

# Simulation-based Digital Twins of Industrial Process Plants: A Semi-Automatic Implementation Approach

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Gerardo Santillán Martínez

# Simulation-based Digital Twins of Industrial Process Plants: A Semi- Automatic Implementation Approach

**Gerardo Santillán Martínez**

A doctoral dissertation completed for the degree of Doctor of Science (Technology) to be defended, with the permission of the Aalto University School of Electrical Engineering, at a public examination held at the lecture hall TU2 of the school on 7th June 2019 at 12:00.

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**Abstract**

Dynamic simulation has been used in the process industry during decades for several important applications over the process plant lifecycle. Recent trends on plant digitalization have resulted on the development of Simulation-based Digital Twins (SBDT) of process plants. In a SBDT, a dynamic first-principles simulation model is used to capture the process plant dynamics. In this application, the first-principles model (FPM) of the plant is run in parallel with the process while dynamic model parameter estimation methods adjust the model results by comparing process measurements with model results to continuously drive the simulated state to the current plant state. As a result, the underlying FPM of the SBDT is continuously synchronized with the operational plant. SBDTs can provide non-measured information of the process and they can be used to obtain high-fidelity predictions that are based on the current state of the process. They can also be utilized to develop operator training simulators, trouble-shooting and fault diagnoses systems. Furthermore, they can be applied for offline and online optimization of the plant. SBDTs are a holistic application for operation support of process plants. However, development of their underlying FPM remains laborious and expensive. Although re-utilization of existing models, developed for plant engineering, could reduce implementation effort and time of SBDTs, these models are still created manually. Moreover, integration of SBDTs with the ICT architecture of the plant could leverage on existing industrial operability standard to seamlessly interface different simulation methods and other SBDT system components with the plant.

In this thesis, these implementation shortcomings are tackled by utilizing a combination of implementation methods proposed in this work. First, laborious FPMs development is addressed by applying an AMG method based on deriving 3D plant model information for automatically generating the FPM of the SBDT. Furthermore, laborious integration between the simulation system and the process plant is addressed by utilizing a method for implementing a lifecycle-wide tracking simulation architecture.

The main results of the thesis show that the model generated using the proposed AMG approach can be successfully applied for implementing SBDTs after its integration into the physical plant. Furthermore, the proposed simulation architecture leverages on the application of industrial interoperability standards for reducing the effort required for configuring the communication between different architecture components and for enabling systematic information exchange between the architecture components and methods.

**Keywords** Digital Twin; Dynamic Simulation; Engineering Automation; Industrial process simulation

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# Preface

This work was carried out at the department of Electrical Engineering and Automation, at the School of Electrical Engineering of Aalto University between 2014 and 2019. During these years, I had the pleasure to meet many people that had an impact in the outcome of this work. Therefore, I would like to thank them.

I would like to start by thanking Prof. Valeriy Vyatkin for giving me the opportunity of carrying out my doctoral studies at the Information Technology in Automation research group. His feedback and advice were always an inspiration for developing the research presented in this work. I would like to extend my deepest gratitude to D.Sc. Tommi Karhela for his technical advice and friendship during the last four years. This thesis would not have been possible without his constant support and guidance. I am very thankful to D.Sc. Seppo Sierla for his always valuable advice and help, as they were of utmost importance for further developing and completing this work. I would also like to thank Prof. Leon Urbas and Prof. Hans Vangheluwe for their valuable feedback provided during the pre-examination of this thesis.

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Espoo, April 22<sup>nd</sup>, 2019.

Gerardo Santillán Martínez.

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# Nomenclature

## Acronyms

3D	Three dimensions
AGM	Automatically generated model
AMG	Automatic model generation
API	Application programming interface
CAD	Computer-aided design
CAE	Computer-aided engineering
CAEX	Computed Assisted Engineering Exchange
CMSD	Core Manufacturing Simulation Data
CS	Control system
CSV	Comma-separated values
DDMs	Data-driven models
DDS	Data distribution service
DEXPI	Data Exchange in Process Industry
DT	Digital Twin
EKF	Extended Kalman filter
EO	Equation oriented
ERP	Enterprise resource planning
FPM	First-principles model
HPP	Heat production plant
ICs	Initial conditions
ICT	Information and communication technology
IEC	Industrial Electro-technical Commission

IFC	Industrial Foundation Classes
ISO	International Standard Organization
MES	Manufacturing execution systems
MIMO	Multiple-input-multiple-input
MPC	Model-predictive control
NRMSE	Normalized root mean squared error
OCL	Object Constraint Language
OMBA	Online Model-based Application
OPC	OLE for Process Control
OPC UA	OPC Unified Architecture
P&ID	Piping and Instrumentation Diagram
PI	Proportional integral
PID	Proportional integral derivative
PLC	Programmable logic controller
RAMI	Reference Architecture Model for Industry 4.0
SBDT	Simulation-based Digital Twin
SCL	Simantics Constraint Language
SISO	Single-input-single-output
SM	Simultaneous modular
SMC	Sliding model control
SP	Set point
SQL	Structured Query Language
SysML	Systems Modelling Language
TH	Thermal-hydraulic
UIs	User interface
UKF	Unscented Kalman filter
UML	Unified Modelling Language
XML	Extensible Mark-up Language

## Latin Symbols

$b_n$	model bias $b$ at the iteration $n$
$D_o$	Elbow fitting diameter
$d$	Implicit dynamic feedback controller output
$K_c$	Implicit dynamic feedback controller proportional term
$R_o$	Elbow fitting bed radius
$y_n$	model variable value at the iteration $n$
$z_n$	measured variable value at the iteration $n$

## Greek Symbols

$\alpha$	noise rejection coefficient
$\delta$	Elbow fitting bend angle
$\zeta$	Head loss coefficient
$\zeta_{fr}$	Friction coefficient throughout the fitting length
$\zeta_l$	Local head loss coefficient
$\lambda$	Elbow fitting friction coefficient
$\tau_i$	Implicit dynamic feedback controller integral term

# List of Publications

This doctoral dissertation consists of a summary of the following publications which are referred to in the text by their Roman numerals

- I.**G. Santillán Martínez; T. Karhela; T. Miettinen; V. Vyatkin. An OPC UA Based Architecture for Testing Tracking Simulation Methods. In The 13<sup>th</sup> IEEE International Symposium on Parallel and Distributed Processing with Applications, Helsinki, 2015, pp. 275-280. doi: 10.1109/Trustcom.2015.644, August 2015.
- II.**G. Santillán Martínez; T. Karhela; A. Rossi; C. Pang; V. Vyatkin. A Hybrid Approach for the Initialization of Tracking Simulation Systems. In IEEE 20th Conference on Emerging Technologies and Factory Automation (ETFA), Luxembourg, 2015, pp. 1-8. doi: 10.1109/ETFA.2015.7301532, September 2015.
- III.**G. Santillán Martínez; A. Aikala; T. Miettinen; J. Savolainen; K. Kondelin; T. Karhela; V. Vyatkin. Parameters Selection in Predictive Online Simulation. In IEEE 14th International Conference on Industrial Informatics (INDIN), Poitiers, 2016, pp. 726-729. doi: 10.1109/INDIN.2016.78192542, July 2016.
- IV.**R. Ruusu; G. Santillán Martínez; T. Karhela; V. Vyatkin. Sliding Mode SISO Control of Model Parameters for Implicit Dynamic Feedback Estimation of Industrial Tracking Simulation Systems. In IECON 2017 - 43rd Annual Conference of the IEEE Industrial Electronics Society, Beijing, 2017, pp. 6927-6932. doi: 10.1109/IECON.2017.8217211, October 2017.
- V.**G. Santillán Martínez; T. Karhela; R. Ruusu; T. Lackman; V. Vyatkin. Towards a Systematic Path for Dynamic Simulation to Plant Operation: OPC UA-enabled Model Adaptation Method for Tracking Simulation. In IECON 2017 - 43rd Annual Conference of the IEEE Industrial Electronics Society, Beijing, 2017, pp. 5503-5508. doi: 10.1109/IECON.2017.8216952, October 2017.

- VI.**G. Santillán Martínez; R. Ruusu; T. Karhela; S. Sierla; V. Vyatkin. An Integrated Implementation Methodology of a Lifecycle-Wide Tracking Simulation Architecture. Accepted for publication in IEEE Access, vol. 6, pp. 15391-15407, 2018. doi: 10.1109/ACCESS.2018.2811845, March 2018.
- VII.**G. Santillán Martínez; S. Sierla; T. Karhela; J. Lappalainen; V. Vyatkin. Automatic Generation of a High-Fidelity Dynamic Thermal-hydraulic Process Simulation Model from a 3D Plant Model. Accepted for publication in IEEE Access, doi: 10.1109/ACCESS.2018.2865206, August 2018.
- VIII.**G. Santillán Martínez; S. Sierla; T. Karhela; V. Vyatkin. Automatic Generation of a Simulation-based Digital Twin. In IECON 2018 - 44th Annual Conference of the IEEE Industrial Electronics Society, Washington, 2018, October 2018.

# Author's Contribution

## **Publication I: “An OPC UA Based Architecture for Testing Tracking Simulation Methods”**

The author wrote the manuscript. The author, in collaboration with Dr. Karhela, developed the conceptual design of the architecture. The author implemented and tested the architecture under the guidance of Dr. Karhela and Prof. Vyatkin.

## **Publication II: “A Hybrid Approach for the Initialization of Tracking Simulation Systems”**

The author wrote the manuscript. The author, in collaboration with Dr. Karhela, developed the conceptual design of the initialization method. The author implemented and tested the initialization method under the guidance of Dr. Karhela and Prof. Vyatkin.

## **Publication III: “Parameters Selection in Predictive Online Simulation”**

The author wrote the manuscript in collaboration with Mr. Miettinen, Mr. Aikala and Mr. Savolainen. The author implemented and tested the proposed method on the Aalto University laboratory process under the guidance of Dr. Karhela and Prof. Vyatkin.

## **Publication IV: “Sliding Mode SISO Control of Model Parameters for Implicit Dynamic Feedback Estimation of Industrial Tracking Simulation Systems”**

The author wrote the manuscript in collaboration with Mr. Ruusu. Mr. Ruusu developed the conceptual design of the proposed method and implemented the parameter controller. The author implemented and tested the proposed method on the Aalto University laboratory process under the guidance of Dr. Karhela and Prof. Vyatkin.

## **Publication V: “Towards a Systematic Path for Dynamic Simulation to Plant Operation: OPC UA-enabled Model Adaptation Method for Tracking Simulation”**

The author wrote the manuscript. The author, in collaboration with Dr. Karhela and Mr. Ruusu, developed the conceptual design of the proposed method.

The author implemented and tested the model adaptation method under the guidance of Dr. Karhela and Prof. Vyatkin.

**Publication VI: “An Integrated Implementation Methodology of a Lifecycle-Wide Tracking Simulation Architecture”**

The author wrote the manuscript. The author, in collaboration with Dr. Karhela, developed the conceptual design of the method. The author implemented the architecture and tested the proposed method under the guidance of Dr. Karhela, Dr. Sierla and Prof. Vyatkin.

**Publication VII: Automatic Generation of a High-Fidelity Dynamic Thermal-Hydraulic Process Simulation Model from a 3D Plant Model**

The author wrote the manuscript in collaboration with Dr. Sierla and Mr. Lapalainen. The author, in collaboration with Dr. Karhela and Dr. Sierla, developed the conceptual design of the automatic generation method. The author implemented and tested the automatic model generation method under the guidance of Dr. Karhela, Dr. Sierla and Prof. Vyatkin.

**Publication VIII: Automatic Generation of a Simulation-based Digital Twin**

The author wrote the manuscript. The author, in collaboration with Dr. Karhela and Dr. Sierla, developed the conceptual design of the automatic generation method. The author implemented and tested the generation method under the guidance of Dr. Sierla, Dr. Karhela and Prof. Vyatkin.



# 1. Introduction

## 1.1 Background and motivation

Dynamic models provide simulation results for the transient responses of a process in terms of the time dimension due to expected and unexpected disturbances. In recent decades, dynamic simulation has been widely utilized for important applications in industrial process plants. Process industry domains, such as oil and gas, power generation, pulp and paper and mineral processing industries, rely on dynamic simulation results for applications ranging from plant engineering [1]–[3] and operation support [4]–[6] to control application optimization [7]–[9]. Dynamic simulation has become essential for strategic decision making throughout the process plant lifecycle [10], [11]. However, beyond traditional dynamic simulation-based applications, recent trends in digitalization, along with advances in computational power and wider industrial adoption of interoperability standards, have resulted in the development of Digital Twins for process plants [12], [13]. A Digital Twin (DT) is a digital replica of an industrial plant, containing the structure of the physical assets of the plant as well as the dynamics describing the operation of its devices and processes [14]–[18]. DT is a high-fidelity reflection of the physical space that interacts and converges with the physical system.

While the physical structure of the plant can be determined in a DT by the plant's design material, model-based approaches are required for simulating the dynamics of the physical assets in order to predict, optimize and analyse its changes [19]. Existing commercially-available DT solutions for process plants [20], [21] are commonly based on data-driven models (DDMs) developed purely from the measured data of the targeted industrial plant [14], [22]. DTs based on data-driven approaches rely on black-box models built to capture relations between the inputs and outputs of the plant [10]. DDMs are fast to develop and can be applied to obtain production forecasts or to detect certain production anomalies. However, since DDMs are based only on historical process information obtained from the plant, they cannot be used to forecast abnormal plant operation states not covered by the available collected data. Additionally, they require expert interpretation and are thus difficult to scale up [10]. Moreover, applications based on data-driven DTs depend entirely on the automation and monitoring system data to provide information on the current plant state.

In contrast, simulation-based DTs (SBDTs) are those based on online first-principles simulation models [10], [22]–[24]. First-principles models (FPMs) utilize physical, chemical or engineering descriptions to represent the behaviour

of the modelled plant [9], [25]. SBDTs use a simulation model of the targeted plant to derive information and predict the dynamics of the modelled system. In these applications, the model runs together with the plant, while model adaptation techniques keep the simulation state in the same state as the targeted device or process [26]. These simulation configurations are also known as tracking simulators [5], [27] and are based on online model-based applications [10]. A SBDT can be used to obtain high-fidelity predictions, including production forecasts of operating regions, from which no measurement data is available [6]. Furthermore, SBDTs can be used for developing operator training simulation systems, for production optimization, or for troubleshooting and failure diagnoses. SBDTs are a holistic and powerful application for supporting the operation of modern industrial plants.

