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**Review of doctoral dissertation
by Reddy Babu Siddareddy, MSc Eng
entitled: "Transient engine simulations using the stochastic reactor model
for driving cycle performance studies"**

The basis for the review of the doctoral dissertation by Reddy Babu Siddareddy, MSc, is a letter from the Chair of the Discipline Council for Environmental Engineering, Mining and Power Engineering at the Silesian University of Technology, Prof. Krzysztof Labus, PhD.

A. Introduction

In the era of transport decarbonisation and the implementation of restrictive Euro 7 standards, the paradigm of powertrain modelling is undergoing a radical transformation. The adaptation of new energy carriers is forcing a shift in the focus of simulation from the offline conceptual stage to the verification and tuning of control systems in a hardware-in-the-loop (HiL) and model-in-the-loop (MiL) environment. In this new research regime, the fundamental technological barrier is the integration of complex chemical kinetics mechanisms, necessary, among other things, for precise emission estimation, while maintaining the requirement for real-time calculations.

In light of the above, the submitted dissertation addresses an important and topical issue, namely the need to optimise internal combustion engines in terms of stringent exhaust emission standards under real operating conditions, which makes the topic chosen by the doctoral student, Reddy Babu Siddareddy, MSc, Eng, should be considered important not only from the perspective of cognitive research, but also due to its high application potential.

B. Scope of the dissertation

The doctoral dissertation submitted for evaluation by REDDY BABU SIDDAREDDY, MSc, Eng, is entitled **"Transient engine simulations using the stochastic reactor model for driving cycle performance studies"**.

The supervisor of the dissertation is Prof. Wojciech Adamczyk, PhD.

The dissertation consists of 118 pages, comprising 5 chapters, an abstract, a list of symbols and abbreviations, a list of 15 publications co-authored by the doctoral student, and a bibliography of 106 items.

In the first chapter, the doctoral student defines the scientific background of the topic, the rationale for undertaking the research problem, as well as the objectives and scope of the dissertation. The author identifies the main research problem, according to which the existing stochastic reactor

model (SRM) is precise but has not yet been adapted for real-time simulation or integrated with control standards such as FMI/FMU.

The second chapter constitutes a literature review, containing in particular a critical analysis of the available literature on the simulation of internal combustion engines in transient states and the use of FMI/FMU standards and MiL/HiL platforms in automotive engineering. The FMI (Functional Mock-up Interface) standard and FMU units are discussed in detail as key technologies enabling the exchange of models between different programming platforms. This chapter also defines MiL and HiL test environments, explaining their role in the verification of control algorithms and virtual calibration of engines prior to the physical testing phase.

In the third chapter, concerning simulation methods and tools, the PhD student presented his own simulation toolchain, including the implementation of a stochastic reactor model (SRM). A key part is the description of the technical integration of the SRM code (written in Fortran) with a C++ wrapper compliant with the FMI 2.0 standard, which enables real-time simulations. The architecture of a meta-model based on artificial neural networks (ANN) is also presented, serving as an ultra-fast surrogate for the physical model.

Chapter 4 constitutes the crucial part of the work, in which the author presents, among other things, the validation of the developed tool and the simulation results for various engines. The author also demonstrates the possibilities of co-simulation of the engine with the exhaust gas treatment system (SCR) and compares the results of the ANN meta-model with the physical model, demonstrating high accuracy with a significant reduction in calculation time.

The work concludes with Chapter 5, which contains a summary and final conclusions. It has been confirmed that SRM integration via FMI/FMU allows deterministic simulation on dSPACE (MiL/HiL) platforms. The chapter also points to potential directions for further work, such as the use of the tool in the concept of digital twins or the optimisation of alternative fuel drive systems.

