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RECENZJA

rozprawy doktorskiej mgr. inż. Reddy'ego Babu Siddareddy'ego pt. *Transient engine simulations using the stochastic reactor model for driving cycle performance studies*

Podstawę opracowania stanowi pismo Przewodniczącego Rady Dyscypliny Inżynieria Środowiska, Górnictwo i Energetyka Politechniki Śląskiej, prof. dr. hab. Krzysztofa Labusa z dnia 31 października 2025 roku.

General characteristics of the dissertation

The doctoral dissertation authored by **Reddy Babu Siddareddy**, entitled *Transient engine simulations using the stochastic reactor model for driving cycle performance studies,* was written in English as a typescript at the Silesian University of Technology in 2025. The supervisor of the work is Prof. Wojciech Adamczyk, and the industry supervisor is Dr Michał Pasternak. Notably, the doctoral procedure follows the so-called implementation doctorate scheme, which has some relevance for my final assessment of the dissertation.

The dissertation has 118 pages and is correctly structured. It includes an introduction with motivation and research objectives, a literature review, a description of the applied methodology and developed tools, followed by the presentation of simulation results and their discussion, and finally a summary. The dissertation lacks a typical conclusion section.

The thesis focuses on the transient simulation of internal combustion engines for the prediction of combustion behaviour, fuel consumption and exhaust emissions during driving cycles such as WLTP and NRTC. To this end, the candidate developed and applied a simulation toolchain in which in-cylinder processes are captured by SRM with tabulated chemistry. SRM is integrated into MiL and HiL environments using the FMI/FMU standard.

There are also additional research tasks, such as replacing SRM with an ANN model and simulation of the aftertreatment system. The research covers both spark-ignition and compression-ignition engines. It also addresses cold-start behaviour. In addition, the author uses various fuels: diesel, natural gas, gasoline, and ammonia as an alternative non-carbon fuel.

Assessment of the dissertation topic

The chosen topic of the dissertation, in my opinion, is highly relevant, up-to-date, and well-justified in the context of current powertrain development trends and regulatory requirements. Reliable prediction of exhaust emissions under realistic, transient operating conditions is today a key engineering and scientific challenge, closely linked with tightening emission standards. Simulations are also grounded by the need to reduce development costs, while the complexity of powertrain systems is constantly increasing. Experimental testing alone is no longer sufficient, as it is expensive, time-consuming, and often limited in flexibility. Therefore, advanced simulation tools are gaining an increasingly important role, efficiently supporting the scope of experimental work.

In this light, the developed transient-capable simulation framework based on SRM, integrated within MiL/HiL environments, represents a well-targeted research direction. Equally important is the optimisation of models to ensure both computational speed and high accuracy, supported by tabulated chemistry and efficient handling of transient engine parameters. The use of machine learning, including ANN meta-models, further increases model autonomy and allows ultra-fast predictions, which is especially valuable in real-time applications. The possibility of using such models for engine calibration is extremely beneficial, particularly when considering the diversity of presently used and emerging fuels, including low-carbon and alternative options.

The topic fits perfectly into the concept of developing digital twins of engines and powertrains, which today play a crucial role in optimisation of operation, improvement of economic efficiency, environmental performance, and transport or energy safety. Finally, the topic is not only scientifically interesting but also highly applicable, addressing real needs of modern engine technology and supporting the transition towards cleaner and smarter propulsion systems.

Assessment of the research methodology

My assessment of the applied research tools is very positive. The doctoral candidate has demonstrated strong competence in the field of research tools and simulation environments used in modern engine studies. His work shows not only confident and independent use of advanced modelling software, but also the ability to develop, adapt, and integrate different tools into one consistent simulation framework. He mastered SRM and its practical implementation, including the use of tabulated chemistry, transient parameter handling, and detailed combustion and emissions modelling. At the same time, he successfully applied the FMI/FMU standard, which requires advanced technical skills related to model export, real-time execution, data exchange and communication between platforms. An important strength of his work is the effective integration of several subsystems, such as engine models, MiL/HiL environments, aftertreatment modules and ANN-based models, into one working toolchain. This means the candidate is not only a user of existing software, but also a developer capable of building advanced, multi-level simulation structures. The thesis shows that he can design simulation procedures, manage complex model architectures and solve technical problems.

Even though the candidate mastered the simulation tools, the scattered research topics and the incomplete coherence of the research raise my concerns. Although the author covers many valuable aspects, the work sometimes gives the impression of being overly broad, combining different engine types, various fuels, several operating conditions, and multiple modelling approaches within one framework. This diversity may suggest an attempt to demonstrate too many capabilities at once, which comes at the expense of a clearly defined, unified research endeavour, an attribute expected of a PhD thesis. The *Results and discussion* section, central to the thesis, places stronger emphasis on the presentation of individual studies than on the development of a coherent research path. In other words, the candidate presented everything he had, but more in a demonstrative form than as a systematically investigated problem.