## **Simulation model development in the process industry**

The industrial process simulation models required for implementing SBDTs are generally created manually using flowsheet-based simulation environments [28]–[30]. These environments allow for manually dragging, dropping and connecting simulated process components into the model configuration canvas of their graphical user interfaces (UIs). In these canvases, model components can be configured according to the structure of the modelled process [31]. A major advantage of these systems is that the development of the model can be performed without a thorough knowledge of the underlying simulation language utilized by the modelling tool. In addition, the structure of the model can be explored through the UIs of the simulation tool. However, since the model development thereof is carried out manually, creating and maintaining industrial FPMs becomes time-consuming and thus expensive [32]–[35]. Reusing existing simulation models created for process engineering could significantly reduce model development effort and cost [33]. However, FPMs development remains laborious [10], making them less attractive than lower fidelity options based on data-driven approaches, which can be developed with less engineering effort [10], [36].

Automatic model generation (AMG) is a promising approach for addressing laborious development and maintenance of FPMs [26]. Existing AMG methods are based on the utilization of plant design data, available from different engineering information sources. These sources include control application programs, technical data sheets of the process equipment, as well as piping and instrumentation diagrams (P&IDs) [28], [37], [38]. However, information on the equipment dimensions and of the piping network structure is highly important for generating high-fidelity FPMs. In particular, pipeline elevations, lengths and head loss coefficients are highly important for generating accurate simulation models required for implementing SBDTs. Head loss coefficients represent head losses caused by abrupt changes on the pipeline network direction. They can only be obtained from information concerning the structure and dimensions of the pipeline and its curved pipe segments [39]. This information

can be obtained only after a 3D pipe routing has been accomplished [40]. Information from 3D computer assisted design (CAD) models of the plant could be used in combination with other plant design information sources to automatically generate the underlying process simulation models of SBDTs [41].

## Implementation of SBDTs

DTs interact with real-time and historical data of the plant in order to remain a high-fidelity representation of the process [42]. Therefore, during their implementation, SBDTs must be integrated with the process and its ICT infrastructure. During this integration phase, also known as Model Deployment [26], the simulation system of the SBDT is connected to the process control application as well as to its monitoring and historical data repository systems. Integration of the simulation system with the process is a safety-critical task, as this is performed during plant operation [4]. At the same time, the complexity of the integration is highly dependent on the information accessibility conditions that can vary according to the plant and its ICT infrastructure [43]. Moreover, expensive integration hampers the scalability of simulation-based applications, particularly when several systems require integration with the process plant [44]. A major limiting factor preventing the exploitation of DTs is the manual work involved in collecting source information and updating the DT over the lifecycle of the plant. Current megatrends, such as Industry 4.0 [45], [46], Industrial IoT [47]–[50] and Cyber-Physical Production Systems [15], [51]–[54], offer solutions to the problem of making all relevant data available in real time throughout the lifecycle of the plant for generating and maintaining as automatically as possible high-fidelity DTs. Industrial interoperability standards often available in modern plants [55], such as OPC and OPC Unified Architecture (OPC UA) [56], could be used for interfacing the simulation system with the plant. Other examples of industrial interoperability standards examples include (but are not limited to) the data distribution service (DDS), proposed by the Industrial Internet Consortium [57].

An SBDT of a process plant is a real-time reflection of the physical plant that maintains synchronization with the physical system. In a SBDT, this is realized by combining model adaptation and dynamic state estimation methods. Model adaptation is based on applying model optimization methods for reducing model residuals. These methods focus on adjusting model parameters utilizing recent plant measurements, obtained from historical process data [58]. In highly complex systems, model optimization results may fail to converge at the required cycle time [59]. Consequently, these methods must be executed offline. In contrast, dynamic estimation methods, such as Kalman filtering [60] or implicit dynamic feedback [58], can be used for real-time model parameter estimation. Dynamic estimation, also known as online calibration [10], can be seen as a feedback process targeted to bring the model results to the real-time process measurements.

Despite significant advances in the application of data-driven optimization and dynamic estimation of FPMs, little research has focused on the development of simulation architectures designed for reducing the time and effort required to integrate simulation systems and simulation methods with the process plant throughout the SBDT lifecycle [43]. These simulation architectures could exploit industrial communication standards for reducing integration effort [10], automating access to historical plant data as well as for managing the exchange of information throughout the SBDT lifecycle [61]. Consequently, there is a need for implementation methods and simulation architectures targeted at reducing not only SBDT development effort but also integration complexity between the SBDT and its corresponding physical plant [26].

## 1.2 Research goals

Due to the aforementioned challenges related to laborious model development and complex integration required to implement SBDTs, this work aims to achieve the following research goals:

1. To propose an automatic model generation method for leveraging 3D CAD plant model information in order to partially automate the development of high-fidelity thermal-hydraulic FPMs.
2. To propose a semi-automatic methodology for implementing SBDTs from FPMs, such as the FPMs generated using the method developed in Research Goal 1. The proposed methodology includes the following simulation methods applied over the SBDT implementation and operation phases: model adaptation, model initialization, predictive simulation as well as online and offline parameter estimation.
3. To propose an SBDT architecture for integrating the simulation methods from the Research Goal 2 in order to enable their utilization over the SBDT lifecycle. This architecture leverages on the application of industrial interoperability standards for reducing the effort required for configuring the communication between different architecture components. Similarly, the industrial communication standards utilized, enable systematic information exchange between the architecture components and methods.

## 1.3 Hypotheses

This dissertation tests two hypotheses:

1. A high-fidelity dynamic thermal-hydraulic FPM can be automatically generated from source information consisting of 3D CAD plant models and other plant design data, such as technical data sheets for plant equipment.
2. SBDTs and their system architectures could leverage on the utilization of standard communication interfaces for automating information exchange between SBDTs components. Similarly, these architectures

could exploit these standards to seamlessly integrate plant ICT systems with different simulation methods required to implement and operate SBDTs.

## 1.4 Contribution to the field

The contributions of this dissertation are three-fold:

1. An AMG method based on 3D CAD plant model information is proposed. The proposed method exploits process information available during the design stage of the plant lifecycle. This enables application of the automatically generated model for other important applications during subsequent lifecycle stages. Experimental results have shown that the proposed method can generate process simulation models with higher fidelity compared to those generated by following state-of-the-art AMG methods. Additional results confirm that the simulation models generated by following the proposed approach can be used for implementing SBDTs.
2. An integrated implementation methodology is proposed for developing SBDTs. The proposed approach integrates various simulation methods required over the lifecycle of SBDTs. This approach consists of a model optimization method, used for model adaptation and offline model parameter estimation, as well as other methods for model initialization, dynamic estimation and predictive simulation. The proposed model adaptation approach can be applied for automatic re-estimation of model parameters for reducing the model residuals in previously existing simulation models or in models generated by following AMG approaches. Furthermore, the proposed model initialization procedure is carried out by modelling the real process control system, which can be run faster than real time to enable faster initialization. Finally, regarding the dynamic estimation needed for the SBDT synchronization with the physical plant, a new estimation method was developed based on implicit dynamic feedback. This novel dynamic estimation method is proposed to overcome shortcomings in similar existing approaches. The results of dynamic estimation experiments show that the simulated state of the adapted model can be continuously synchronized with the physical process state, thus confirming that the proposed approach can be applied for implementing the SBDTs of process plants.
3. Finally, a simulation architecture is implemented based on the industrial interoperability standard OPC UA. This architecture enables seamless system integration of the SBDT components into the ICT infrastructure of the plant. During connection of the model with the physical plant, the utilization of an industrial interoperability standard reduced the time required for connecting the simulation model with the physical plant and its ICT infrastructure. Finally, the architecture utilizes OPC UA for systematically retrieving historical process data as

well as for reducing the configuration effort needed to interface the SBDT components by avoiding the need for point-to-point connections.

## 1.5 Summary of the publications

This thesis consists of eight publications. Two have been published as journal papers, and the six remaining have been published as conference papers. The publications are summarised as follows:

**Publication I.** This paper presents tracking simulation architecture based on the OPC UA industrial interoperability standard. The proposed architecture was designed for testing dynamic estimation methods required for model parameter adjustment of SBDTs. In the proposed system, OPC UA is used for interfacing the physical system with the simulation system. This work first introduces the structure of the testbed. To test the proposed system, a previously published dynamic estimation method based on the tuning of the model parameters using PI controllers is implemented and tested using the laboratory process described in Section 4.1.

**Publication II.** This paper presents a hybrid approach for initializing the underlying simulation model of a SBDT. The presented approach exploits OPC UA-enabled communication between the simulation system and the process to initialize the simulation model. The proposed initialization method performs model initialization in two steps. First, the simulation model is provided with initial conditions closely corresponding to the current plant state. In the second step, the model is run in the same state as the physical system using a model of the process control system. Possible mass or energy errors in the state of the simulation model are corrected before starting the dynamic parameter estimation. In this paper, the proposed initialization method is implemented and tested using the laboratory process described in Section 4.1.

**Publication III.** This paper presents two case studies focusing on dynamic estimation, in which the controlled parameters are selected using different techniques. The first case study deals with a laboratory-scale hot water generation process, described in Section 4.1, in which the parameters are selected manually. This paper presents the laboratory process, its online simulation system and ICT architecture. In addition, presents the parameter selection procedure followed and the dynamic estimation results. The second case study investigates a combined heat and power production process with major uncertainties in the process structure. In this case, the paper introduces a variance decomposition method for determining the most suitable controlled parameters for dynamic estimation.

**Publication IV.** This paper presents a dynamic estimation method based on implicit dynamic feedback estimation. The proposed approach applies sliding mode controllers (SMC) for dynamically adjusting model parameters. SMC controllers can be more easily tuned than PI or PID controllers. Furthermore, they are more robust against uncertainties caused by simulation model behavior or

by plant measurement noise. In this work, an SMC-based approach for tracking simulation is described, implemented and tested using the laboratory process described in Section 4.1.

**Publication V.** This paper presents a model adaptation method for implementing SBDTs. The method utilizes a model optimization method to adapt simulation models developed during the engineering phases of the process plant and then apply them in the operation and maintenance stages. The model adaptation method proposed in this work utilizes OPC UA to seamlessly connect the simulation system to the physical plant without disrupting the process operation and to retrieve the historical data of the plant in a systematic manner. In this work, the method is described, implemented and tested using the laboratory process described in Section 4.1.

**Publication VI.** This work integrates the methods presented in Publications I-V into a novel SBDT architecture to address the laborious development of FPMs as well as high costs of integrating with the process or with other systems and simulation methods. The developed simulation architecture applies the proposed methodology during various phases of the tracking simulation. Furthermore, the architecture exploits the industrial communication standard OPC UA to avoid the need for point-to-point integration of various simulators and other systems used over the course of the SBDT lifecycle. The work is demonstrated with the laboratory process equipment described in Section 4.1.

**Publication VII.** This paper presents a method for automatic generation of a thermal-hydraulic process simulation model from a 3D CAD plant model. The process structure, dimensioning and component connection information included in the 3D CAD plant model is extracted from the machine-readable export of the 3D CAD tool and used to automatically generate and configure a dynamic thermal-hydraulic simulation model. In particular, information concerning piping dimensions and elevations is retrieved from the 3D plant model and used to calculate the head loss coefficients of the pipelines and to configure the piping network model. This step, not considered in previous studies, is crucial for obtaining high-fidelity industrial process models. The proposed method is tested using the laboratory process described in Section 4.1, and the results of the automatically generated model are compared with experimental data from the physical system as well as with a simulation model developed using design data utilized by existing state-of-the-art methods.

**Publication VIII.** This paper focuses on applying the methods developed in Publications I-VII for reducing the implementation effort of SBDTs. First, laborious simulation model development is tackled by applying the automatic model generation method presented in **Publication VII**. Second, the integrated implementation methodology presented in **Publication VI** is followed for developing an SBDT. The SBDT of a laboratory-scale process is implemented to demonstrate the proposed method. The results show that the method proposed in this work reduces the implementation effort required for developing industrial SBDTs, thereby increasing industrial adoption of these systems.

## 1.6 Structure of the thesis

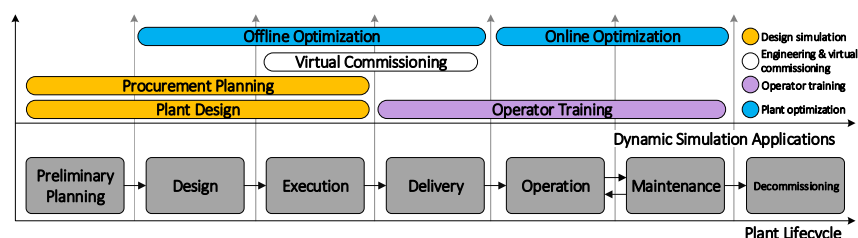
This thesis presents a novel method for semi-automatically generating the SBDT of an industrial process plant. In this work, laborious model development is addressed by applying an AMG generation that utilizes 3D plant model information for automatically generating the underlying simulation model of a SBDT. Furthermore, laborious system integration of the simulation model with the plant is overcome by applying an integrated implementation method for a lifecycle-wide tracking simulation architecture. Chapter 2 reviews related work on the development of SBDTs for the process industry. Chapter 3 presents the proposed SBDT implementation method. This chapter also describes the proposed AMG method as well as the integrated tracking simulation architecture and implementation method. A description of the case study, as well as the results of the proposed implementation method, are presented in Chapter 4. Chapter 5 provides a critical discussion of the results of this work. Finally, conclusions are presented in Chapter 5.

## 2. Related work

### 2.1 Simulation-based applications in process industry

Simulation technology has become highly important for decision support across the lifecycle of the process plant in various industries, including chemical, power generation, oil and gas, pulp and paper and mineral processing [10], [11]. Simulation is based on mimicking the physical, chemical, energy or information-related behaviour of the system based on a mathematical model [62]. Simulation can be understood as a virtual experiment to better understand or predict the modelled system. First-principles simulation models use rigorous physical, chemical and engineering relations to model the behaviour of the targeted system [9], [25]. They capture more detailed process information than data-driven modelling alternatives [10], as DDMs solely focus on finding empirical relations based only on the input and output data collected from the modelled system.

FPMs can be divided into either static or dynamic models. Static FPMs describe a system without the time dimension; thus, they can predict only time-independent system responses [63]. In contrast, dynamic FPMs can predict process transient responses to both unexpected and expected disturbances [64] even before measurement data from the physical plant becomes available [43]. Therefore, dynamic FPMs have become essential for several applications throughout the plant lifecycle, including lifecycle stages during which the plant is not yet functioning. Common industrial simulation-based applications over the plant lifecycle are shown Figure 1.

