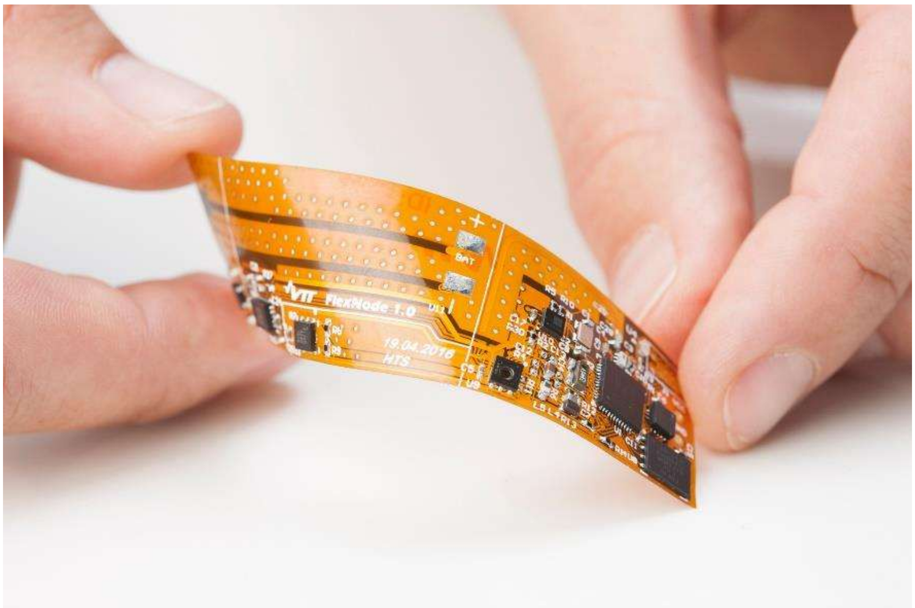
RESEARCH REPORT VTT-R-00442-25



Development of Artificial Intelligence and Machine Learning for Online Perception and Operating Mode Optimization in Process Industry (AIMODE) – Project results

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Summary

This report summarises the VTT research project results from Business Finland project called Development of Artificial Intelligence and Machine Learning for Online Perception and Operating Mode Optimization in Process Industry (AIMODE). Already, during the project, the participating researchers have published their results in academic papers, thus, this report gathers the achieved results by topic and communicates where these results have been published. As such it is a shortcut document to quickly find the project results and point-out where more information can be found.

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Preface

This research has been conducted as a part of the Development of Artificial Intelligence and Machine Learning for Online Perception and Operating Mode Optimization in Process Industry (AIMODE) project, which was funded by Business Finland and VTT. This project developed artificial intelligence (AI) methods to understand the interactions between the variables necessary for improved operational knowledge and performance. The project started on 9/2022 and ended on 8/2025. The companies and research institutes in the project were: VTT, Aalto, Metso Oyj, LightningChart Oy, and Quva Oy. The steering group members are: Anssi Laukkanen (VTT), Juha Kortelainen (VTT), Lauri Palva (Aalto), Simo Särkkä (Aalto), Jani Kaartinen (Metso), Jari Moilanen (Metso), Pasi Tuomainen (LightningChart), Terho Häkkinen (LightningChart), Olli Pasanen (Quva), Janne Korhonen (Quva). Business Finland contact person was Mika Niskanen.

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Contents

1. Introduction to the project

The minerals and metals processing systems are typically multidimensional, inherently complex, and dynamic. Thus, they are characterized by incomplete, high uncertainty information. One of the root causes for the current operational challenges is the limited adaptability due to the lack of valid dynamic, either measured or estimated, process information. This project developed new insights with artificial intelligence (AI) to understand the interactions between the variables necessary for improved operational knowledge and performance.

The work combined digitalization, control engineering, and first-principles modeling and simulation. The proposed solutions are basis for pragmatic day-to-day operational tool for process operators, e.g., for proactively compensating for feed material-based disruptions and visualization technologies for enhanced process advisor systems.