C . Evaluation of the dissertation

1. In the reviewer's opinion, the research topic addressed in the dissertation is important, interesting and in line with the latest global research trends in environmental engineering and energy, making a significant contribution to its development. The clear structure of the study demonstrates a systematic approach to the analysed issue. The doctoral student has demonstrated a broad cognitive horizon, skilfully operating the conceptual apparatus of measurement techniques and mathematical modelling.
2. The dissertation proposes an original, innovative solution consisting in the development of a novel methodology for system integration and architecture (toolchain), which allows for the application of advanced combustion chemistry in real-time simulations.
3. The methodology applied deserves recognition for its interdisciplinary nature, combining thermodynamics, combustion chemistry and software engineering.
4. The dissertation is not limited to model validation, but provides specific conclusions on the impact of gas quality on emissions, which is crucial in the context of decarbonisation.

5. It is worth noting that the PhD student not only combined the engine with the exhaust system model, but also performed a sensitivity analysis of the physical parameters of the catalyst.

6. From a technical point of view, the way in which the author solved the problem of integrating legacy code with modern standards deserves great recognition. The author developed a proprietary wrapper in C++ compliant with the FMI standard for the SRM solver written in Fortran. This made it possible to compile the model into a dynamic library (DLL/SO) and implement it directly in industrial real-time platforms, which was not possible before.

7. In the summary of his work, the doctoral student clearly positions his tool as a technological basis for Digital Twins. The created 'physics-based driving cycle simulator' can be used not only for the development of controllers, but also as a virtual sensor in a vehicle or a tool for predictive maintenance, which goes beyond standard HiL applications.

8. The presented research material is characterised by scientific maturity, which predestines it for dissemination in the global scientific community. Its quality meets the standards of highly rated international specialist journals.

D. Critical and debatable comments

- The neural network-based model is trained on the results from the physical model (SRM) rather than on experimental data. This means that the ANN replicates the model's errors and cannot function as a standalone tool without first running a full physical simulation.
- The choice of artificial neural network architecture, with hidden layers containing 64 and 128 neurons, should be justified, as the correctness and accuracy of the calculation results generated using artificial neural networks strongly depends on the topology (architecture) of the network.
- Why is the model based on an artificial neural network introduced in subsection 3.7 on page 36 treated as a meta-model?

This issue should be justified in more detail.

- The inputs and outputs used in neurocomputing have not been clearly defined.
- The amount of training and test data used in the neural network training process is not specified.
- I suggest that further development should focus on the implementation of a flame extinction model, which will significantly improve the accuracy of hydrocarbon emission predictions under cold start conditions, which are key to Euro 7 standards and future regulations.

E. Specific comments

- The work has been prepared with care. Minor linguistic and stylistic errors do not detract from its substantive value.
- Some acronyms, e.g. NRMM, RMSE, EDGAR, have been omitted from the Abbreviations section.
- ReLU stands for Rectified Linear Unit instead of Reflective Linear Unit (p. 37).
- When discussing the artificial neural network model, the doctoral student uses the term second layer instead of hidden layer.

F. Final conclusion

The work has been conducted reliably, and the results obtained and the software created constitute a modern research tool, ready for use in industry.

The doctoral dissertation of Mr Reddy Babu Siddareddy, MSc, Eng entitled "Transient engine simulations using the stochastic reactor model for driving cycle performance studies" contains an original and important formulation and solution of a scientific problem for environmental and energy engineering, as well as an original application of the results of his own scientific research in the economic sphere, in line with current global research trends. The assessed work, therefore, constitutes a significant contribution to the development of the represented scientific discipline.

The doctoral student has demonstrated general theoretical knowledge in the scientific discipline of environmental engineering, mining and power engineering. The work constitutes a well-thought-out, logical and coherent whole, confirming the doctoral student's ability to conduct independent scientific work.

I believe that the reviewed dissertation by MSc Eng. Reddy Babu Siddareddy meets the statutory requirements for doctoral dissertations defined in the relevant regulations.

In view of the above, I hereby request that it be admitted for public defence at the Faculty of Energy and Environmental Engineering at the Silesian University of Technology.

[signature]: Jarosław Krzywański