A more strictly focused and consistently structured methodological concept could strengthen the scientific message. Importantly, the research results disseminated in the PhD thesis should be described in sufficient detail to allow their replication and validation by others. It is also evident from subsection 1.2 that the objectives of the dissertation are predominantly technical and engineering-oriented, while the strictly scientific dimension is somewhat lost in the background. To some extent, this may be justified by the implementation doctorate scheme.

Assessment of the dissertation content

The following section provides a critical assessment of the dissertation content. My remarks are intended to support a scientific discussion and to indicate areas where the dissertation could be further strengthened.

Although Chapter 2 contains useful information on available simulation tools and offers a structured overview of existing modelling environments, it functions primarily as a descriptive survey and would benefit from a more developed critical literature review. Even the author notes at the bottom of page 8 that it "provides a brief overview of commonly used simulation tools...", which accurately reflects its character.

However, in a doctoral dissertation, the reader typically expects not only a presentation of tools, but also a deeper, analytical synthesis of the state of the art. In particular, it would be desirable to discuss what the current level of knowledge is regarding combustion and emission simulation under transient conditions, what has already been achieved, and what challenges remain open. The reader would also benefit from learning which models are commonly used by other researchers to address similar problems, what accuracy they provide, and where their limitations lie. Questions such as which emission components can currently be predicted reliably, which still pose difficulties, and why, deserve clearer attention.

In this sense, Chapter 2 would gain significantly from extending the discussion towards a more comprehensive and critical summary of the existing knowledge base and remaining research gaps.

Subsection 3.5.3 *Uncertainty quantification in transient simulations* provides only a limited quantification of uncertainty and focuses on the typical error level in research. Table 3.2 contains interesting information on emission estimation uncertainty from different studies or recommendations, but the caption is misleading. This subsection would be more appropriate in a state-of-the-art review, where one critically evaluates the accuracy of different models against specific applications.

When reading the research section (Chapter 4), one may feel that the individual subchapters are largely self-contained studies. This shows the richness and diversity of the work, but it also means that the subsections sometimes read as separate research pieces rather than parts of one coherent investigation. The fact that different engines and fuels are analysed is not a problem in itself, since the declared aim of the thesis is methodology verification. However, difficulties appear when the level of model simplification and the analytical approach differ significantly between sections. As a result, direct comparison of results becomes difficult. Different datasets are used and evaluated with different criteria, and the links between the individual parts are not always clearly explained. In practice, the strongest common feature is the use of the developed simulation tools in various case studies.

The stages of research and the analytical approaches are not fully consistent and vary in their level of detail. Instead of limiting the amount of presented data and focusing on their thorough interpretation, the author appears to have attempted to include almost every available result, rather than concentrating on a clearly defined scientific problem. More detailed remarks follow.

In Section 4.1, the author states that the presented studies correspond to works [24–27], yet later sections reference additional publications. Furthermore, publication [27] appears to be identical to [44]. In Section 4.3, "reference engine data" are mentioned, but neither the thesis nor the publication [44] explains their origin. It is unclear whether these are measured data, how measurements were performed, or what their uncertainty is. The reader knows only that some unspecified reference data exist. It is also not stated what kind of toolchain was used for the simulations: HiL or MiL.

In many cases, the simulation tasks are carried out correctly, but the results are presented with limited discussion. For example, Fig. 4.6 shows a comparison of emissions at selected operating points, yet the analysis is restricted mainly to indicating which values are overestimated and which are underestimated, without further interpretation. Although the total simulated emissions of CO and HC in Section 4.3.4 are close to the reference values, in the middle of the cycle (Figs. 4.13 and 4.14) the underestimation reaches almost 50%. The author does not explain why CO and HC deviate so significantly, while NOx predictions remain accurate. There is no detailed investigation of when and why these discrepancies occur. This naturally raises the question of why the candidate did not attempt to improve model calibration.

The analysis of emission variability based on the data from Subsection 3.5.3 is also questionable. Subsection 3.5.3 presents typical emission estimation errors reported in various studies, including simulation-based ones, but these values are not necessarily appropriate for the engine research presented in this thesis. At this stage, the work would benefit from including results of several repeated emission measurements of a real engine under WLTP conditions. The largest discrepancies would likely appear under dynamic engine operation.

In Section 4.4, the CNG engine is simulated using a simplified (smoothed) WLTP cycle. Emission results, especially for NOx, CO, and HC, obtained under a less dynamic cycle cannot reasonably be compared with those from a fully dynamic one. Furthermore, in Section

4.3 emission limits are not discussed at all, while in Section 4.4 they are analysed in detail, although the thesis focuses on cylinder-out emissions and legal limits apply to complete powertrains, including aftertreatment systems. Additionally, emissions in these sections are presented in different domains: grams vs. grams per kilometre.