2. AIMODE project description

Research was organized into seven work packages, and the general structure of the project is shown in Figure 1. WP1 started the project with gathering historical operational data from the plant, setting up simulation environment for the project (to generate synthetic data and to work as a state-of-the-art simulation benchmark). Work was continued in WP2-WP4 to develop novel ML/AI methods for enhancing accuracy of predictions at sub-systems and at system level, and to develop decision-making tools for automated process control. The developed computational steps and ML/AI methods were to be lab-evaluated in WP5 and real-life assessed in WP6 at the demonstration site. WP7 concentrated on project management and dissemination of the project results.

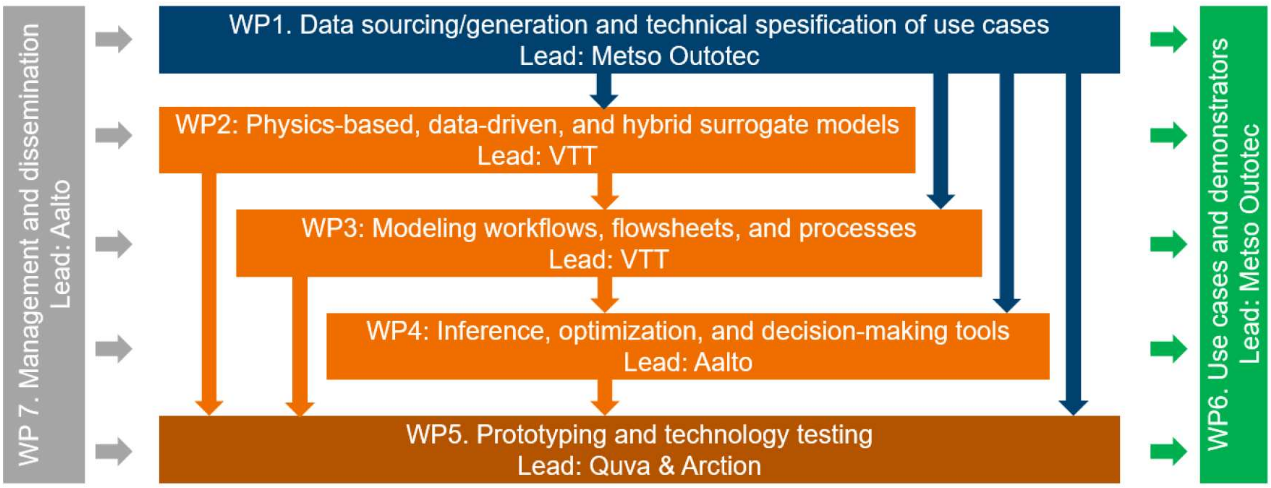

Figure 1. Project structure and high-level tasks (note: Arction was renamed to LightningChart during the project).

VTT's research focused on work packages 2, 3 and 4. WP2 developed various forecasting surrogate models covering selected equipment, process stages, and processes. The methodology was based on a combination of first-principles physics and data-driven machine learning through deep learning models. WP3 addressed the interactions and modeling workflows associated with system level flowsheets and processes. The aim was to analyse the available datasets and create sensor-data-processing and management methodology. Finally, WP4 was concerned with the artificial intelligence associated capabilities related to analysis, inference, and optimization to support decision-making using dynamic and steady-state simulation combined with forecasting surrogates.

3. VTT research project implementation

Project started with exploration and visualisation of the data, understanding the use cases and the digital twin simulator provided by Metso. In addition to our internal workshopping, we discussed with domain experts about the characteristics of the data and visited a mine site. The components and subprocesses to be modelled with surrogates were selected. We further studied and created soft sensors to increase the predictability and correlation between selected inputs and outputs variables. Literature reviews with Aalto were performed to identify previous research done on time-series forecasting using data-driven and hybrid deep learning models, especially in the mineral engineering domain. Based on the literature review, we selected three deep learning model architectures (LSTM, CNN and GRU) as best candidates [1], [2]. An example of a flotation process flowsheet is shown in Figure 2.

