Poznań, 15.11.2023

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REVIEW

The doctoral dissertation of Mr. Michał Jędrzejczyk, M.Sc. Eng., entitled

"ESTABLISHMENT OF BEST PRACTICES IN REDUCING UNCERTAINTIES IN MULTIGROUP CROSS-SECTIONS WITH BAYESIAN METHODS"

1. FORMAL BASIS FOR THE PREPARATION OF THE REVIEW

The formal basis for the review was the *Work Agreement* regarding the preparation of a review in the proceedings for awarding a PhD degree to Mr. Michał Jędrzejczyk, concluded in Otwock on October 17, 2023, in which the National Center for Nuclear Research is represented by Dr. Hab. Aneta Malinowska – Scientific Secretary.

The review was prepared based on the copy of the doctoral dissertation of M.Sc. Michał Jędrzejczyk provided both in an electronic (pdf file) and traditional forms.

The review was conducted in accordance with Article 187 of the Act of July 20, 2018, Law on Higher Education and Science. According to article the doctoral dissertation presents the candidate's general theoretical knowledge in the discipline or disciplines and the ability to independently conduct scientific work. The subject of the doctoral dissertation is an original solution to a scientific problem. A doctoral dissertation may be a written work, including a scientific monograph, a collection of published and thematically related scientific articles.

The scope of this review includes assessing whether the doctoral dissertation meets the criteria outlined in the Act, as well as the evaluating the relevance of the topic undertaken, the correctness of the formulated goal, verification of the research methodology used, research results presented in the work, conclusions formulated and the ability of the PhD candidate to independently conduct scientific work.

2. GENERAL CHARACTERISTICS AND EVALUATION OF DISERTATION

Doctoral dissertation of M.Sc. Michał Jędrzejczyk is a theoretical research work. The dissertation was prepared in English. The work has 120 pages and consists of 6 sections preceded by contents, list of figures, list of tables, nomenclature and summary in Polish and English. The above organizational part of the PhD thesis takes up 19 pages. The work ends with a list of references containing 50 items. Unfortunately, the list of literature does not include any works by a doctoral student. The literature is dominated by articles from international journals such as: *Progress in Nuclear Energy, Nuclear Engineering and Design, Nuclear Science and Engineering, Nuclear Technology, Reliability Engineering and System Safety, Annals of Nuclear Energy, Energies, Atmospheric Environment, Mathematics of Computations, Technometrics, International Journal of Forecasting, Biometrica, Theory of Probability and Its Applications, Journal of the American Statistical Association, Journal of statistical Software, Journal of Computational Physics*. The bibliography also contains chapters in monographs, user manuals for appropriate software, research reports and conference materials.

In the introduction (10 pages) the author formulated two objectives and one hypothesis of the work. The objectives are as follows:

1) "*to compare the algorithms GLLS, MOCABA, and SMC-ABC and check whether the rigorousness and universality of SMC-ABC are worth the additional computational power required to execute the algorithm*",

2) "*to present a validation technique that hasn't been applied yet in nuclear engineering. The method is based on the so called "synthetic experiments", which are computationally generated data used in place of experiments*".

The proposed hypothesis is: "*There exist improvements in the methodology of conducting Bayesian calibration of neutron cross-sections, which allow for obtaining improved results with a more reliable validation*".

Both the objectives of the work and the hypothesis were defined clearly and precisely. The problem of reducing uncertainties in multigroup cross-sections is important and constitutes an appropriate challenge for a doctoral thesis.

In Section 2 (14 pages) the author described three Bayesian calibration methods GLLS, MOCABA, and SMC-ABC, which in the PhD thesis were compared in terms of neutron cross-section calibration performance.

In Section 3 (7 pages) an overview of the simulation software used for multiplication factor k_{eff} calculations is presented.

The application and comparison of the GLLS, MOCABA, and SMC-ABC algorithms in calibrating 23 cross-sections that contribute significantly to k_{eff} uncertainties in highly enriched uranium fast systems are presented in Section 4 (29 pages). Also in this section a validation procedure of the synthetic experiment is described.

In Section 5 (28 pages) the most effective algorithm, namely MOCABA is applied to calibrate 1904 cross-sections across 34 thermal systems. Additionally, an enhanced synthetic cross-section validation procedure is introduced, along with an examination of the influence of uncalibrated cross-sections on Bayesian calibration results. The consequences of neglecting the influence of uncalibrated parameters are also investigated through the formulation of appropriate inverse problem.

A summary of the work is presented in Section 6 (5 pages). The main part of this Section is description of a step-by-step procedure for Bayesian calibration of neutron cross-sections, incorporating the best practices established in sections 4 and 5.

The assessed doctoral thesis falls within the discipline *"Natural sciences, physical sciences"*. In my opinion, the planning and writing of the PhD thesis were executed properly.

3. EVALUATION OF THE SUBJECT SELECTION OF THE DISSERTATION

The research topics of M.Sc. Eng. Michał Jędrzejczyk are associated with the issues of reducing uncertainties in experimental data used in nuclear power engineering, and the search for unconventional theoretical methods of improving the data quality. The dissertation focuses on applying approximate Bayesian computation to reduce uncertainty in multigroup U-235 neutron cross-sections. The calculations aim to determine the multiplication factor (k_{eff}) value, reduce its uncertainty, and improve knowledge of neutron cross-sections, which is crucial for operation, safety, and economic reasons.

The subject of the doctoral thesis is current and important from the point of view of the quality of nuclear reactor calculations. The presented calculation method is a valuable step not only on the way of reduction of the uncertainty of the integral experiment parameters like k_{eff} but plausibly it might be use for calibration of continuous energy neutron cross-section libraries.