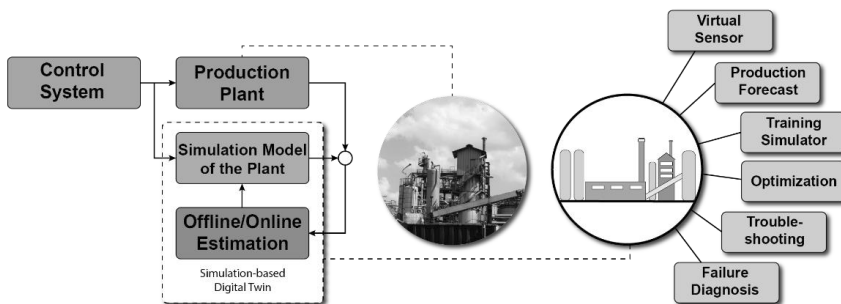


**Figure 1.** Industrial simulation-based applications over the plant lifecycle and their classification based on [65].

Industrial simulation-based applications have been classified in [35] according to their target as: *Design simulation*; *Simulation-supported engineering and virtual commissioning*; *Operator training*; and *Simulation-supported plant optimization*. This classification over the plant lifecycle is shown in Figure 1. *Design simulation* applications are targeted to define the process layout as well

as to investigate the plant behaviour during start-up, shut-down, steady-state and possible production transients. Examples of these applications are presented in [66]–[68]. *Simulation-supported engineering and virtual commissioning* applications are developed after control system engineering to aid engineering activities, such as procurement planning, further layout refinement as well as virtual commissioning. Virtual commissioning refers to the use of a process simulation model for testing the control application during plant engineering when the physical process is yet not available [34]. *Operator training* applications are developed to prepare operating personal on how to handle the plant [69]–[71]. Finally, *Simulation-supported plant optimization* applications focus on the use of simulation models to support decision making for optimal process design and operation [43], [72], [73].

SBDTs of production plants, also known as tracking simulators [6], [26], [27], are a relatively new simulation-based application that has started to be developed, driven by recent trends in plant digitalization. SBDTs are digital replicas of the targeted plant, which rely on first-principles simulation models to represent its dynamics [22], [23], [54], [74]. These applications leverage the persistent communication between the simulation and physical systems in order to permanently synchronize their underlying dynamic simulation model with the operational plant. Offline and online model estimation methods are utilized to continuously update the simulation model for ensuring that their results correspond to the current process state. SBDTs integrate other simulation-based applications used during process operation and maintenance, such as operator training and online optimization systems. Additionally, since they are based on FPMs, non-measured plant data can be derived from the simulation model. This application is known as a virtual sensor [10]. Finally, SBDTs can also be used for obtaining production forecasts, for trouble-shooting and for diagnosing plant failures. Thus, SBDTs are a holistic tool for plant operation support.



**Figure 2.** A simulation-based digital twin and its applications during the operation and maintenance phases of the plant lifecycle [75].

## 2.2 Development of FPMs in the process industry

Industrial simulation models based on FPMs have been utilized in the process industry for several critical applications. Development of industrial FPMs involves three steps [10]. First, mathematical descriptions based on physics, chemical or engineering relations of the system are obtained. Next, the actual

simulation model is created and configured in the selected simulation environment. Finally, the simulation model undergoes model initialization, in which initial solutions of the model equations are obtained utilizing best-available estimates of the simulation variables [61].

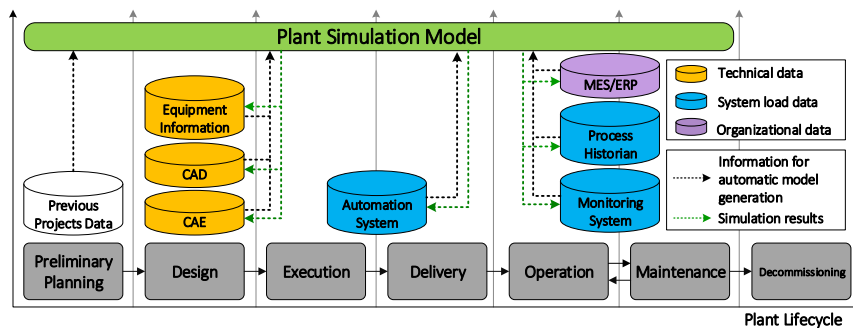
The amount of effort required for model development depends on the complexity of the application. Similarly, it is also dependent on the solver characteristics of the simulation environment in which the model is being developed [76]–[78]. Simulation environments are classified as equation oriented (EO) or as simultaneous modular (SM), according to the solver they utilize [10], [79]–[81]. In EO tools, the model solution directionality is not unique nor pre-defined. Therefore, model equations in EO systems can be solved concurrently [43], [73]. In SM tools, simulation streams and units must be solved starting with the input feed streams, following a specific unit sequence. EO and SM approaches have been compared in [82], and their trade-offs have been shown to be mainly related to the amount of effort required for initializing the simulation model [83], [84].

Irrespective of the solver characteristics utilized by the simulation tool selected, simulation models of industrial processes are generally created manually using flowsheet-based simulation tools [28]–[30]. These tools allow simulation process components to be manually dragged, dropped and connected into the model configuration canvas of their graphical user interfaces (UIs). In these canvases, model components can be manually configured in accordance to the structure of the modelled process [31]. In this work, model components refers to all the simulation elements comprising a given model, such as models of process piping network segments as well as models of process equipment and thermal-hydraulic points (TH points). Model configuration is based on providing model components with nominal parameters derived from structural data of the physical plant. A major advantage of these systems is that the development of the model can be performed without a thorough knowledge of the underlying simulation language utilized by the modelling tool. In addition, the structure of the model can be explored through the UIs of the simulation tool. However, since this model development is carried out manually, creating and maintaining industrial FPMs is time-consuming and thus expensive [32]–[35]. Consequently, FPMs are less attractive than other lower fidelity modelling approaches based on data-driven modelling, as DDMs are generally faster to develop [10], [36]. Reusing models created for process design can reduce the maintainability costs of simulation-based applications [33], [37], [66]. However, the actual development of FPMs remains laborious, limiting broader adoption of these systems in the process industry [10].

## 2.3 AMG of industrial process simulation models

AMG could be applied to enable broader utilization of simulation-based applications during early plant lifecycle stages and to reduce maintenance costs and the development effort of FPMs [26], [40]. AMG methods are based on generating a simulation model from the design information of the targeted plant [61].

These methods automatically map the available plant information into the model configuration defined by the selected simulation tool [85]. AMG methods exploit different plant data sources available over the plant lifecycle stages, as shown in Figure 3. For this reason, the applicability of specific AMG approaches is determined by the availability of the data sources required by the AMG method. Data sources for AMG have been classified in the industrial manufacturing domain according to their information as *Technical*, *System Load* and *Organizational* [86]. No equivalent classification is available for industrial process plants, in which there are additional sources from which historical data can be obtained describing the process dynamics of common operating regions. For this reason, Figure 3 extends the classification presented in [86] and positions AMG data sources available in process plants according to the corresponding lifecycle in which they are available.



**Figure 3.** Data source availability for automatic model generation during the plant lifecycle and their classification [41].

AMG methods have been classified in [87] according to the implementation techniques followed. This classification groups AMG as *Structure*, *Parametric* and *Hybrid-knowledge-based*. *Structural* AMG utilizes CAD and CAE information for generating the simulation model [88]. *Parametric* methods focus on generating the model after connecting components from their corresponding simulation libraries [89]. *Hybrid-knowledge-based* methods combine *Structure* and *Parametric* approaches. They are the most common approach followed by existing AMG methods [28], [88], [90], [91], as plant information is seldom accessible only from structural or only from parametric sources.

Some of the earliest implementations of AMG methods in industry have been developed in the manufacturing domain. *Parametric*-based approaches for AMG of manufacturing systems have been presented in [31], [92]–[94]. Since manufacturing systems dynamics can be captured as discrete sequences of actions in time, these studies have been implemented utilizing discrete-event simulation tools. However, this restricts their utilization for automatic generation of industrial process models, as the dynamics of industrial process systems must be captured using continuous models to track the process transient responses over time.

In the industrial process domain, although some research has been dedicated to the automatic generation of plant control applications during plant design

[33], [34], [88], [95], [96], these methods have mainly been targeted at developing the control application configuration of their application for virtual commissioning. Consequently, these techniques do not tackle the AMG of the process to be controlled. Automatic generation of the process model during plant design stages is desired, as the simulation models generated during early stages could be utilized in a wider number of applications at subsequent lifecycle stages [35], [82], [97]. In addition, simulation results available during plant design are key for achieving system-wide optimization throughout the entire plant lifecycle [98]. Existing methods for AMG of industrial process models during plant design [28], [37], [91], [99] have been based on automatically generating a simulation model of the plant after accessing plant information from computer-aided design (CAD) and computer-aided engineering (CAE) systems. Plant information available from these systems includes technical data sheets of process equipment as well as P&IDs. A major advantage of the approaches presented in [28], [37], [91], [99] is that, since they utilize data available from P&IDs, the AMG based on these methods can be performed during very early plant design. This is possible, as P&IDs are one of the earliest design documents created during plant engineering. P&IDs are developed before other design documents, such as isometric drawings, equipment data sheets and 3D plant models. However, important structural information on the process piping network and equipment, required for developing and configuring highly accurate FPMs of the plant, is not available from these sources [39].

In recent decades, engineering and procurement companies have started creating and utilizing 3D models of process plants for process design and as a reference document for early plant commissioning [100]. This raises the possibility that 3D plant models could be utilized as an information source for AMG. Particularly, piping network elevations, lengths and head loss coefficients could be derived from the plant structural data included in their 3D models. However, such utilization of 3D model information has only been suggested for finite-element-based flow calculations [28], [90]. Consequently, the information available from 3D plant models could potentially be also exploited for AMG of industrial process simulation models.

## 2.4 Digital twins

A DT has been defined as a digital copy of a physical asset, which contains models of its structure and of its behaviour [14], [23]. It is a digital description of the physical and functional aspects of a component, product or system [101]. DTs present information based on previous and current lifecycle phases and are able to seamlessly transfer this information to subsequent phases [54]. Additionally, a DT must be able to predict future states of the physical asset through simulation [102]. According to the definitions presented in [19], [102], DTs fulfil the following characteristics: 1) They are a real-time reflection of the physical asset. This is achieved through continuous synchronization between the real asset and the DT states. 2) They are fully integrated with the real asset as well as interact

with current and historical data of the physical asset, enabling continuous improvement of the DT. 3) A DT can directly compare and analyse predicted and measured values of the physical asset. As a result, a DT can be used for simulating, monitoring, optimizing and verifying various activities throughout the entire lifecycle of the asset.

Various DTs have been implemented in different industrial domains since its introduction over a decade ago [103]. Although, the interpretation of DT is relatively homogeneous across different technology fields, the functional characteristics of these systems and their implementation methods vary significantly depending on their end-applications. In the automotive and aerospace industries, DTs have been used as an ultra-high fidelity simulated replica of a vehicle. They have been applied for anomaly diagnoses and for predicting future states and remaining useful life [22], [24]. In the construction industry, DTs have been implemented after combining virtual building models with physical data in order to obtain more accurate information regarding structure fatigue [101].

In manufacturing, DTs of production assets have been applied for product lifecycle management. In these applications, DTs mirror the entire lifecycle of end-products, resulting in applications for product lifecycle design as well as for services design and optimization [13], [42]. On the other hand, DTs of the actual manufacturing system [19], [103], [104] have been mainly based on virtualization for achieving improved flexibility, scalability and efficiency. Simulation functionalities in the DTs of manufacturing systems utilize discrete-event models in which the dynamic changes of a system can be represented and predicted as discrete sequences of events over time [61].

In the process industry domain, applications which fulfil some of the characteristics of DTs have been proposed in recent decades. They follow implementation approaches for capturing the process dynamics that differ from those followed in the manufacturing domain, as discrete-event modelling cannot be applied for prediction of continuous systems [43], [58]. The commercially-available DTs for process plants [20], [21], are based on DDMs for representing the plant dynamics. Although these models are fast to develop, data-driven-based DTs have limited capabilities, as they are strongly dependent on the quality and quantity of measurement information available from the targeted plant. Moreover, while DDMs can predict a set of system outputs given a set of inputs, they offer limited information on sub-systems states and their process values. This is because they are only based on finding relations between the inputs and outputs of their targeted systems.

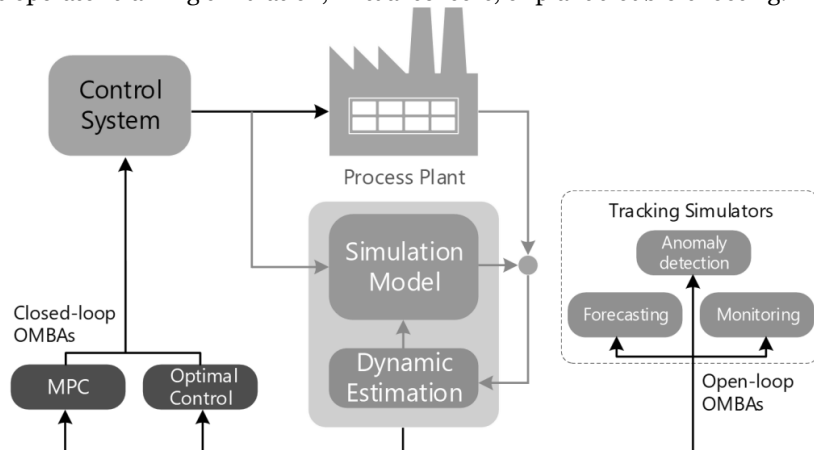
In contrast, existing SBDTs [4], [6], [27], [105] rely on online FPMs based on an up-to-date condition of the physical plant that can be built from plant design data and that can be applied to explore operating regions not captured by the process measurement systems. SBDTs are based on online model-based applications (OMBAs) [10], which consist of an online simulation configuration that runs a dynamic FPM in parallel with the modelled plant, while being controlled by the plant control application. Consequently, these applications are implemented during the operation and maintenance phases of the plant, when it is

possible to interface them with the physical system through connections between the simulation system and the control application of the plant.

## 2.5 Online model-based applications in process industry

OMBAs [10], [58] are online simulation systems that are continuously adjusted by dynamic estimation methods to ensure that their result will correspond to the current process state. These systems, also known as symbiotic simulation systems [106]–[108], have been developed for applications ranging from virtual sensors [109] and prediction systems [5] to model-based control [110]. In OMBAs, the online simulation system interacts with real-time measurements of the plant and benefits from these by continuously adjusting its results through dynamic estimation [58]. In contrast, the layout of the feedback connection from the simulation system to the plant [111] determines the way in which the physical system benefits from the online simulation results. Consequently, OMBAs are classified into *Closed-loop control* and *Open-loop advisory online model-based* applications [10], [106], as shown in Figure 4.