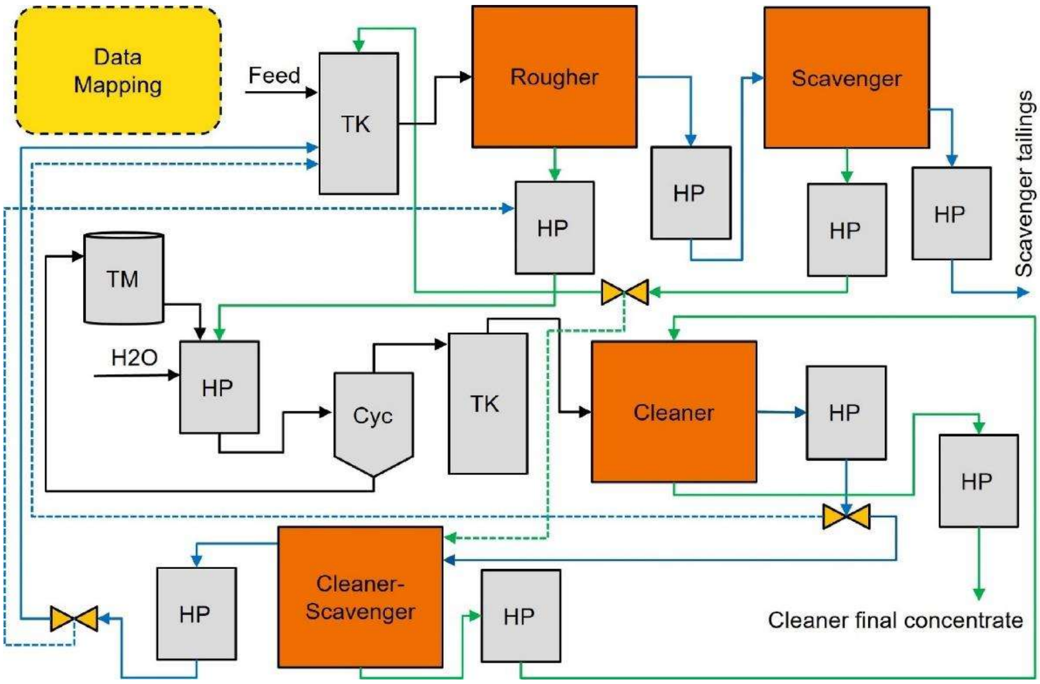

Figure 2. Example of case study flotation flowsheet from [2].

Next, we created forecasting surrogate models of the selected process subsystems (e.g. the Cleaner subsystem from Figure 2). We started with pure data-driven surrogates trained on process and simulation data from a case plant and found them capable of forecasting outputs six steps ahead (30-minute horizon), an example is shown in Figure 3. We published our findings in [2]. Next, we studied how to integrate process-related physics to our forecasting surrogate models, transforming them into hybrid models (or physics-informed machine learning models). A review and a comparison of the hybrid methods is presented in [1]. The most promising method was a modified cost function, tracking the mass flow error of the predicted and the real system, in addition to the regular training error. Learning was more stable, and the accuracy of the model enhanced, but at the cost of increased model complexity. Figure 4 shows an example of comparing data-driven and physics-informed models. We compared the six surrogate models (3 data-driven and 3 hybrid models) and published the results in [3]. We have also summarized the development work of forecasting surrogates in [5] and [4].

