Revision of doctoral (PhD) thesis

Name of the candidate: Balázs Palotai

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

Reviewer: Gyula Ádám Dörgő; Data Intelligence Department Manager; Borouge International

Balázs Palotai's outstanding work offers significant novelty in the increasingly relevant topic of reliable and automated digital twin applicatons in the process industry. The work systematically identifies crucial pain points in the practical application of digital twins (primarily presented in the chapter „Moving towards digital twins in the process industry") and presents corresponding solutions to three of these pain points. Each solution is presented in a separate chapter: the chapter "Surrogate-based calibration of flowsheet models" formulates flowsheet model maintenance as an adaptive calibration problem and introduces a surrogate-based methodology that significantly reduces the computational cost, the chapter "Online learning for incremental surrogate model maintenance" examines how different online update mechanisms can sustain surrogate accuracy under evolving conditions, while the chapter "Integrated framework for adaptive flowsheet model maintenance" integrates the previously presented surrogate-based flowsheet calibration and online surrogate learning into a coherent framework. Each of these chapters concludes with case studies: a heat exchanger network model provides continuity and comparability between the different chapters, while two industrial case studies are presented in Chapter 5. In addition to the industrial case studies, a software prototype presented in Chapter 6 further underpins the intention and readiness of practical applications. The systematically and incrementally improving nature of these chapters perfectly demonstrates how the toolboxes of process engineering, data analysis and machine learning form a powerful synergy which is universally applicable to enhance the chemical industry, moreover, they highlight the widespread knowledge of the candidate in the fields of chemical engineering and data-based modelling.

It was particularly insightful to observe how the candidate identified complex practical problems in the modeling of chemical technologies and the application of these models as digital twins, elevated these problems to a higher level of integration, and proposed practical solutions after data-based evaluation. The chosen methods are well justified, the case studies

and results are thoroughly evaluated, and the conclusions drawn are sound and clearly demonstrate the candidate's professional competence. Overall, the work was a pleasure to read.

Formal and structural evaluation

From a structural perspective, after the introduction, a more structural summary of the digital twins is presented, which is followed by the three methodological improvement proposals providing the main findings of the thesis work. The software prototype is presented in a separate chapter projecting towards the further industrial applications. As all of these chapters describe independent and standalone analysis results, which in addition build on top of each other, in my view, the selection of this structure is favorable and advantageous.

The sections build on the already accepted journal articles of the candidate, underpinning the scientific foundations of the results. The main part of the thesis consists of 152 pages and contains 149 references. It is well-edited and constructed in a transparent and easy-to-follow structure. The figures are high-quality and well-explained in the text.

Theses:

All theses are well-formulated, transparent, and clearly state the novelty and candidate's contribution. All of them are supported by at least one internationally accepted research paper, and some have already received independent citations, showing the cascading effect of the research.

Thesis #1: "I developed a framework supporting the industrial adoption of digital twins and demonstrated that one of the most critical prerequisites for their successful deployment and long-term operation is the automated maintenance of the underlying flowsheet models."

(3 sub-theses)

The thesis results were published in a journal article and five conference abstracts.

Thesis #2: "I demonstrated that the proposed surrogate-based calibration methodology substantially reduces the computational cost of flowsheet model calibration while improving its robustness without compromising the required accuracy, thereby supporting the efficient application of flowsheet models in digital twin systems."

(3 sub-theses)

The results of the thesis were published in a journal article and one conference full paper, for which the candidate has received an independent citation according to the MTMT.

Thesis #3: “I demonstrated that online (incremental) learning enables the continuous adaptation of surrogate models to changing operating conditions while preserving the previously acquired global knowledge of the system. Furthermore, I demonstrated that the timing of model updates and the selection of training data are independent design decisions, allowing different update strategies to be freely combined.”

(3 sub-theses)

The results of the thesis were published in a journal article and two conference abstracts.

Thesis #4: “I developed an integrated framework that combines surrogate-based flowsheet model calibration with online learning of surrogate models, thereby reducing the computational effort required for flowsheet model calibration and improving calibration efficiency, while effectively supporting the long-term adaptation of flowsheet models in digital twin systems.”

(3 sub-theses)

The results of the thesis were published in a journal article, one conference full paper and two conference abstracts, for which the candidate has received an independent citation according to the MTMT.

Question:

After receiving the answers from the candidate to my comments and discussing them during the internal presentation, I have no formal comments left. I had no serious critics or concerns even during the previous evaluation round of the thesis work. My more forward-looking question to the candidate:

Chapter 1 states that “Despite their conceptual maturity and demonstrated potential, DTs are significantly less prevalent in the process industry than in discrete manufacturing”, along with the key issues of the application of digital twins. If, in theory, we had infinite resources to tackle the problem, what would be the candidate’s roadmap to sustainably solve it? And what would be the first element to address: the technological, computational, organizational, financial, or any other aspects?

Summary and Evaluation:

Considering the importance of the topic, its scientific significance, its novelty, the high standard of professional achievement, the thoroughness demonstrated in the discussion of the analyses, and the publication record covering the topic (4 journal articles, 2 conference articles and 9 conference abstracts), the dissertation is an outstanding scientific achievement. The candidate has met the requirements of a PhD dissertation. In my opinion, the PhD dissertation of Balázs Palotai satisfies the conditions to present the findings at a public debate. Following the successful defense of Balázs Palotai's dissertation, I highly recommend that the candidate be awarded the PhD degree.



Vienna, 13.10.2026

Gyula Ádám Dörgő
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