In *Closed-loop control* OMBAs, the direct feedback connection from the simulation system to the plant is directly interfaced with the control application of the plant for directly implementing control actions. Model-predictive control (MPC) and optimal control are the most common applications of these systems [8]. Consequently, the real-time requirements of industrial control applications often limit *Closed-loop* OMBAs to focus on specific process subsystems. Similarly, they often utilize DDMs derived from collected process data, further limiting their application to study specific process operating regions [110] and limiting their utilization for other important operation support applications, such as operator training simulation, virtual sensors, or plant trouble-shooting.



**Figure 4.** Closed-loop and Open-loop online model-based applications (OMBAs). Tracking simulators integrate the different variations of Open-loop OMBAs [26].

In contrast, *Open-loop advisory* OMBAs require no feedback connection from the simulation system to the physical system. These systems can be developed based entirely on either FPMs or hybrid models. In hybrid models, model equations utilize physical principles, though data-driven methods are applied for

modelling process uncertainties. *Open-loop advisory* OMBAs are decision support applications which can be used to study entire plants or specific plant subsystems. Furthermore, they can also be used for simulating any plant operating region and their underlying simulation model can be used for obtaining current and future state information regarding the process. *Open-loop* OMBAs can be further divided into three classes: *Anomaly Detection*, *Monitoring*, and *Forecasting Open-loop advisory* OMBAs. *Anomaly detection Open-loop* OMBAs are applied for plant anomalies and fault diagnoses [81], [112]. In *Monitoring Open-loop* OMBAs, unmeasured plant data is obtained from the results of the online simulation model [6]. *Forecasting Open-loop* OMBAs are utilized for production forecasting.

## 2.6 Tracking simulation systems

Simulation-based systems that integrate the applications of different *Open-loop advisory* OMBAs are known as Tracking Simulation Systems [4], [5]. Similar to OMBAs, tracking simulators consist of dynamic FPMs, which are continuously adjusted by dynamic estimation to synchronize the states of the model and the physical plant. These systems provide information that can be used for supporting operator training [113], process operation [35], process maintenance [105] and plant optimization [114]. Tracking simulators serve as the SBDTs for process plants, as they provide a holistic set of simulation-based applications for operation support. However, the drawbacks of tracking simulators in terms of expensive and laborious development of FPMs, restrict broader adoption of these systems in industry [10]. Existing systems [4], [6], [27], [105] have mainly focused on proposing different methods for parameter estimation of FPMs. Moreover, no work has attempted to address issues related to time consuming model development or laborious implementation of tracking simulators. Therefore, there is a lack of implementation methods that would allow model reutilization, or that could exploit AMG approaches for developing SBDTs.

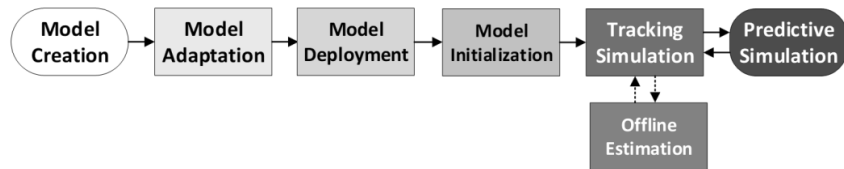
Wider adoption of tracking simulators has been further limited by the complex integration needed to interface the simulation system and architecture with the plant. There is also a need for simulation architectures that could enable reduction of integration time and effort [43]. A possible approach to overcome this particular challenge would be to utilize industrial interoperability standards for three purposes: to automate access to the historical data of the plant; to reduce the effort needed for establishing communication between the simulation and physical system [10]; as well as to manage information exchange more efficiently over the tracking simulation lifecycle [61], [83].

To further improve the model results, a tracking simulation system is presented in [105] that applies offline dynamic data reconciliation [115] for adjusting multiple model parameters. This and other existing model optimization methods could be applied not only to aid online dynamic estimation but also to optimize existing outdated models or models generated automatically based on AMG methods. This would further reduce tracking simulation implementation effort and time. However, dynamic data reconciliation and other methods for

optimization of deterministic models require direct access to information in the Jacobian matrix of the model. This is necessary for determining the dependencies between the model results and the model parameters [43], [73]. Moreover, the analytical values of the Jacobian matrix are not always available in simulation software utilized in industry [116], such as the simulation system used in the case study of this work. This is a critical issue preventing adaptation of previously created simulation models.

### 2.6.1 Tracking simulation lifecycle

The tracking simulation lifecycle, shown in Figure 5, corresponds to the implementation and operation phases, in which tracking simulation systems undergo [26]. The first phase of this lifecycle involves Model Creation. As previously explained, plant simulation models are generally created and configured manually. This occurs immediately before the implementation of the tracking simulator. Alternative model development approaches, such as applying AMG methods or reutilizing existing models created during process design, would reduce model development effort. However, applying these approaches would require re-estimation of their model parameter for their results to closely correspond to the current plant behaviour. Therefore, a Model Adaptation phase is proposed in this work. During Model Adaptation, the model parameters from existing models or from models developed following AMG methods are readjusted for enabling their results to capture the process behaviour represented by recent plant historical data. At the Model Deployment stage, the simulation system is connected to the process plant. This is a safety-critical task, as the simulation system must be seamlessly interfaced with the plant during process operation. At the Online Model Initialization phase, the simulation model is provided with a set of initial conditions (ICs) corresponding to the current process state. The simulation model can be initialized using a nominal set of input parameters as well as best-available estimates of the simulation variable values. The Tracking Simulation phase starts after the model, previously initialized, starts being adjusted online by the dynamic estimation method after comparing plant measurements with the online simulation results. During Offline Estimation, offline optimization is applied to aid dynamic estimation for further improving the model results. Finally, during Predictive Simulation, an instance of the tracking simulator is utilized for obtaining predictions. These predictions are based on the current state of the process and are obtained using a simulation model that has been adjusted to mimic the real process.



**Figure 5.** Tracking simulation lifecycle stages [26].

### 2.6.2 Model adaptation for tracking simulation

Model adaptation involves re-estimation of model parameters for their results to represent the newly observed behaviour of the physical system [117]. Several methods for model adaptation of DDMs have been developed in a number of application domains [117]–[119]. The steady increase in computational power has continuously reduced the development time of DDMs, making them easier to develop on demand from recent information. This approach is faster than adapting and reutilizing previously created DDMs.

Model adaptation of FPMs can be seen as a model validation procedure, which involves finding the level of agreement between the system modelled and the actual physical system. Similarly, model validation is a procedure in which the model is iteratively refined until the behaviour best representing the physical system is found [44]. A thorough review of existing model validation methods has been presented in [120], [121]. However, the methods reviewed in these surveys are not targeted for adapting online or tracking simulation models that can exploit persistent communication between the simulation model and the ICT infrastructure of the plant in order to decrease model adaptation time and effort.

### 2.6.3 Initialization of tracking simulation systems

Model initialization procedures are required for obtaining initial solutions for the model equations [61], [122]. These procedures vary according to the simulation tool utilized. Although it is possible to directly write an estimate of the initial state into the model of some SM simulation tools [80], full plant state information is not available or is not accessible until the process operation phase [83]. For this reason, in SM simulation tools, state observers can be utilized to obtain estimates of the unknown information of the plant [123]–[125]. On the other hand, EO simulation tools cannot directly write the state of simulation variables [26]. Therefore, initialization based on the utilization of state observers cannot be applied for EO simulation tools. Steady-state process models have been used to estimate initial values for dynamic simulators [10], [126]. However, steady-state models are not always available, or their configuration may not be updated to correspond to the process represented by the underlying dynamic model of the tracking simulation system.

In tracking simulation systems, persistent communication between the simulation system and the plant can be used to feed data from the real system into the model for achieving model initialization. Theoretically, it is possible to copy the current state of the real process into the online simulation system of the tracking simulator. However, in reality, sufficient plant state information needed for model initialization might not always be available from the plant ICT infrastructure [61], [83]. An online model initialization method is proposed in [83] based on the initialization of a *Parent simulation* and then creating simulation instances called *Child simulations*. In this approach, a *Parent simulation* is first initialized by retrieving available plant data and then providing it to the model. Next, the *Parent simulation* model is connected to the plant and is run

together with the process. *Parent simulation* instances, called *Child simulations*, are created on demand according to the required application. Creating simulation instances of the online simulation model according to the required application is an interesting approach. However, the authors did not present their initialization method. Moreover, it cannot be assumed that all information required for initialization is always available from the plant measurements of every facility. In cases involving limited availability of measurement information, the initial simulation state may differ from the current plant state.

The work in [61] proposes initialization of discrete-event models by using the core manufacturing simulation data (CMSD) specification developed by the Simulation Interoperability Standard Organization [127]. CMSD is an XML-based specification for data exchange between manufacturing systems and discrete-event-based simulation tools. The initialization approach in [61] is based on selecting, classifying and mapping the input data required for the initialization into an XML format. This XML file can be later read by the targeted simulation system. Although this method addresses the need for systematic model initialization methods based on standards, the procedure followed is only applicable to manufacturing applications that use discrete-event models to represent discrete states of machines, jobs, or parts.

#### 2.6.4 Dynamic estimation methods for tracking simulation

Dynamic estimation is based on dynamic adjustment of model parameters for reducing model residuals. This estimation is performed after comparing simulation results with real-time measurements of the modelled plant. This method is targeted to determine a best estimate of the current state of the process. Single-input-single-output (SISO)-based dynamic estimation methods pair a measurement with an unmeasured disturbance for estimating the state of a model variable [58]. Although SISO approaches are simple to implement, they are limited to pair only a single measurement with a single disturbance. Nevertheless, since they add very little computational overhead, they provide faster responses compared to similar methods. Filtered bias update [58] and implicit dynamic feedback [128] are two of the most widely utilized SISO approaches for dynamic estimation of industrial dynamic systems.

Filtered bias update assumes a constant disturbance to update the initial condition offset of a controlled variable by calculating an additive model bias  $b$  at the iteration  $n$  with an exponential filter  $\alpha$ , as shown in Eq. (1).

$$b_n = \alpha(z_n - y_n) + (1 - \alpha)b_{n-1}, 0 \leq \alpha \leq 1 \quad (1)$$

Where  $z_n$  and  $y_n$  represent the measured and model variables, respectively. The value of  $\alpha$  is the only tuning parameter to balance noise rejection. The calculated value of the bias  $b$  can be restricted by validity limits in order to not violate physical constraints of the system in context. A major drawback of this method is that directly updating offset values of energy or mass may result in state instability. Moreover, directly updating the state of variables is not always

possible in causal models, as they are not explicitly described as equations but as algorithms for solving these equations.

Implicit dynamic feedback can be seen as a feedback process that aims to align the simulated results with the process measurements in the same manner feedback is used in a control application to drive measured process variables to their set points [10]. This method focuses on adjusting model parameters to match the simulated and process outputs by using feedback controllers (called parameter controllers), as explained in [27], [58], [128]. Parameter controllers can be tuned to avoid abrupt changes in the mass or energy balance of the targeted system, thereby reducing spurious transients. Furthermore, implicit dynamic feedback is also applicable to causal models. PI controllers have been the obvious choice to implement tracking simulators based on implicit dynamic feedback [27], [105]. The PI-based approach updates parameter values as shown in Eq. (2).

$$d = K_c(z - y) + \frac{K_c}{\tau_i} I, \quad \frac{dI}{dt} = (z - y) \quad (2)$$

Where  $z$  and  $y$  are the measured and model variables, respectively, and  $K_c$  and  $\tau_i$  are the tuning parameters. PI tuning is required to balance adjustment speed. The application of autotuning techniques is proposed in [27]. An obvious drawback of this method is the potential instability caused by the integral term. This can be avoided by adequate controller tuning. However, aggressive estimation of simulation model parameters can result in poor prediction results [58].

Other previously studied dynamic estimation methods have included moving horizon estimation [59] and Kalman filters [60], as well as variations such as the extended Kalman filter and the unscented Kalman filter. Moving horizon estimation [59] is based on optimization of the states or parameters of the targeted model. It is an estimation method applicable mainly to simple systems, expressed with a low number of ordinary differential. However, this method becomes computationally infeasible in large systems, due to the need for iterative model evaluations.

Kalman filtering is based on calculating a gain after comparing differences between the real and estimated states. This gain is used for directly updating model states. For linear systems with Gaussian noise, Kalman filtering can produce optimal state estimates. The most straightforward application of Kalman filtering to non-linear models applies linearization (Extended Kalman Filter, EKF [129]). A more robust approach is offered by the Unscented Kalman Filter (UKF) [60], which is based on an unscented transformation approach to the estimation of state uncertainties. It eliminates some of the biases in covariance estimation that result in the linearization of the EKF but requires the ability to evaluate each simulation time step multiple times from different starting points. To be able to utilize the Kalman filtering approach, the simulation model must be implemented to allow direct modification of the state variables. In more complex system models that include partial differential equations across a spatial domain, the option of making updates to a limited number of state variables is not always possible without the introduction of spurious transients. Such is the

case in the thermal-hydraulics simulation that is the focus of this research. For this reason, Kalman filtering approaches were ruled out in this case.

## 2.7 Comparison of existing DT implementation examples

Different examples of DT implementations for the process industry have been presented in this chapter. These examples are compared in Table 1. In a DT, the plant structure information can be obtained from plant design and operation material, such as the P&IDs, 3D plant models, equipment technical data sheets, control configuration programs and automation systems. In [20], [21], which are two of the most popular commercially-available solutions for plant digitalization, plant structure is obtained after integrating different CAD/CAE and automation systems, such as COMOS [130] in the case of [21]. In these systems, plant structure information is contextualized after being presented in an interface based on the P&ID of the targeted plant. In [6], [105], the structural information is also presented in an interface based on the P&ID. Since these systems mainly focus on providing support to plant operators, their user interfaces are very similar to those used for developing operator training simulators. An alternative option for DT visualization would be to utilize the simulation model configuration canvas as the user interface where the structure information is presented. The model configuration canvas contains key process data, such as process components connections and locations as well as equipment nominal and operational data. However, the interfaces of simulation tools are rather simple compared to those obtained after integrating structure data from CAD/CAE plant material. Moreover, navigation through different plant sub-systems using the model configuration canvas can be time-consuming in large processes.

**Table 1.** Comparison of existing examples that implement digital twins for process plants. (The notation "N/A" indicates that no information is available for the approach).