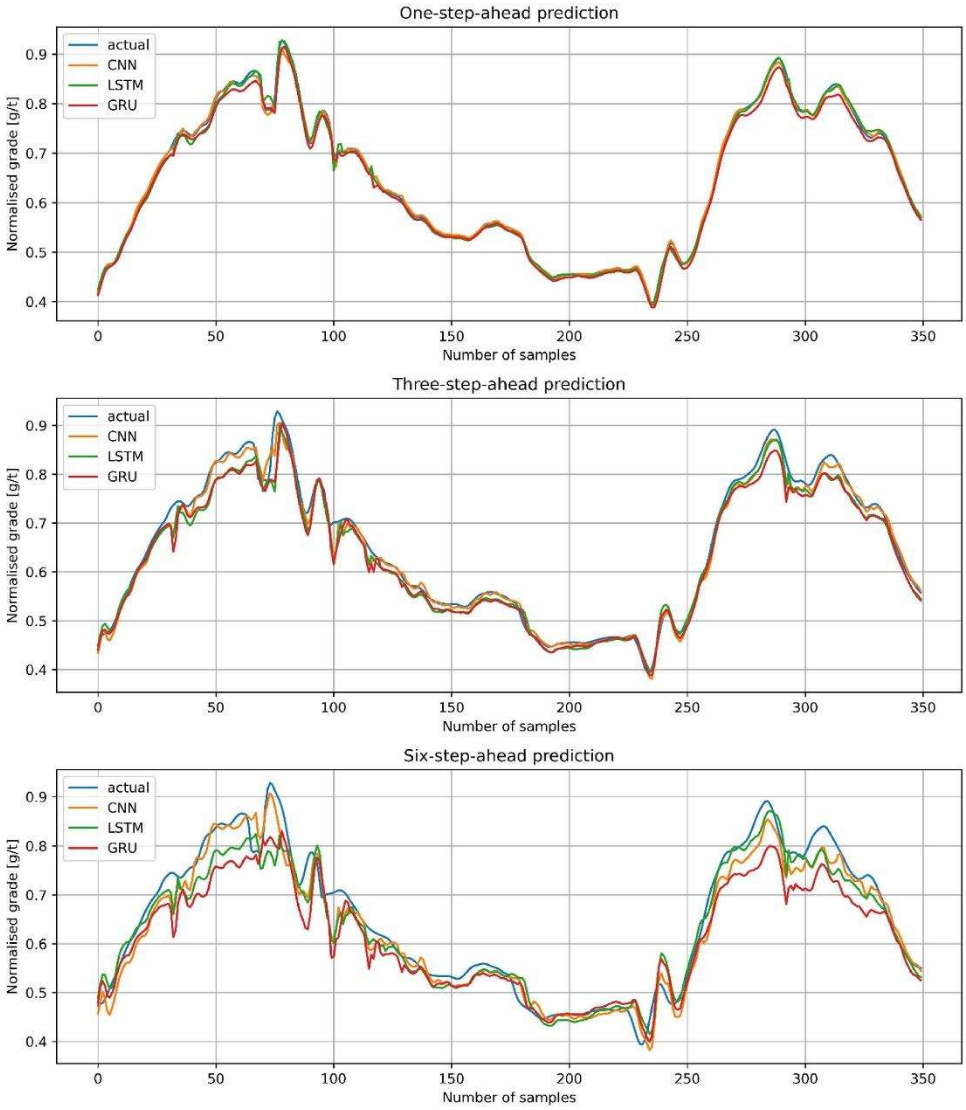

Figure 3. Examples of one-, two-, and six-step-ahead process output forecasts using CNN, LSTM, and GRU data-driven surrogate models. One step corresponds to 5 minutes of real process time [2].