In Section 4.5, another CNG engine is analysed under NRTC conditions, however with a speed profile different from that previously shown in the methodology section (see Fig. 3.7). Model validation at steady conditions clearly shows systematic emission errors, yet there is no attempt to calibrate the model. The comparison in Fig. 4.54 reveals substantial torque discrepancies throughout the cycle. The author notes that simulated indicated torque is higher than brake torque, which is natural, and that there should be a constant difference between these two values determined by engine drag torque. Why then, in the right-hand part of Fig. 4.54, do these values converge? Additionally, while fuel flow is simulated accurately (Fig. 4.53), the CO_2 concentration profiles in Fig. 4.55 do not match. Notably, large discrepancies in emissions of CO and CH_4 are reported, but the author merely acknowledges potential model shortcomings without attempting recalibration.

Section 4.6 introduces two entirely new and complex topics: ammonia–biodiesel combustion and exhaust aftertreatment. Neither of them is validated, and both are examined only at a single operating point, despite the thesis being devoted to transient simulations. It is also unclear whether the emissions in Fig. 4.63 represent engine-out or tailpipe results. Moreover, no validation of the aftertreatment model is provided, and neither aftertreatment model is described in the methodology section. Consequently, these results seem somewhat detached from the main scientific narrative of the thesis.

In this section, the author mentions that the content is based on previously published results (e.g., work [25]). However, not only are the results reused, but the complete artwork of this section is copied directly from the referenced paper. In such a case, good practice would be to re-edit the figures. This would avoid potential self-plagiarism and ensure graphical consistency across the dissertation.

The last result presented in Section 4.7 introduces ANN into the simulation tool. SRM is replaced by an ANN model to simulate combustion and emissions. The author compares the results obtained using these two simulation tools. As expected, ANN reproduces the simulated combustion and emission characteristics of the SRM model well. However, the simulation results used as a reference (from Section 4.3) do not accurately reproduce real emissions. Why, then, was the ANN model not trained using real measurement data? The performance of the ANN model is demonstrated only on a single WLTP run, the same one with which the model was trained. This does not confirm the predictive capability of such a model.

Summarising this part of the review, it should be emphasised that although the presentation of the research is incomplete in places, the results themselves are valuable and interesting. In several cases, the discussion of the results is too limited; it lacks cause-and-effect reasoning. To understand the complete picture of the research, the reader must refer to the individual research papers.

The dissertation does not include a separate conclusions chapter. Introducing such a chapter could strengthen the synthesis of the presented findings and the formulation of scientific conclusions.

Assessment of editorial quality

The overall editorial quality of the dissertation is good, and the work is generally well prepared in terms of structure, formatting, and technical presentation, with only minor formal inconsistencies. The thesis is written in good technical English, and the nomenclature used is well established for engine research. Although the thesis is generally understandable, some sentences are too long and complex, which in places makes the reading experience demanding. The number of grammatical and typographic errors is small. For the future, please remember that torque is 'indicated', not 'indicative', and 'brake', not 'break' (p. 84). Some figures would benefit from being redrawn instead of copied from the published papers, to ensure a consistent graphical style.

Originality and individual contribution of the candidate

The originality and contribution of this work come from developing a unified transient engine simulation framework. It connects all components into one stable and reliable toolchain and is suitable for both MiL and HiL environments. The thesis moves the field forward by enabling SRM-based prediction of combustion and emissions under fully transient conditions. At the same time, the model keeps good combustion simulation accuracy (while emission prediction is less convincing) and high computational efficiency. The modular FMU architecture is another strength of the work. It is supported by an ANN-based surrogate model that can operate faster than real time. Together, they create a scalable and portable platform linking detailed combustion physics with practical needs in control development and real engineering applications. Therefore, this work represents a real methodological contribution rather than just an integration of existing software tools.

As already mentioned, the results themselves have archival value. There is high potential for continuation of the research and publication in the form of high-quality scientific papers.

The research data used in the dissertation have already been published in several multi-author articles, which appeared in journals such as *Renewable Energy*, *Energies* and SAE journals. Given the multi-author nature of these publications, it would be advisable to clearly indicate in the dissertation the personal contribution of the candidate to the obtained research results and to the preparation of these publications. This information can be extracted from the *Contribution* sections of the papers, but it should also be explicitly stated in the thesis itself.

Conclusion

The dissertation submitted for evaluation represents an original scientific contribution, and the research results and analyses presented in the thesis confirm the author's reliability and scientific diligence. The candidate has demonstrated advanced theoretical knowledge in the scientific discipline of *environmental engineering, mining, and energy*, combined with the ability to translate this knowledge into practical research and to conduct independent scientific research.

The critical remarks presented above constitute part of a scientific discussion. They are not intended to diminish the value of the dissertation, but to engage in a scholarly discussion with the author and to reflect the reviewer's perspective on the doctoral thesis. This perspective may naturally differ from that of the supervisors and the doctoral candidate.

Therefore, I conclude that the dissertation of Mr **Reddy Babu Siddareddy**, entitled *Transient engine simulations using the stochastic reactor model for driving cycle performance studies,* supervised by **Prof. Wojciech Adamczyk** and co-supervised by **Dr Michał Pasternak**, meets the requirements for doctoral dissertations as specified in Article 187 of the Polish Law on Higher Education and Science of 20 July 2018, and the author may be admitted to public defence.

Podpisał Jacek Hunicz