Implementa- tion	Industrial Do- main	Approach for Presenting Asset's Struc- ture	Modelling Approach for Presenting Asset's Dy- namics	Model Generation Approach Followed
[20]	Process and Manufacturing	Integration with CAD/CAE systems.	DDMs	Model cre- ation on demand from pro- cess data.
[21]	Process and Manufacturing	Integration with CAD/CAE systems.	DDMs	Model cre- ation on demand from pro- cess data.
[27]	Process	N/A	FPMs	N/A
[4]	Process	N/A	FPMs	N/A
[6]	Process	Through UIs based on the Asset's CAD/CAE ma- terial.	FPMs	N/A
[105]	Process	Through a UI based on the Asset's CAD/CAE ma- terial.	FPM/Data- driven	N/A

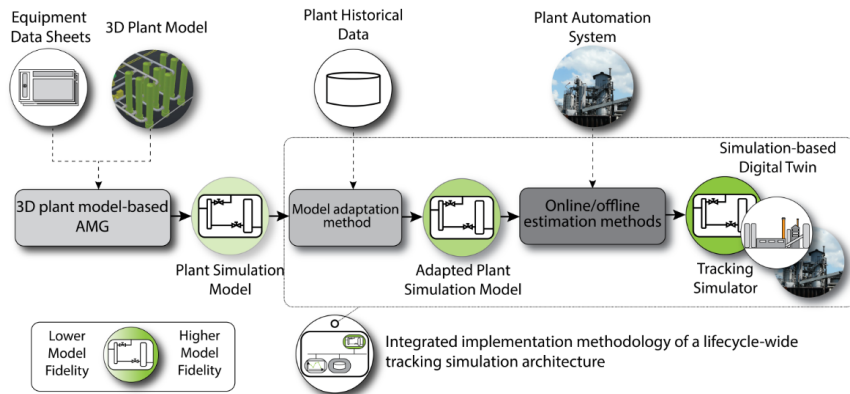
The modelling approach followed for capturing plant dynamics determines the model development method utilized. In [20], [21], plant modelling is based on data-driven methods. These methods use plant data for creating a data-driven model of the targeted plant. Since data-driven models can be developed relatively fast, these models can be developed on-demand when the DT is under implementation. However, the reliability of their results is strongly dependant on the plant data that has been collected. Moreover, it cannot be assumed that sufficiently accurate data-driven models can be developed for every facility, as the conditions for data availability change from one plant to another. In contrast, the SBDTs presented in [4], [6], [27], [105] utilize FPMs to represent the plant dynamics. Since no particular information regarding the model creation approach utilized is given, it is assumed that these systems follow the manual simulation model development practices described in Section 2.2 for developing their underlying plant models.

### 3. Proposed method

#### 3.1 Overview of the proposed method

Based on the shortcomings of existing methods for implementing SBDTs, it is clear that although these systems can bring significant benefits to the operation of industrial process plants, their development remains laborious and expensive. Although research on the reuse of existing simulation models could reduce implementation effort and cost [33], development of FPMs remains time-consuming, and thus expensive [10]. Moreover, wider industrial adoption of SBDTs is limited by the lack of integrated approaches for SBDT implementation, which could address complex integration of the process with simulation systems and the various simulation methods required over their lifecycle [26].

In this thesis, these implementation shortcomings are tackled by utilizing a combination of implementation methods proposed in this work. First, laborious FPMs development is addressed by applying an AMG method based on utilizing 3D plant model information for automatically generating the underlying FPM of the SBDT [41]. Furthermore, laborious integration between the simulation system and the process plant is addressed by utilizing a method for implementing a lifecycle-wide tracking simulation architecture [26]. A conceptual diagram of the proposed implementation method is shown in Figure 6.



**Figure 6.** Conceptual diagram of the proposed SBDT implementation method.

### 3.1.1 Scope of the proposed method

This work is limited to study thermal-hydraulics-based systems and their corresponding models. Thermal-hydraulic simulation models are based on FPMs, which rely on physics, engineering and chemical relations for calculating the thermodynamic properties of hydraulic flow [9], [25], [131]–[133]. Dynamic thermal-hydraulic simulation models are broadly utilized in the process industry for various important applications, including engineering support [1]–[3], operation planning [4]–[6], and online process optimization [7]–[9].

## 3.2 Automatic generation of a high-fidelity thermal-hydraulic process simulation model from a 3D CAD plant model

Laborious and expensive development of simulation models based on FPMs, has hindered wider industrial adoption of these systems. This is evident from the information provided in Table 1, which assumes that the underlying model is created manually, since no information is provided regarding the method followed to develop the FPM in the surveyed SBDTs examples. 3D plant models are created at the process design stage of the plant before building the plant. For this purpose, CAD models could be utilized as a source of information for applying AMG methods, thereby enabling a more efficient and rapid generation of simulation models.

In order to address Research Goal 1 described in Section 1.2, this work proposes an AMG method that leverages the information available from 3D plant models for automatically generating dynamic thermal-hydraulic process simulation models. In this work, information on 3D pipe routing is obtained and applied for calculating and configuring the simulation model based on pipeline lengths and their head loss coefficients. Similarly, elevations of process equipment and of piping sections are derived from the 3D plant model for configuration of the corresponding model components. This information is highly important, as the thermal-hydraulic simulation methodology follows mechanistic modelling, which models in detail the structure and characteristics of the target process, and uses the first principles of physics to describe process phenomena, such as fluid flows and heat transfer [131], [132]. Consequently, the accuracy of the dimensions is of utmost importance. The cross-sectional areas, lengths and shapes of the pipeline sections affect the flow rates and process delays, system volumes, and hydrodynamic losses. Furthermore, the elevations of the equipment and pipe sections affect the pressure levels of the system. This information is not available from a typical PI&D.

The conceptual diagram of the proposed 3D plant model-based AMG method and its comparison with existing P&ID-based AMG approaches is shown in Figure 7. The implementation steps of the proposed AMG method are shown as Unified Model Language (UML) activity diagrams in Figure 8 and Figure 9. The method is divided into Model Generation and Model Initialization, as shown in Figure 8. During Model Generation steps, information is retrieved from the 3D plant model. Next, the model components are generated and then connected. During Model Initialization, the model is first configured and connected to its

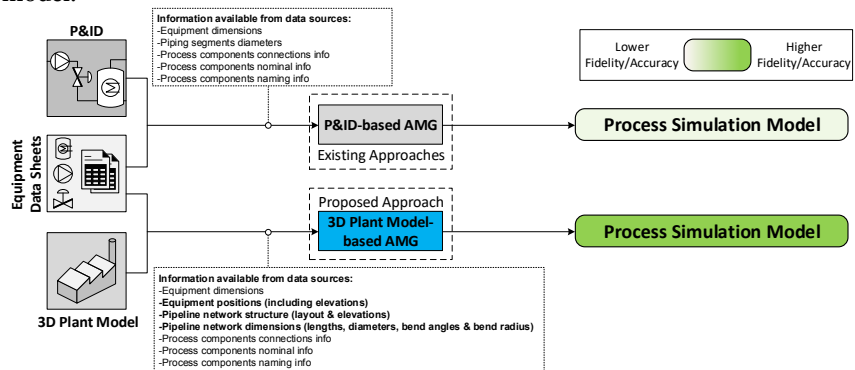
control application before being finally initialized. The proposed method is intended to be implemented utilizing flow-sheet-based simulation tools, as these are widely used in the process industry to develop thermal-hydraulic simulation models. Furthermore, flow-sheet-based simulation tools offer two advantages for implementing AMG:

1. They offer libraries of modelled process components, which can be configured and connected according to the corresponding physical system.
2. They commonly offer script-based commands which can be applied to ease model development.

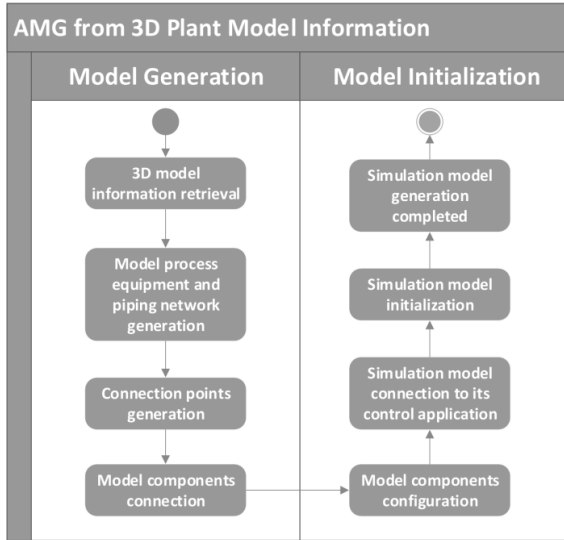
The Model Generation and Model Initialization steps in the proposed method are explained in the following sections.

### 3.2.1 Model generation

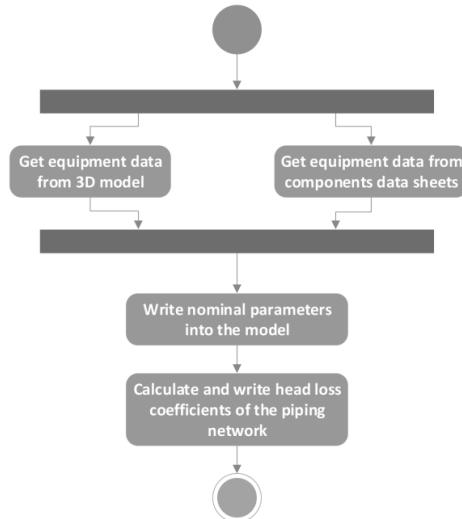
Model Generation starts when the proposed method retrieves information from the 3D plant model. Accessing this information is a non-trivial task which is dependent on both the communication interfaces of the 3D modelling tool used as well as the data access options offered by the tool interfaces. Industrial 3D modelling tools typically offer direct communication to their data bases through their application programming interfaces (API). Alternatively, some 3D modelling systems also offer options for exporting 3D model information as tables of comma-separated values (CSV). The 3D modelling tools *Aveeva E3D* [134] and *Cadmatic* [135] offer export options of files compliant with the Industry Foundation Classes (IFC) data model format. IFC is an XML-based format, standardized in ISO 16739. It is mainly used in the construction industry for describing building data, including their heating and ventilation systems. However, IFC currently supports only air conditioning, heating and ventilation piping systems. Therefore, 3D information regarding the complex pipeline and equipment utilized in thermal-hydraulic systems cannot be represented using the IFC data model.



**Figure 7.** Comparison of the proposed 3D plant model-based AMG approach and existing state-of-the-art AMG approaches which are mainly based on utilizing P&ID data and equipment data sheets [41].



**Figure 8.** Flow diagram of the proposed method for automatic simulation model generation from 3D model information [41].



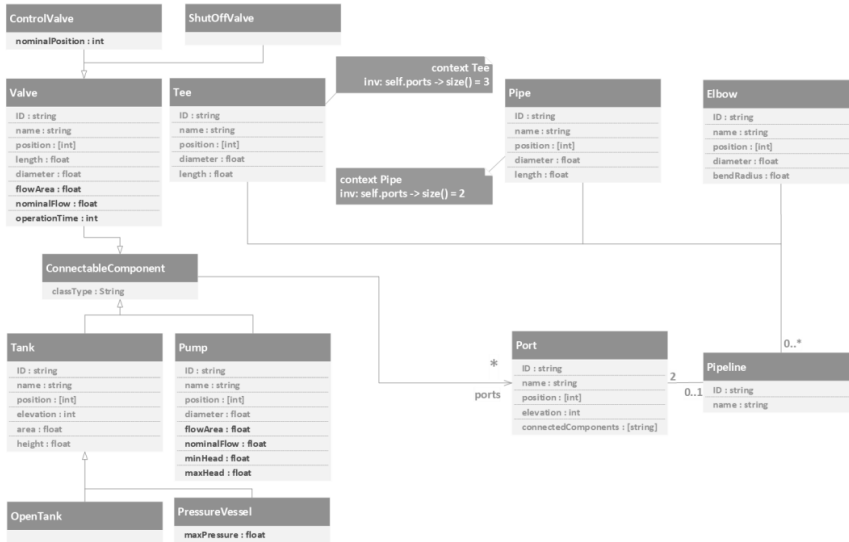
**Figure 9.** Flow diagram of the model components in the configuration subprocess shown in Figure 8 [41].

During recent decades, some efforts have been devoted to the development of industrial standards for data modelling and exchange between process plant engineering systems, including 3D modelling tools. The Computed Assisted Engineering Exchange (CAEX) [136] specification is a promising example of these standards. CAEX is an XML-based neutral data format for plant information modelling and exchange. It is defined in the IEC 62424 specification and has been adopted by the industry-driven initiative AutomationML [137]. However, commercial 3D modelling tools do not support export or import of CAEX format. Recently, the Data Exchange in Process Industry (DEXPI) [138] initiative has been developing a neutral data exchange standard for the process industry. The DEXPI specification is the result of this initiative. It is an extension of the ISO 15926 [139], originally intended for information exchange between P&ID

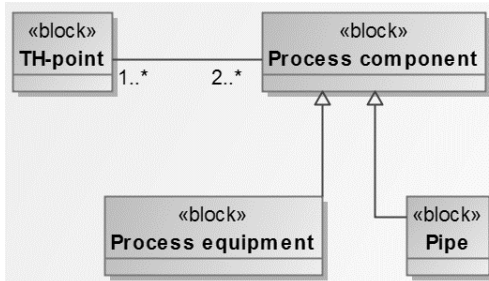
and 3D modelling tools. The DEXPI specification is currently supported by a group of process owners and most vendors of the main CAD tools. However, DEXPI is currently limited to information exchange only between P&IDs tools. The study in [140] presents a comparison of CAEX and ISO 15926 specifications. Broader industrial adoption of standards, such as CAEX and DEXPI, would reduce the effort required for integration of 3D modelling tools with other systems, including industrial simulation systems.

Due to the lack of widespread industrial adoption of information exchange formats, the AMG method proposed in this work uses 3D plant model information retrieved in CSV format directly from the 3D modelling tool database. Information available from 3D plant models includes equipment dimensions, positions, elevations and connections as well as pipe section lengths and elevations. It also includes data related to the piping structure, especially elbows and branches, needed to calculate the head loss coefficients of the process pipelines. In this work, position and elevations are classified separately. Positions refer to XY positions on the horizontal plane. Elevations are defined as the Z coordinate in respect to the XY plane. Finally, the 3D models also contain process equipment naming and nomenclature information. This is required when connecting the simulation model to a real control application or an automation system emulator during plant operation and maintenance phases. Figure 10 shows an UML class diagram of the information available from the 3D plant model of a process comprised of some of the most common components in thermal-hydraulic systems, such as tanks, vessels, valves and pumps. Figure 10 also lists various pipe geometries, including tees and elbows.