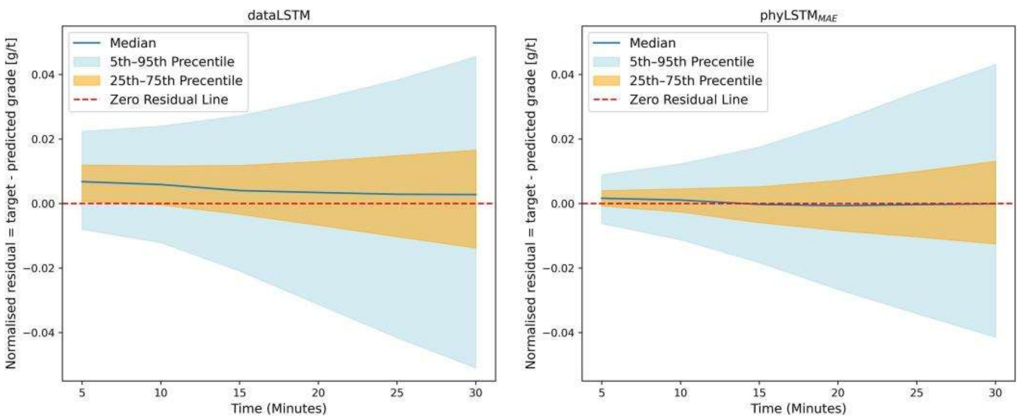

Figure 4. Comparison of average residual errors for a data-driven and a physics-informed LSTM surrogate model, from one- to six-step-ahead forecasts [3].

Additionally, we studied how to create forecasting surrogates just with synthetic data generated with HSC Sim, e.g., in situations of limited historical data or for green-field plants. This modelling workflow is illustrated in Figure 5 and reported in [6] and [7].

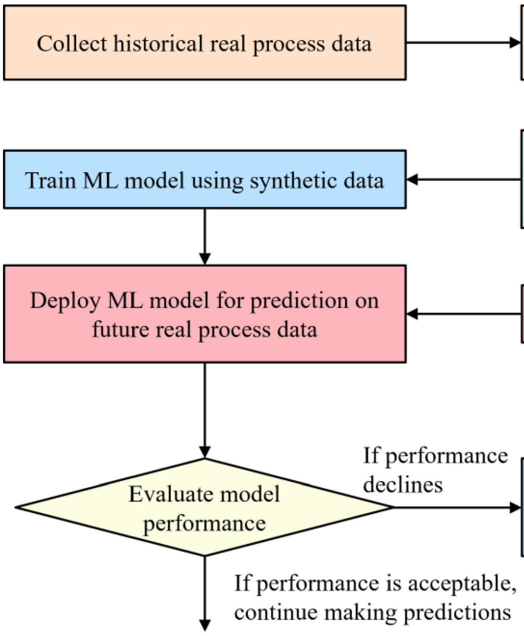

Figure 5. Synthetic surrogates' creation and deployment methodology [6].

We also experimented and published results using our surrogates with streaming data (simulating live plant data) and made a live demonstrator visualizing the forecasting and uncertainty capabilities with the help of LightningChart plots [8] using 5-second input data, as shown in Figure 6. However, we did not integrate our surrogates to directly read data from plant systems for online prediction. A study with Aalto was done into sensor and model data accuracy estimation and visualization, including data imputation activities, and the results are to be published at the time of writing.

Figure 6. Visualization of online 30-minute-ahead surrogate forecasts with uncertainty estimates.

To work on the optimization tasks from WP4, we updated our forecasting surrogate models to incorporate future process control variables as additional inputs. To determine the optimal future control settings, three optimization strategies were evaluated—Random Search (RS), Gaussian Process Bayesian Optimization (GP-BO), and Tree-structured Parzen Estimator Bayesian Optimization (TPE_BO)—with the objective of maximizing the forecasted process outputs [10]. Figure 7 compares the actual process values with the optimized 30-minute-ahead average forecasted outcomes generated by the surrogate model using historical data. The results are preliminary and have not yet been validated in the plant environment. Another effort was an ore blend and plant configuration optimizer done in cooperation with Metso. A Python-based TPE optimizer could select optimal plant settings and ore blend for maximizing the process profit within the simulator environment, refer to Figure 8 for an example of the optimization run. A conference paper was published about the results [9], and another is being written about the methodology.

