Response to the Reviewer's Evaluation

Title of PhD thesis: Reliable Digital Twin Operation via Surrogate-Based and Online Learning-Driven Flowsheet Model Maintenance

Reviewer: Dr. Péter Baladincz, Chief Operating Officer (MA-Coding Kft.)

Dear Dr. Péter Baladincz,

Thank you for your thorough and constructive evaluation of my PhD dissertation, as well as your positive assessment of its methodological contributions and scientific results.

My responses are provided in blue text directly below the corresponding sections of your review.

Sincerely,

Balázs Palotai

1. Significance and novelty of the topic:

The dissertation addresses one of the central challenges of industrial digital twin deployment: maintaining model fidelity under evolving real-world conditions. As digital twins and data-driven methods spread across the process industry, this topic is highly timely. In the reviewer's view, the principal novelty of the work lies in its systems-oriented framework and in the way it is built on engineering logic. By bridging the methodological silos between process engineering, surrogate modelling and online machine learning, the candidate establishes a common operational and conceptual platform that allows experts from different disciplines to understand one another and work together effectively.

The industrial relevance is substantial. As the candidate points out, appropriate production planning and the identification and improvement of optimal operating parameters can be worth millions of dollars annually, and the reliability of such decisions depends directly on how faithfully the simulation reflects the current state of the plant. Ensuring exactly that is the ultimate goal of the work.

I sincerely appreciate your positive assessment of the significance, novelty, and industrial relevance of my research.

2. Scientific foundations:

The candidate's treatment of the relevant literature is thorough and of high quality. The dissertation draws on 149 references, primarily peer-reviewed academic publications and relevant standards, and provides a very good overview of the fields it covers, including the key scientific antecedents. The review is contextualised with concrete industrial examples, effectively grounding the theoretical contributions in the practical realities of refinery and

process plant operation. The literature is not merely summarised but processed analytically and critically: the candidate surveys existing approaches, positions his own work in relation to them, and builds on this to formulate his research objectives and proposals. As a result, the contributions of the dissertation are clearly placed within the current state of the art.

Thank you for your positive evaluation of the scientific foundations and literature review.

3. Methodology and results:

The dissertation presents the candidate's own results: it constructs the framework and its components incrementally, and each step is supported by experiments. The case studies are carried out on real industrial systems or on purpose-built simulations that faithfully reproduce real plant behaviour, using both real operating data and simulated scenarios. The experimental validation is therefore well suited to examining the stated objectives, and the experiments attached to each chapter clearly show the role each component plays in the system as a whole.

The methods applied are modern and well chosen. The online learning component deserves particular recognition, as it is the very core of the framework. It keeps the flowsheet model maintainable over time, continuously aligning it with the actual state of the plant instead of relying on periodic, labour-intensive recalibration. Since surrogate models can become silently misleading without principled and wellgoverned retraining, the online learning component is critical to the practical reliability of the entire framework. The software platform developed by the candidate is transparent in its architecture, provides coherent monitoring of the models and their performance over time, and puts cross-disciplinary collaboration into practice.

The metrics applied and the presentation of the results are appropriate, and the comparative analysis is clear: the candidate convincingly explains why different approaches yield the observed outcomes. The conclusions follow consistently from the results presented, and the overall concept is both intellectually well grounded and practically well executed.

I am grateful for your thorough evaluation of the proposed methodologies, experimental validation, and results. I would also like to express my gratitude for the constructive comments and valuable suggestions provided during the previous evaluation round and discussed during the internal defense. These discussions helped me identify opportunities to further improve the clarity, consistency, and scientific presentation of the dissertation.

4. New scientific results and publication activity:

Based on the dissertation, the candidate formulates four new scientific results in his thesis statements, all of which are accepted by the reviewer. The candidate has 15 Hungarian and international publications related to the dissertation, in which he appears as first author. This demonstrates both his active participation in the scientific community and his leading role in the research. The reviewer considers his publication performance adequate for the award of the doctoral degree.

Thank you for accepting the four thesis statements as new scientific contributions and for your positive evaluation of my publication activity.