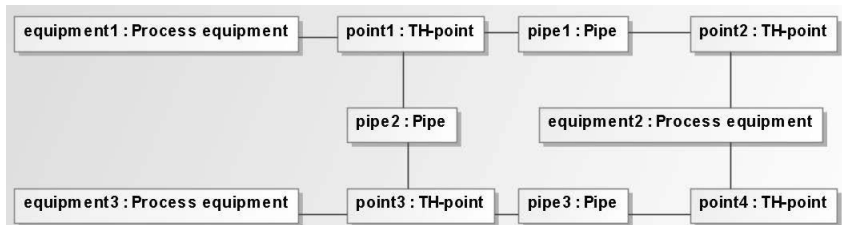
The proposed AMG method first retrieves process information from the 3D modelling tool as a CSV file. Next, model components are generated automatically according to the process information included in the retrieved CSV file. As previously defined, model components are all elements comprising the simulation model, including models of the pipeline network, the process equipment as well as the TH points. TH points are defined as coordinate locations in space which define the elevations and positions of the connections between process components and pipelines. These points play an important role in the thermal-hydraulic solution, as they represent a calculation volume with state information. Model components are generated and positioned on the model configuration canvas of the flowsheet modelling tool using configuration commands offered by these tools. Elevations of pipelines and process components are also highly important, as they are required for calculating hydrostatic pressures in the process. This information is essential for obtaining accurate simulation results and is not available from P&IDs. Generated model components are positioned at their corresponding XY coordinates specified by the 3D model information. After their generation, the model components and the pipeline network are connected using TH points. Figure 11 shows a Systems Modelling Language (SysML) block definition diagram that depicts the simulation model components. Figure 12 shows an internal block diagram that uses the block types defined in Figure 11 to illustrate examples of connections between process equipment and pipes through TH points.



**Figure 10.** UML class diagram of the information available from the 3D plant model comprised of common components in thermal-hydraulic systems [41].



**Figure 11.** SysML block definition diagram of simulation model components. TH-points refer to thermal-hydraulic points [41].



**Figure 12.** Internal block diagram that uses the block types defined in Figure 11 for the purpose of illustrating examples of connections between process equipment and pipes through TH points [41].

### 3.2.2 Model Initialization during AMG

During Model Initialization, model components are first configured by assigning nominal values to their corresponding parameters. Nominal equipment information is defined as the de facto information that represents the conditions in which the process equipment is expected to function under normal operation. Nominal information includes positions, flows, pressure heads, head loss coefficients, power coefficients, and heat coefficients. Nominal values for process

equipment, marked in purple in Figure 10, may or may not be included in 3D models, depending on the level of detail required by the engineering company developing the 3D model. Since it cannot be assumed that nominal equipment information is always available from the 3D model, the proposed AMG method, retrieves this information from technical data sheets. The sub-step for configuring simulation model components is shown in Figure 9. During this step, the retrieved nominal information is utilized to configure the corresponding model component.

Model configuration includes calculation of the head loss coefficients of the pipeline network. Head loss coefficients, also known as pressure loss coefficients or as form loss coefficients [141], are a nominal parameter of pipes that represents head losses due to friction and turbulence. These head losses are caused by abrupt piping direction changes or by cross-section areas of pipelines [142]. Consequently, head losses occur mostly in piping fittings such as elbows, expansions, reducers, tees (a 3-way connector) and 4-way connectors. Analytical methods for obtaining head loss coefficients in pipelines are generally based on the Herschel-Bulkley model [143]–[147]. Alternatively, numerical models commonly used in industry can be obtained from process engineering handbooks, such as [148], [149].

Calculation of head losses in the pipeline network is very important for generating accurate thermal-hydraulic simulation models. In the proposed AMG method, head loss coefficients are obtained utilizing the geometrical pipe fittings information included in the 3D plant model. This information cannot be obtained from other engineering sources. The geometrical information needed for calculating head loss coefficients includes the fitting type, its length, diameter ( $D_0$ ), bend angle ( $\delta$ ) and bend radius ( $R_0$ ). The proposed AMG method calculates head loss coefficients for fittings utilizing the equations in [149]. As an example, equations (3) - (6) correspond to the calculations followed to obtain the head loss coefficient of 90° elbow fittings, shown in Figure 13. The total head loss coefficient  $\zeta$  of a 90° elbow fitting is the sum

$$\zeta = \zeta_l + \zeta_{fr}, \quad (3)$$

where  $\zeta_l$  is the local head loss coefficient of the elbow fitting; and  $\zeta_{fr}$  is the friction coefficient throughout the fitting length.

$$\zeta_l = A_l B_l C_l \quad (4)$$

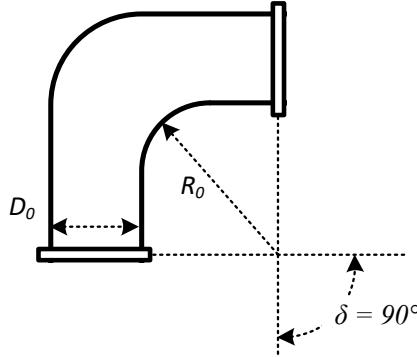
$A_l$  is determined as a function of the fitting bend angle  $\delta$ . In the case of a 90° degrees elbow,  $A_l = 1.0$ .

$$B_l = 0.21 / \sqrt{(R_0 / D_0)} \quad (5)$$

$C_l = 1.0$  for circular or square cross sections.

$$\zeta_{fr} = 0.0175 \lambda (R_0 / D_0) \delta \quad (6)$$

where  $\lambda$  is the friction coefficient of unit length of the curved pipe.  $\lambda$  varies according to the relation  $R_0 / D_0$  of the elbow and can be calculated using equations 6-12 to 6-14 in [149].



**Figure 13.** Elbow fitting and its diameter ( $D_0$ ), bend angle ( $\delta$ ) and bend radius ( $R_0$ ) [41]. Figure adapted from [149].

After completing the model configuration, model initialization must be performed in order to find initial solutions for the set of model variables which define the starting simulation state. Therefore, the proposed AMG approach performs model initialization using a control system for driving the simulation model to a given initial state. This approach is suitable for model initialization of SM and EO dynamic simulators and can be followed even if no steady-state models of the plant are available. For this reason, before initialization, the automatically generated simulation model is connected to its control application. Upon initialization, the AMG method is completed, and the simulation model can now be used for the targeted application.

### 3.3 Integrated implementation methodology of a lifecycle-wide tracking simulation architecture

After AMG, the implementation of a SBDT is followed by integration of the automatically generated model with other plant information systems. This integration must be carried out in a non-disruptive manner while the process plant is under operation. Furthermore, the various simulation methods utilized over the tracking simulation lifecycle must also be integrated into the simulation system. In order to accomplish this, this work proposes applying an integrated tracking simulation methodology of a lifecycle-wide tracking simulation architecture. The proposed methodology aims to address Research Goals 2 and 3, described in Section 1.2. The proposed architecture, originally designed for developing tracking simulation systems from previously existing models, is applied to develop SBDTs from automatically generated FPMs. The remaining of this chapter focuses on the description of the proposed approach which integrates an implementation method and a lifecycle-wide tracking simulation architecture.

### 3.3.1 Lifecycle-wide tracking simulation architecture

The proposed tracking simulation architecture is shown in Figure 14. It is comprised of a Simulation System and a Historical Data Repository. The Simulation System contains three simulators: Online, Optimization and Predictive. The Online Simulator is permanently running in parallel with the plant, controlled by the process control application. The Optimization Simulator is used to run an offline model optimization to adapt simulation models after adjusting their parameters during Model Adaptation. The Optimization Simulation is also used to apply model optimization during Offline Estimation to aid in online dynamic estimation. The Predictive Simulator is utilized to obtain production forecasts.

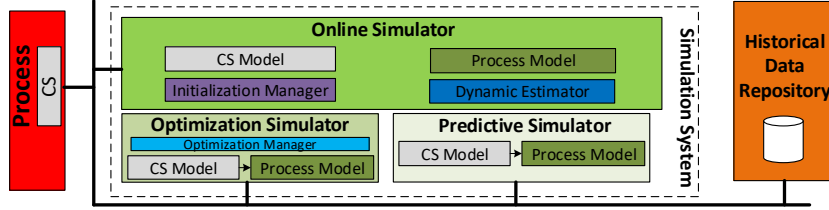


Figure 14. Proposed tracking simulation architecture components [26].

During Predictive Simulation, the simulation model requires to be controlled faster than real-time. Unfortunately, commercial control systems do not offer options for faster than real time execution. Moreover, different simulation instances must be created for different applications throughout the tracking simulation lifecycle. Additionally, having a dedicated control system for each simulation instance would involve significant implementation effort. Thus, due to differences in their operation cycle approaches, an additional experiment manager would be required to handle the synchronization between the control and simulation systems. In order to overcome this, the proposed architecture includes a model of the process control system (CS). The CS model, developed and integrated into the same simulation tool, is used to independently control the process model when required, even during Predictive Simulation, when the model is run faster than real time. The CS model is a replica of the structure, equations and tuning parameters of the real CS. In addition, having a CS model included in the simulation tool reduces the time and effort needed to integrate the process simulator into other control systems. The architecture consists of four components:

- **Online Simulator:** Prior to Tracking Simulation, Online Model Initialization is handled by the Initialization Manager. Later, during the Tracking Simulation stage, the Online Simulator runs in parallel with the plant, controlled by the real CS, while the Dynamic Estimator component adjusts model parameter to align the simulated results with the process measurements. As a result, the Online Simulator and the process states are continuously synchronized. A snapshot of the Online Simulator is always used for initializing the Optimization and Predictive simulators during the Offline Estimation and Predictive Simula-

tion stages, respectively. This guarantees that their ICs always correspond to the current state of the process. A model snapshot is defined here as an executable copy of a simulation model that includes its ICs.

- **Optimization Simulator:** This component consists of a snapshot of the Online Simulator that runs a model optimization that is needed to find a set of model parameters that best represent the behaviour of the plant described by historical process data. Model optimization is applied during Model Adaptation to adapt a previously developed or a model created following AMG methods using historical data of the process. Model optimization is also used during Offline Estimation for offline optimization to aid in dynamic estimation. The latter is achieved using recent historical process data. The Optimization Simulator is run faster than real time and controlled by its CS model in order to reduce the time required to obtain the optimization results. The Optimization Manager is responsible for starting the optimization by obtaining a snapshot of the Online Simulator; retrieving the data relevant to the optimization from the Historical Data Repository; and managing the automatic execution of the method.
- **Predictive Simulator:** This simulator consists of another snapshot of the Online Simulator. It is executed faster than real time to obtain predictions. The CS model is used to control the process model during Predictive Simulation.
- **Historical Data Repository:** This component consists of a process historian that stores into a database the information generated by the process and the simulation system. Many existing process plants already have this component, as historical data can be used not only for implementing SBDTs but also for creating DDMs of the plant.

### 3.3.2 Tracking simulation methodology

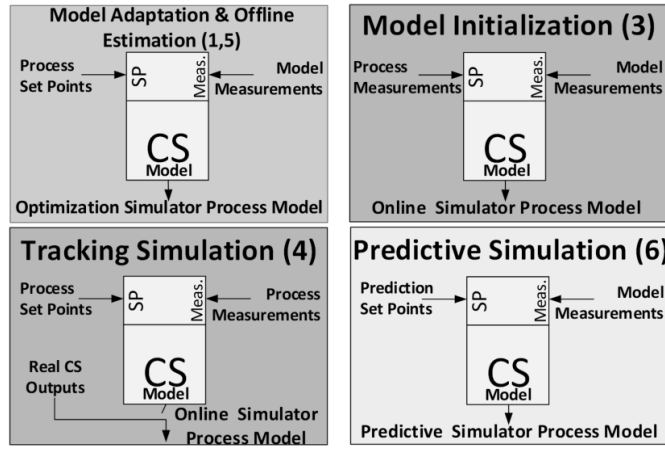
This section describes the tracking simulation methodology followed, along with the way the proposed simulation architecture components are utilized during each Tracking Simulation stage.

#### *Model Adaptation*

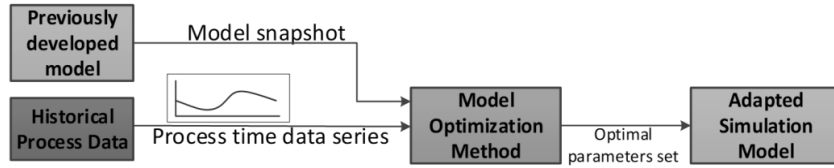
AMG can eliminate much of the laborious work required for FPM development. However, the results of the automatically generated FPM of the SBDT does not always fully correspond to current process measurements. This is also the case for models created manually from plant design material. One possible reason for this is either that the physical system was not built exactly according to the design specifications that were used to generate the FPM, or that the design specifications lacked some detail. Another possible reason is that although the physical system has long been in use, some parameters, such as friction in the piping network or valves, may have changed over time. Thus, the proposed method requires a Model Adaptation step to optimize either existing models or automatically generated models using historical data from the physical system.

This step is required to obtain results representing the current behaviour of the physical system. For this reason, adapted simulation models can be used as the underlying models for implementing tracking simulators of SBDTs.

Model Adaptation is based on a multi-parameter model optimization. This differs from the online model parameter adjustment performed by the dynamic estimation methods, as online calibration is limited to adjusting only a few model parameters for synchronizing the states of the model with the process [105]. The proposed Model Adaptation method, described in detail in **Publication V**, is carried out using the optimization method described in Section III C of **Publication VI**. During the execution of this method, the Optimization Simulator is controlled by its CS model. The connections between the CS model during this and other phases of the tracking simulation lifecycle are presented in Figure 15. Model Adaptation is automatically started and handled by the Optimization Manager.



**Figure 15.** Control system (CS) model set point (SP) & measurement (Meas.) connections during tracking simulation lifecycle [26].



**Figure 16.** Model optimization for Model Adaptation [26].

### Model Deployment

Model Deployment is the procedure during which the simulation system is connected to the running process. This is a safety-critical task, as this integration is carried out during process operation [9]. Furthermore, it must be performed although the conditions for accessing information from the plant ICT infrastructure may vary significantly in different facilities [88]. The expensive and laborious work required for integration can restrict the scalability of simulation-based applications, especially when multiple systems must be integrated with the process plant [44]. In contrast, the proposed implementation approach only re-

quires integrating the simulation architecture, as the architecture already includes the components required for model optimization, initialization and dynamic estimation. Industrial interoperability standards can be used as communication mechanisms to interface the simulation system with the physical plant. Examples of these standards include (but are not limited to) the OPC and OPC Unified Architecture (OPC UA) industrial interoperability specifications [56], often available in modern plants.