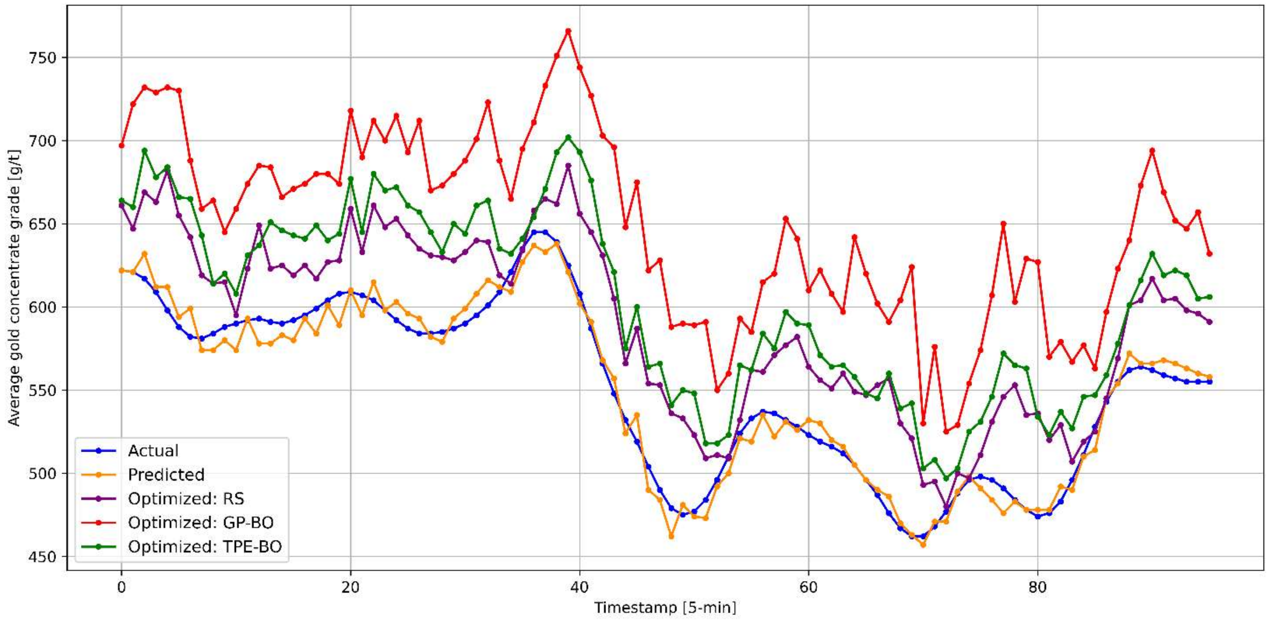

Figure 7. Comparison of actual and optimized 30-minute-ahead average process outcomes obtained using Bayesian optimization and random search. Results are based on surrogate model predictions from historical data and require further validation in the process simulator and plant [10].

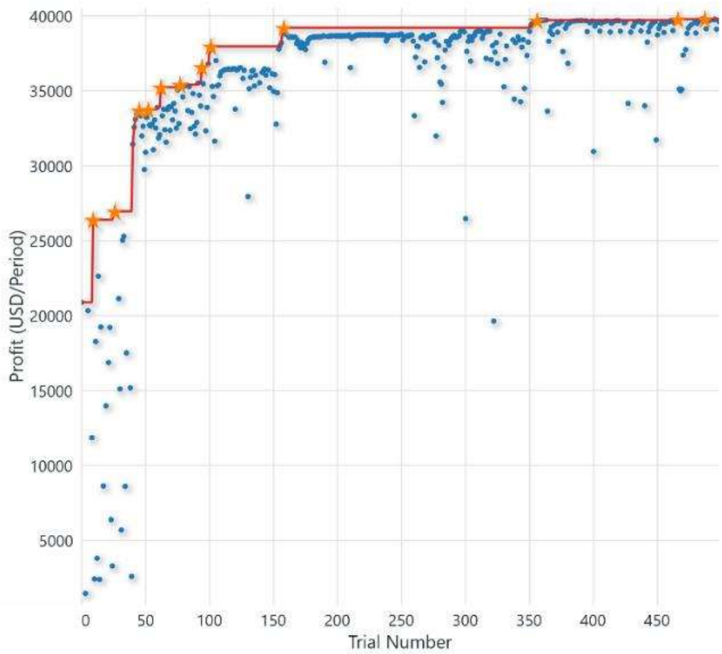

Figure 8. Example case of TPE optimization algorithm trial results for maximising process output by feed ore blending and equipment configuration. Blue dots are single trials while red line and stars are highlighting currently best found combination as the trial's progress [9].