I believe that the doctoral thesis submitted for review by M.Sc. Eng. Michał Jędrzejczyk fits well into the issues of nuclear reactors core design and the results obtained should have an impact on the core strength and economic results.

The topic of the work was chosen correctly, and the formulated goal of the work has a significant practical aspect.

4. SOLVED SCIENTIFIC ISSUES

The most important and original issues constituting a scientific novelty of the work are:

1. Proposing a best-practices algorithm for reliable calibration of neutron cross-sections.
2. Demonstrating that computationally expensive procedures like SMC-ABC are not necessary; similar results can be obtained with MACABA and GLLS methods.
3. Identifying a disadvantage of the MOCABA procedure, where even a minor skew in the prior distribution can result in noticeable differences in posterior keff.
4. Showing that although cross-section uncertainties may be reduced during Bayesian calibration, it's not guaranteed they will converge to true values.
5. Improving validation procedures in nuclear engineering by proposing a synthetic experiment validation procedure.
6. Demonstrating that neglecting the uncertainty of uncalibrated input parameters in Bayesian statistics can lead to incorrect computational results.

The research challenge undertaken was a complex task. A huge number of advanced calculations were carried out, and the way they were planned and executed indicates a well-thought-out and consistently implemented research procedure. The presented calculations confirm the PhD student's good knowledge of computational techniques and appropriate software. The content of the dissertation proves that he is well-placed in the subject matter. The adopted computational methods and advanced software and hardware (Świerk Computing Center) allowed the PhD student to achieve the assumed research goals.

I did not find any significant shortcomings and I rate the knowledge of the subject matter highly. In my opinion, the goals of the doctoral dissertation have been achieved and its thesis has been proven.

5. COMMENTS / QUESTIONS

While reading the dissertation, I have drawn attention to the following issues:

- How can the credibility of the calculation results be assessed; Is it possible to obtain experimental confirmation in Polish laboratories?
- Which of the three basic sources of uncertainty, i.e. model discrepancy, measurement uncertainty (i.e. uncertainty of the reference experiment), and error stemming from uncertainty in unadjusted parameters, contributes most to the total uncertainty, and how can its contribution be reduced?
- In traditional uncertainty analysis, the final result consists of three numbers: the expected value, its total uncertainty and the confidence level of the total uncertainty (usually 95%).

Is there any guidance on preferred values for the total uncertainty and its confidence level with respect to the multiplication factor k_{eff}?

- Are Bayesian methods related to machine learning and artificial intelligence? If so, to what extent?
- What is the most important advantage and most important disadvantage of Bayesian methods in engineering applications?

Minor remarks and editorial suggestions that came to mind while reading the PhD thesis:

- There is no need to present general information in the doctoral dissertation. For example, subsection 1.1 is not necessary. Moreover, the quality of Fig. 1 in this subsection is low.
- On page 15 it is stated that the dissertation is based in part on the publication "Application of Approximate Bayes Calculations to Reduce Uncertainty in Multigroup 235-U Sections Using ICSBEP Experimental Data" by Jędrzejczyk M., Kopka P., Foad B., and Kozłowski T., but there is no information where and when this publication was published or where it has been accepted for publication.
- On page 81, the first sentence in section 5.1 is the same as the sentence a little earlier on the same page. There is no substantive justification for such repetition.

6. CONCLUSIONS

M.Sc. Eng. Michał Jędrzejczyk became interested in important issues related to the innovative computational methods of reducing uncertainties in multigroup cross-sections and multiplication factor. Research work has been undertaken, which can lead to the development of a nuclear power engineering. The methods and calculation results should be considered valuable, current and original from the point of view of further development of procedures for performing neutron-physical calculations of nuclear reactors.

The PhD student demonstrated his ability to independently formulate scientific problems and plan research leading to their solution, together with the presentation of results and their interpretation.

In my opinion, the doctoral thesis of M.Sc. Michał Jędrzejewski meets the conditions outlined in the Act of July 20, 2018, Law on Higher Education and Science (Journal of Laws of 2018, item 1668), and thus I apply to the *Doctoral Committee of National Center for Nuclear Research Świerk* for admission to the next stages of the doctoral procedure.

PODSUMOWANIE I WNIOSEK KOŃCOWY

Praca doktorska mgr inż. Michała Jędrzejczyka dotyczy poszukiwania innowacyjnych metod obliczeniowych mających na celu zmniejszenie niepewności eksperymentalnie wyznaczonych przekrojów czynnych reakcji jądrowych wywoływanych przez neutrony oraz zmniejszenia niepewności ważnego w energetyce jądrowej makro-parametru jakim jest efektywny współczynnik mnożenia neutronów. Zastosowanie zaawansowanych metod wnioskowania bayesowskiego do realizacji wyżej wymienionych celów ma w dużym stopniu charakter oryginalny. Uzyskane wyniki są wartościowe i mogą przyczynić się do poprawy dokładności obliczeń neutronowo-fizycznych rdzeni reaktorów jądrowych.

Doktorant wykazał się umiejętnością formułowania problemów badawczych oraz realizacji obliczeń w sposób prowadzący do ich rozwiązania. Przedłożona dysertacja świadczy o umiejętności prezentacji uzyskanych wyników i ich interpretacji.

Uważam, że praca doktorska mgr inż. Michała Jędrzejewskiego spełnia wymagania określone w ustawie z dnia 20 lipca 2018 r. Prawo o szkolnictwie wyższym i nauce (Dz. U. z 2018 r. poz. 1668) i wnioskuję do Komisji Doktorskiej Narodowego Centrum Badań Jądrowych w Świerku o przyjęcie rozprawy i dopuszczenie jej do publicznej obrony.