#### *Online Model Initialization*

In tracking simulators, direct, persistent communication between the simulation system and the plant can be exploited to achieve efficient model initialization. The proposed Online Model Initialization method is similar to that applied for initialization of models generated using AMG methods, as it based on controlling the simulation model to an initial simulation state. However, during Online Model Initialization, instead of controlling the process to any given initial state, the CS model guides the Online Simulator model to the current state of the process, as described by plant measurements. The model initialization sequence starts when the adapted, deployed simulation model is connected to the CS model, as shown in Figure 15. Next, the process model is controlled to the current process state. The initialization stage is completed when the Online Simulator and plant states are at the same state, as shown by the example Process and Simulated Variables in the uppermost part of Fig. 4 in **Publication VI**.

#### *Tracking Simulation*

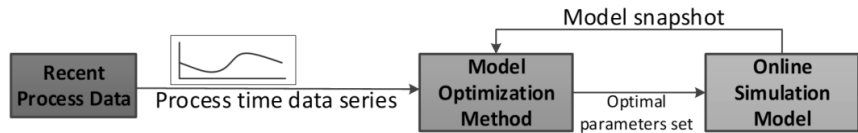
A SBDT must remain an accurate twin of the physical plant throughout the operation and maintenance phases of the plant lifecycle. Therefore, the state of the SBDT plant requires continuous alignment. This is accomplished during Tracking Simulation by applying dynamic estimation while at the same time running the Process Model of the Online Simulator together with the plant, controlled by the real control application. Concurrently, the CS model of the Online Simulator is connected to the process measurements and set points in order to synchronize its state with the real control application state. This synchronization is shown in Figure 15. The layout of the simulation architecture during Tracking Simulation is presented in Fig. 4 of **Publication VI**. As explained in Section 2.5.4, direct state adjustment can result in spurious transients that can negatively affect the simulation results [150]. This is a critical issue if the tracking simulation is applied as a virtual sensor which requires an accurate estimate of the current of the process. Therefore, the proposed architecture applies implicit dynamic feedback [128] as the dynamic estimation mechanism.

Implicit dynamic feedback is a SISO-based dynamic estimation method which pairs a single process measurement with an unmeasured disturbance for estimating the state of a single model variable. The advantage of this method is that any SISO feedback controller can be applied for its implementation. PI controllers have been the most popular controllers for implicit dynamic feedback estimation. Alternatively, this work proposes the utilization of sliding mode controllers [151]. The advantage of sliding mode control (SMC) over PI controller-

based implicit dynamic feedback is that SMC can eliminate bounded disturbances in finite time in the presence of bounded uncertainties, whereas PI-based controllers always exhibit a discrepancy that is proportional to the magnitude of the disturbance. Although SMC is not applicable to systems that exhibit significant real delays, such delays can mostly be eliminated for tracking simulation purposes. Additionally, SMC controllers are more robust in terms of controller tuning requirements. They are also very robust against uncertainties related to the presence of noise. However, industrial application of this approach might be limited by pending patents regarding the utilization of PI controllers for dynamic estimation [152]. The proposed dynamic estimation method based on SMC controllers is explained in detail in **Publication IV**.

### *Offline Estimation*

SISO-based dynamic estimation can adjust a limited number of model parameters [105]. Therefore, the proposed architecture applies offline multi-parameter estimation to prevent bias concentration on a low number of simulation variables. This approach can also be applied for obtaining specific sets of model parameters to improve the simulation results of specific plant operating regions. Offline Estimation is carried out by using the Optimization Simulator to optimize a snapshot of the Online Simulator. This is accomplished using the same model optimization method employed for Model Adaptation. However, during Offline Estimation, the optimization is performed using recent process time data series or data series from common operating regions or transients, instead of historical plant information. This is shown in Figure 17. Fig. 4 of **Publication VI** shows the layout of the proposed architecture during Offline Estimation. Figure 15 shows the connections of the CS model connected during this phase. Although model optimization can be performed faster than real time, this method cannot be utilized for dynamic estimation, as optimization results may fail to converge in the required cycle time, depending on the complexity of the modelled system [43]. For this reason, model optimization for Offline Estimation is mainly applied for further improving the Predictive Simulation results. Model optimization during Offline Estimation is also managed by the Optimization Manager. Once model optimization is completed, the values of the found optimal set of model parameters are provided to the Online Simulator and a new optimization is started.



**Figure 17.** Model optimization method for Offline Estimation [26].

### *Predictive Simulation*

At the Predictive Simulation stage, a snapshot of the Online Simulator is run faster than real time for a simulation length through an operation sequence specified by the system operator. During this stage, the simulation model is controlled by the CS model, as shown in Fig. 4. of **Publication VI** and in Figure

15. During Predictive Simulation, the calibrated model parameters remain constant at the mean value obtained from the Online Simulator before forecast execution. This approach has two advantages. First, since predictions are obtained using a snapshot of the Online Simulator, they are based on the current state of the process. Second, the resulting forecasts are based on a simulation model that has been adjusted during Tracking Simulation and Offline Estimation to closely match the plant's behaviour.

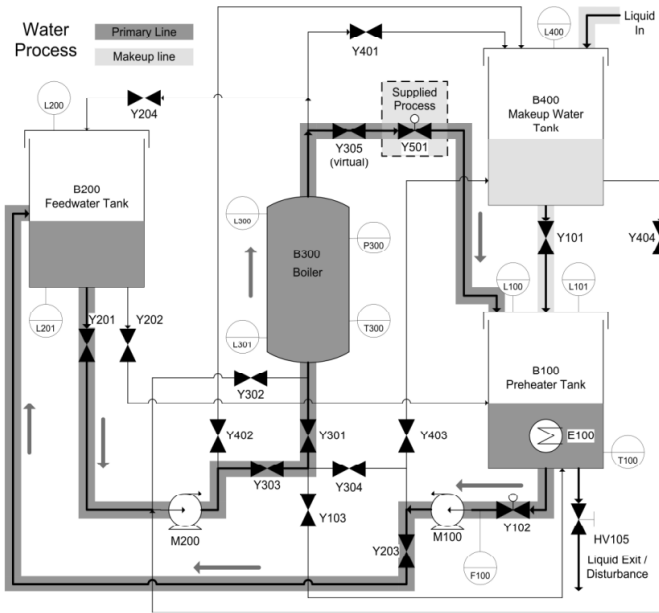
## 4. Results

### 4.1 Description of the case study

The described methodology was implemented and tested using a laboratory-scale heat production plant (HPP) process. The HPP, shown in Figure 18, is a hot water production system that is simpler than real process plants. However, it has been designed by automation experts and includes key automation functionalities found in industrial processes [153]–[156]. Figure 19 shows the P&ID of the HPP process. The process is comprised of three open tanks (B100, B200 and B400), a vessel (B300), two pumps (M100 and M200), a heating element (E100), various shut-off valves and two control valves (Y102 and Y501). During operation, the water in the tank B100 is heated by the heating element E100. The water temperature of tank B100 is controlled by an on-off controller. The water level L200 of tank B200 is controlled by a cascade PID controller which adjusts the position of proportional valve Y102. The pressure P300 in tank B300 is controlled by a PID controller, which adjusts the speed of pump M200. Load on the consumption of hot water can be changed by adjusting the position of valve Y501. The consumed hot water flows back into tank B100 where it is re-heated. The control application for the process runs on a soft programmable logic controller and was developed following the IEC 61131-3 standard. The CS of the HPP offers an OPC UA server for accessing process measured information.



**Figure 18.** Heat production plant (HPP) process used as the case study for the proposed methodology [41].

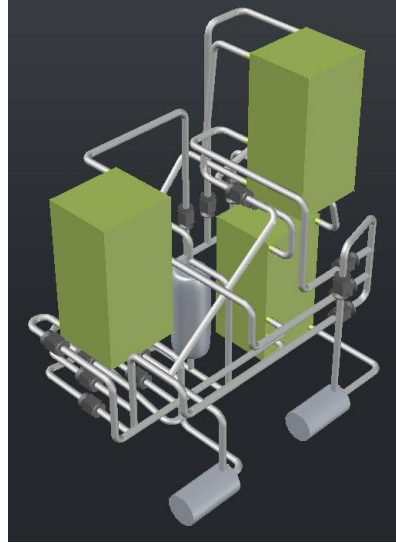


**Figure 19.** P&ID of the HPP process [153], [157].

HPP system dynamics exist mostly in the tanks, as they have the largest share of the total volume, which can vary. Similarly, the control valves are dynamic elements that are used to control flows. Furthermore, since a portion of the system volume resides in the pipelines, they also introduce a portion of the system heat and fluid flow delay. However, since the system in this study is always operated at a constant temperature, thermal inertia or heat transfer remain negligible. In this work, the simulation model is controlled by a CS model. This CS model is an exact copy of the equations, structure and tuning parameters in the real control application. An exact copy of the real control application is utilized to reduce the impact on the system dynamics and to reduce discrepancies between physical and modelled systems.

## 4.2 Automatic model generation method results

The HPP system was developed before starting the implementation method proposed in this work. No 3D model of the system was created during its design. Therefore, in order to test the proposed AMG methodology, a 3D model of the HPP was developed in AutoCAD Plant 3D [158] after measuring physical dimensions of the real process. AutoCAD Plant 3D is a 3D modelling tool utilized in industry. The 3D model of the physical system is presented in Figure 20.



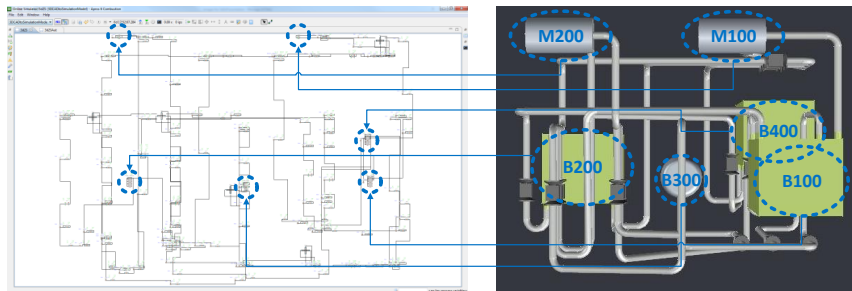
**Figure 20.** 3D model of the HPP process developed in AutoCAD Plant 3D [41].

The proposed AMG method was implemented using Apros [159]. Apros is a commercial flowsheet-based tool for modelling and dynamic simulation of thermal-hydraulic processes. Apros has been used for modelling and simulating various industrial thermal-hydraulic systems, including nuclear power plants [71], combined heat power plants [160], renewable energy production systems [161], [162], as well as pulp and paper mills [70]. This simulation tool offers libraries of simulation components for common process equipment. Model components are connected through pipes and TH points. The simulation tool also offers communication interfaces for connecting the process simulation model to industrial automation systems. Alternatively, Apros includes simulation components with functionalities for developing a model of the process automation system. This is particularly useful for independently controlling the simulation model or for faster than real time simulation. Detailed descriptions of the thermal-hydraulics model, equations and calculation methods in Apros are available in [70], [71], [161]. Apros utilizes the Simantics Constraint Language (SCL) [163] to manage different model configuration tasks. This script language is based on the integration platform Simantics [164]. Consequently, the proposed AMG method was developed using SCL.

The proposed AMG method, utilizes information from the 3D plant model for automatically generating a thermal-hydraulic simulation model. In AutoCAD Plant 3D, this information can be accessed either directly from the 3D model database or through the API of this 3D modelling tool. Additionally, AutoCAD Plant 3D offers the possibility of exporting the 3D model information in CSV file format. The main drawback of the latter option is that the exported CSV format is not compliant with any industrial information exchange standard. Moreover, the exported CSV file does not contain information on the process equipment connections. Consequently, the proposed AMG method directly retrieves information from the AutoCAD Plant 3D database. This information is accessed

through an SQL server which connects to the data base client of the 3D modelling tool and then exports the required data as CSV files.

After the 3D plant model information is retrieved, the AMG method generates model components of the HPP process equipment, such as the vessel, open tanks, pumps and valves. Next, the pipeline network, including the pipe fittings and TH points are created. Model components are generated and located at the corresponding XY position specified by the HPP 3D model information. Information on the elevations of the process components is provided as a parameter to the TH points. Next, the connections are generated between all the model components. The resulting model and its comparison with the lower isometric view of the HPP 3D model are shown in Figure 21.



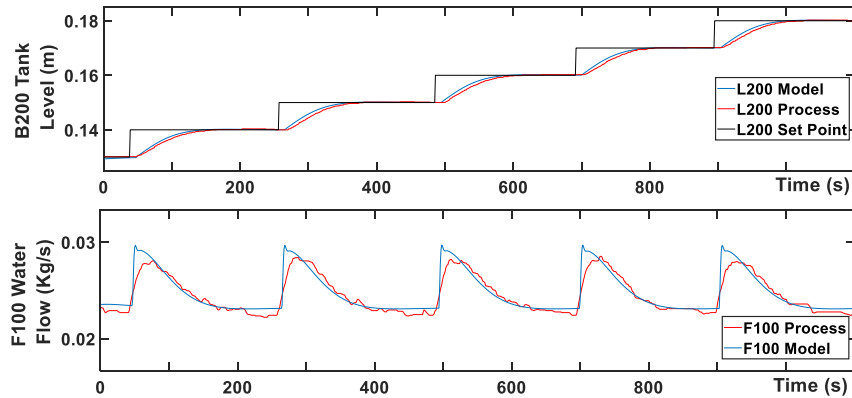
**Figure 21.** Apros' configuration canvas of the simulation model generated using the proposed method, and its comparison with the lower isometric view of the HPP 3D model [41].

Some industrial 3D plant models include equipment nominal information on the modelled system. However, it cannot be assumed that this information is always available from a single information source. Therefore, in the proposed AMG method, the model configuration is performed using data obtained from both: the HPP 3D model and the process equipment data sheets. Equipment nominal data obtained from the data sheets is provided to the AMG method as CSV tables. Equipment nominal parameters, such as nominal flows and positions of valves as well as nominal pressure heads and nominal flows of pumps are provided to the corresponding process equipment. Finally, Model Configuration is complemented after calculating head loss coefficients of the pipeline fittings (using the equations presented in Section 3.2.), and then providing these to the corresponding piping fitting.