Additional, throughout the project, a systematic approach to data preprocessing was developed to ensure methodical and transparent data transformation. We wanted distinct and reproducible stages of data preprocessing and built a modular, scalable, and maintainable DVC-based solution. We published the principles of our three-tiered data management framework (Figure 9) in a [11].

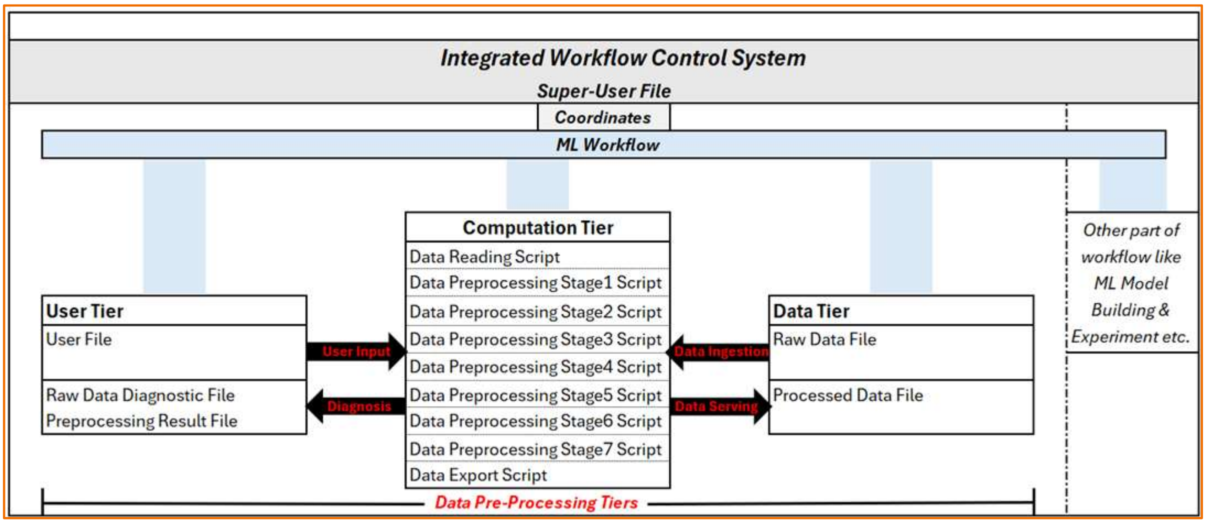

Figure 9. Methodology for three-tiered data preprocessing framework for ML workflow [11].

4. The key results of the project

VTT's research topics and the progression of research is depicted in Figure 10.