5. Formal assessment:

The structural organisation of the dissertation is excellent. The chapters build on one another logically and guide the reader toward a comprehensive understanding of the subject. Notably, each chapter is largely self-contained: introductory summaries of prior findings at the opening of each chapter ensure that the individual contributions can be understood and evaluated independently, which is a mark of disciplined scientific writing. The style is professionally rigorous yet accessible to a broad academic readership. The tables and figures are, in general, well composed, clear and informative. In some places, the reduced size of the figures combined with the density of the data series shown together is somewhat disturbing; the figures nevertheless remain interpretable, and the candidate explicitly draws the reader's attention in the text to the parts to be evaluated. The references are cited correctly and consistently, and the bibliography is complete. The external appearance of the dissertation is appropriate: it is well formatted and well structured.

I appreciate your favorable assessment of the dissertation's structure, clarity, and overall presentation. I acknowledge that presenting multiple data series within limited space can affect readability.

6. Further remarks:

A significant strength of the proposed system is its strict adherence to the human-in-the-loop principle. Models issue recommendations; intervention and decision-making remain exclusively within human authority. While this design choice positions the system closer to the paradigm of a digital shadow than a fully autonomous digital twin, it is a deliberate and justified decision. In the context of hazardous chemical and refinery operations, maintaining human oversight is not a limitation but a prerequisite, and it meaningfully supports the incremental trust-building that the industrial adoption of advanced modelling techniques requires.

Thank you for highlighting the importance of the human-in-the-loop principle in the proposed framework. I fully agree that maintaining human oversight is particularly important in safety-critical industrial environments, such as chemical and refinery operations.

7. Questions:

What effort would be required to apply the framework to a new process unit or plant? Which components of the framework are generic, and which require case-specific adaptation?

The proposed surrogate-based and online learning-driven flowsheet model maintenance framework is designed to be generally applicable to different process units and plants. Its main workflow components, including flowsheet model sampling, surrogate model development, calibration, validation, and online learning, can be considered generic and therefore transferable to new applications without fundamental methodological changes.

However, the framework intentionally provides flexibility in selecting the most appropriate sampling strategy, surrogate model architecture, optimization algorithm, and online learning strategy. These components require case-specific configuration depending on the characteristics of the process, the complexity of the flowsheet model, the availability and quality of operating data, and the required prediction accuracy.

For example, while Latin Hypercube Sampling (LHS) is suitable for independently varying operating parameters within predefined ranges, it may not be appropriate for directly sampling constrained variables, such as feed compositions, where component fractions must sum to unity. In such cases, constraint-aware sampling or an appropriate parameterization of the input space would be necessary.

Similarly, the online learning strategy should reflect the dynamics of the process and the frequency of significant changes in operating conditions. For relatively stable processes, event-driven or threshold-based model updates may be more computationally efficient than continuous incremental updates, provided that model performance is monitored between updates.

Therefore, the implementation effort would primarily depend on the availability of an existing flowsheet model and representative operating data, as well as the case-specific configuration of the individual framework components.

Under what conditions does the candidate consider it realistic to move from the current human-inthe-loop operation towards greater autonomy, such as closed-loop intervention?

The feasibility of moving from human-in-the-loop operation towards greater autonomy depends primarily on the complexity and criticality of the specific use case. If the problem addressed by the digital twin is well-defined, the recommended actions are clearly understood, and the results have been consistently validated and accepted during open-loop operation, transitioning towards closed-loop intervention could be a reasonable next step.

However, such a transition requires appropriate safeguards to ensure that autonomous actions are only executed when the process is operating within predefined conditions, the model predictions are sufficiently reliable, and the recommended interventions remain within established operational and safety constraints. This would require continuous monitoring of

model performance, validation of proposed actions, and mechanisms to prevent or suspend autonomous interventions when these conditions are not satisfied.

One practical approach could be to integrate the digital twin's recommendations into an existing Advanced Process Control (APC) system, which is already established and well understood in process industrial operations. In this configuration, the digital twin could provide optimized operating targets or constraints, while the APC system would manage their implementation within its defined control and operational limits. This approach would build on existing control infrastructure while maintaining appropriate safeguards, human oversight, and the possibility of manual intervention when necessary.

Budapest, 2026.11.04

Balázs Palotai