane conversion was determined from corresponding alkane molar flow in the inlet and outlet gas mixture (Eq. 1). How was the alkane molar flow at the reactor outlet determined?

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- It is stated in the paper V that the catalytic experiments were performed in a plug flow fixed-bed tubular shaped reactor using 100 mg of catalyst. Reactors used for presented experiments had id from 9 to 15.5 mm. Can you discuss if the approach to plug flow is sufficient and criterions for negligible axial dispersion and plug flow velocity profile are fulfilled? In which way can these phenomena influence conversion and selectivity?
- Were checked that the reaction rate is not influenced by internal and external diffusion limitations? For instance, total flow rate of 20 ml min^{-1} in reactor with id of 15.5 mm resulted in quite low velocity in catalyst bed (Fig. 38) and catalysts grains are quite big (0.3- 0.5 mm).
- To interpret the results of the catalytic tests, it is necessary to mention the error of conversion of alkanes.
- The PhD candidate used a number of experimental methods and collected a relatively large set of experimental data in his work. What works did he perform himself?

Formal remarks

- Page numbering is missing.
- In the Abbreviations / Nomenclature part, it will be useful to mention all the symbols used even though they are explained under the relevant equations.
- Variables in the text should be italicized.
- In lattice parameter a = 0.38907, unit is missing (text regarding to Eq. 6).
- The labels of Figure 33 are illegible.
- There is an incomplete sentence at the end of the paragraph after Fig. 33.

Conclusion

I declare that I studied the presented dissertation thesis written by Mehran Sajad and that the thesis meets all requirements of the doctoral thesis. Therefore, I recommend it for the doctoral thesis defense.

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