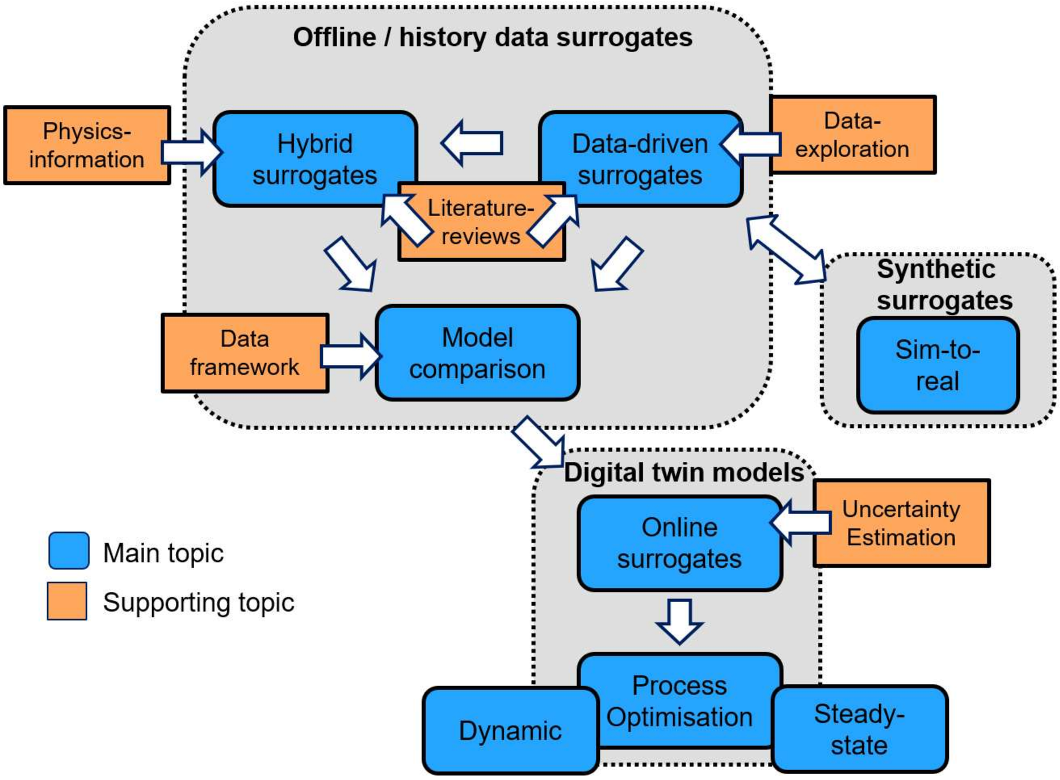

Figure 10. VTT's research topics.

The following section lists and categorises the main results of the project, with references to the corresponding publications where further information can be found (note: some of the papers are still under publication at the time of writing this report).

From the preparation phase (WP3):

1. Data exploration on the project datasets and creating needed soft sensors to help surrogate training [1,2,3].
2. Literature review to data/PINN/hybrid multivariate multistep forecasting surrogates in minerals engineering to select the most promising deep learning models [1,2,3]

These results prepared the group for the modelling work. They have been published as part of the other studies.

From forecasting surrogate studies (WP2):

3. Review and comparison of methods to integrate physics information to data-driven surrogate models, creating physics-informed machine learning models [1].
4. Developing, training and testing of data-driven multivariate multi-step forecasting surrogate models based on CNN, LSTM, and GRU architectures with a 30-minute-ahead forecasting horizon [2].
5. Integrating the work of physics-informed and data-driven models by creating common model baselines for thorough comparison [3][4][5].

6. Synthetically trained surrogates and real-time synthetic data gathering scheme with HSC Sim [6][7].
7. Studying forecasting surrogate behaviour and visualization with online/streaming Geminex data [8].

These are the main contributions of VTT. All the results utilized the datasets and simulator provided by Metso.

From optimization tasks (WP4):

8. Ore blend optimizer for Geminex steady state simulation [9].
9. Dynamic process profit optimizer concept using scenario design and forecasting surrogates [10].

We worked in cooperation with Metso and LightningChart on these case problems.

From supporting activities (WP4):

10. DVC-based structured and modular data preprocessing framework [11].
11. Sensor and model data accuracy estimation and visualization scripts [to be published].

These were our internal work to support the other activities.

5. Conclusions

The project examined how artificial intelligence and machine learning can be applied to produce fast data-driven surrogate components to a first-principles digital twin, when the process is slow to simulate or try in real-time. In addition, our studies produced insights into using physics-informed machine learning for surrogate modeling of industrial processes, supporting robust digital twins and process optimization.

In addition, optimization using surrogate models were studied. For example, a steady state optimizer can efficiently explore different plant configurations and ore blending ratios, potentially leading to improved operational decision. For dynamic process control optimization, a trained surrogate model can quickly discover control strategies that maximize the output of mineral processing plant.

Developed data framework significantly enhances the reproducibility, version control, and reliability of cleaned data obtained from an offline dataset in a project.

Before implementation, future research and development should include an ML pipeline alongside standard software development. Technology integration, piloting, and evaluation with existing IT/OT systems are necessary. Next steps for optimization tool development include validation and further plant system integration. Expanding the data framework for online data will also require extra development.

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