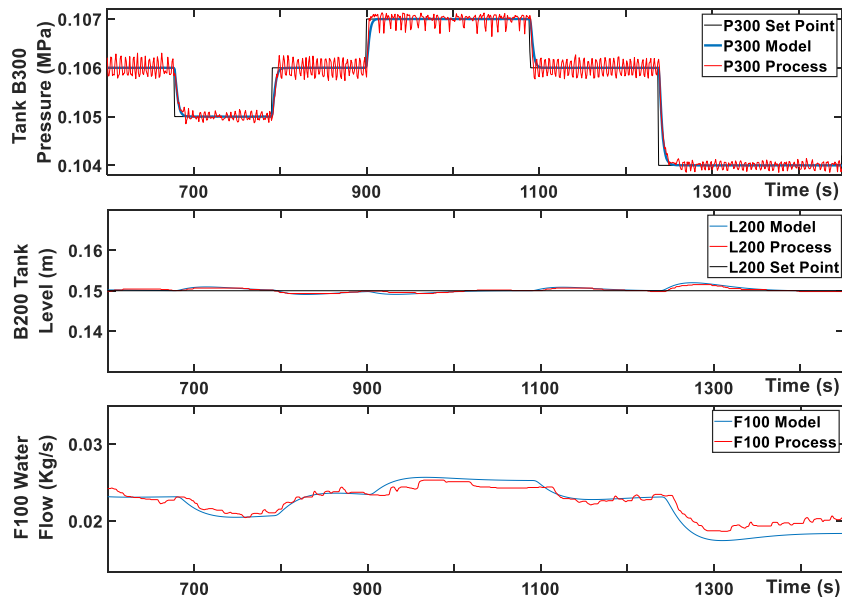
Model initialization of the automatically generated model is performed by connecting the simulation model to its control application and controlling the model to the desired initial state. In order to test the method, a CS model was manually developed in Apros. The CS model replicates the HPP control application equations, structure and tuning parameters. In this work, model initialization during AMG was carried out by independently controlling each process sub-system to the desired initial state and then verifying model stability at that state. This is iteratively carried out until the entire system reaches the desired initial state. Once the initialization is completed, the automatically generated model can be utilized for the desired application.

The results of the model generated using the proposed AMG method were compared with experimental data from the HPP process. The experimental

setup during these experiments is explained in the Results section of Publication VII. Figure 22 compares the simulation results with the HPP experimental data during transients caused by changes in the set point of the B200 tank water level L200. The flow F100 is the water flow between tanks B100 and B200, measured between valve Y102 and pump M100. Figure 23 shows a comparison between the simulation results and the HPP experimental data during transients caused by changes in the set point of the pressure in vessel B300. The results of these comparisons show that the behaviour of the model generated using the proposed AMG method is in good agreement with the HPP experimental data.



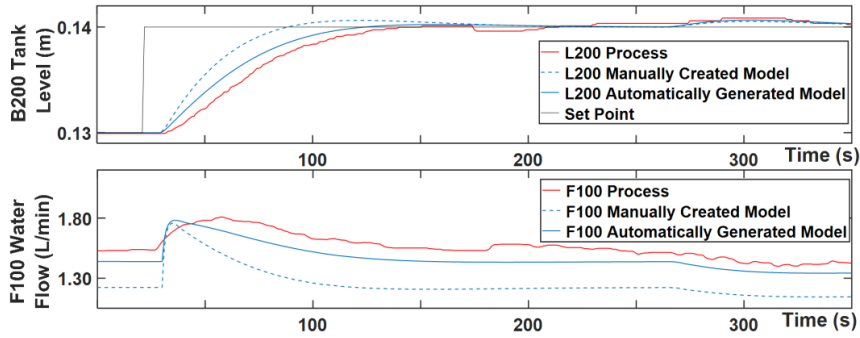
**Figure 22.** Simulation results of the automatically generated simulation model and its comparison with the HPP measurements. Transients are caused by changes in the set point of the water level L200 of the tank B200.



**Figure 23.** Simulation results of the automatically generated simulation model and its comparison with the HPP measurements. Transients are caused by changes in the set point of the pressure P300 in the vessel B300.

The automatically generated model is further assessed by comparing its results to those obtained from a model created manually using the plant P&ID and equipment nominal data. This source information corresponds to the data utilized in the closest state-of-the-art methods for AMG of industrial processes [28], [37], [91], [99]. Therefore, the manually created model was developed with limited information concerning the pipeline network structure. Nevertheless, the pipe lengths and the elevations of process equipment and pipes were measured and then configured on the manually created model. This is done to highlight the improvements due to differences in the head loss coefficient values. Therefore, in this respect, the manually created model included even more parameter information than the models created with data used by AMG state-of-the-art methods.

The experimental setup during these comparisons is explained in detail in the Results section of **Publication VII**. Figure 24 compares the automatically generated and the manually created models with experimental data from the HPP plant. The figure also compares the water level L200 in tank B200 and the flow F100 during transients due to a change in the L200 set point. The same ICs have been used in both experiments for the tank B200 level. However, the difference between initial conditions for the flow F100 in Figure 24 is an unavoidable result of the fact that the head loss coefficients of the manually created and the automatically generated simulation models are different.



**Figure 24.** Comparison of the simulation results between the automatically generated model and the manually created model. Transients are caused by a change in the set point of the water level L200 of the tank B200.

Table 2 shows a comparison between the normalized root mean squared error (NRMSE) of the automatically generated model and that of the manually created simulation models in respect to the process data series for the experiments depicted in Figure 24. NRMSE is used to facilitate the comparison between datasets with different units and scales [165]. These results show that configuring the automatically generated model using 3D plant model information can reduce model residuals.

**Table 2.** Comparison between the normalized root mean square errors (NRMSE) of the automatically generated and that of the manually created model in respect to the HPP experimental data.

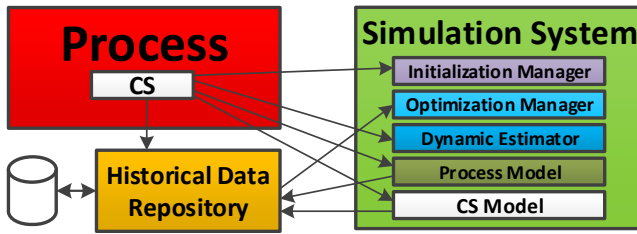
Description	NRMSE
Automatically generated model	102.8
Manually created model	386.9

A direct comparison between the proposed AMG method and the state-of-the-art works [28], [37], [91], [99] is not possible, as the case studies are different. Nevertheless, the source information utilized for developing the manually created model is the same as that suggested by the cited state-of-the-art methods. Furthermore, the results of the comparisons shown in Figure 24 are based on the same case study and the NRMSEs are calculated from the same transient scenarios. Consequently, the obtained NRSME can be considered representative of a performance improvement resulting from the proposed approach, as shown through comparison with state-of-the-art methods. Tracking simulation system implementation

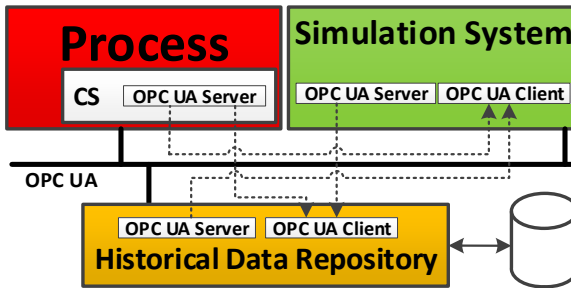
### 4.3 Implementation of the proposed tracking simulation architecture

The tracking simulation architecture proposed in this work, relies on OPC UA for interfacing the architecture components with the HPP plant. OPC UA is an industrial interoperability protocol, standardized in IEC 62541 [166]. It has been selected as the only standard for the communication layer in the Reference Architecture Model for Industry 4.0 RAMI [74], which will further consolidate its relevance in the future [55]. The OPC UA standard offers a set of specifications for information exchange between various industrial systems, including specifications for systematically retrieving historical process data from plant historians.

Figure 25 shows the point-to-point connections required for communication between components of the tracking simulation architecture during its lifecycle. Point-to-point communication requires laborious configuration of a high number of connection points. For this reason, the proposed system avoids this by utilizing OPC UA, enabling a simpler communication layout based on client-server connections. This is shown in Figure 26. In this approach, servers provide access to an information model with which clients can connect and interact to retrieve data and functions through a set of standardized services. OPC UA-based connections between the architecture components are implemented utilizing the subscription service of the OPC UA standard. Utilizing this communication standard results in a reduction in the effort required for configuring the connections between the architecture components. Furthermore, it reduces the number of connections required to interface different components. This is critical for reducing integration effort throughout the proposed architecture lifecycle. This finding addresses research goal 3, described in Section 1.2.



**Figure 25.** Point-to-point communication required for information exchange during operation of the tracking simulation architecture. Based on [26].

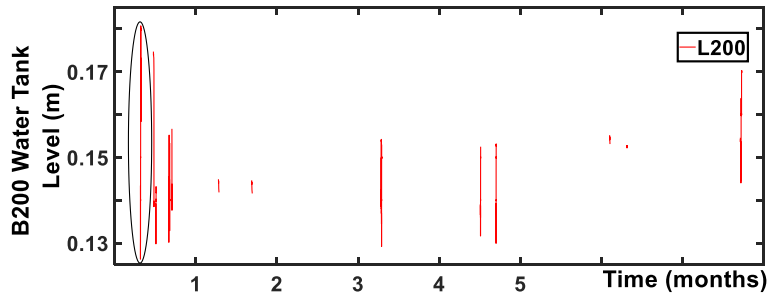


**Figure 26.** Communication enabled by OPC UA during the tracking simulation lifecycle. Based on [26].

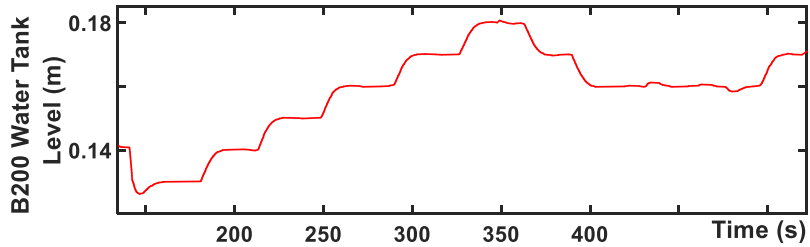
The Prosys OPC UA Historian [167] is the OPC UA-based historian utilized for implementing and testing the proposed architecture. The historian client connects to the OPC UA servers of both the HPP plant and the simulation system in order to collect their data into an SQL database. The automatically generated model was developed in the described simulation tool Apros. Therefore, the tool is also used as the simulation system for implementing the proposed architecture. A further benefit is that Apros offers an OPC UA client and server.

#### 4.3.1 Model Adaptation results

Model Adaptation is required for finding an optimal set of parameters to represent the plant behaviour in terms of its historical data. Model Adaptation is based on applying the multi-parameter model optimization presented in Section III C of **Publication VI**. As shown in Figure 16, Model Adaptation starts by accessing historical process data from the Historical Data Repository. Historical data is systematically retrieved utilizing OPC UA historical access functions. This adaptation method, based on leveraging the OPC UA communication standard, is explained in detail in **Publication V**. To illustrate this process, Figure 27 shows 8 months of historical data from the B200 tank and water level L200. Figure 28 presents a close-up view of the data enclosed by the ellipse in Figure 27.



**Figure 27.** Eight months of historical process data of the B200 tank water level L200 [26].



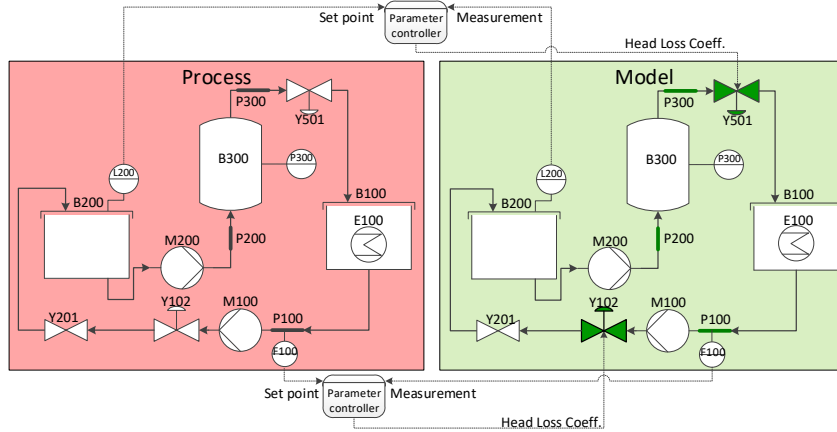
**Figure 28.** Close-up view of the historical data enclosed by the ellipse of Figure 27 [26].

During Model Adaptation, the model optimization method adjusts five parameters of the automatically generated HPP simulation model. These parameters are selected using a sensitivity analysis performed to determine how the uncertainty in the output of the model can be apportioned to different sources of uncertainty in its inputs. The method utilized for selecting parameters is the variance decomposition global sensitivity analysis [168]. This method, based on Monte-Carlo simulation, was selected as it is possible to measure the effect of varying the value of a parameter on the variance of an examined process variable. Additionally, it measures the effect that varying a single parameter has on all of the other process variables. Results of this analysis can be used to select parameters suitable for adjustment during Model Adaptation as well as during the Tracking Simulation phases. A detailed description of the parameter selection method used is available in **Publication III**. This method is reviewed and compared with similar alternatives in [84], [169], [170].

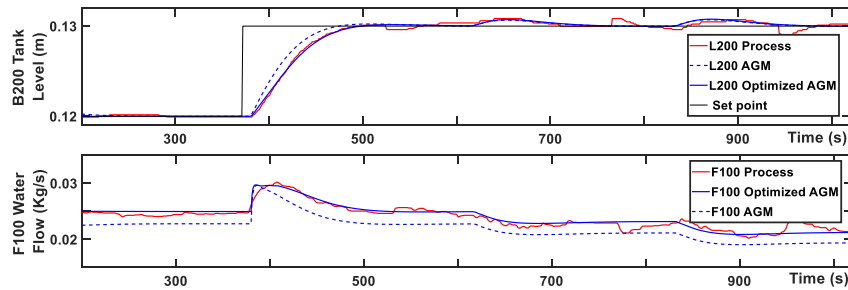
In the HPP process, five parameters are adjusted during Model Adaptation: the nominal flows of proportional valves Y102 and Y501 as well as the head loss coefficients of piping sections P100, P200 and P300. Model components that include a parameter adjusted during Model Adaptation are marked in dark green in the model diagram of Figure 29. The nominal flow parameter of a proportional valve represents the expected flow rate at different pressure levels. Different equipment aging factors, such as static friction, can cause variation in head loss coefficients or in nominal flow values over time. Consequently, it is expected that equipment parameters available from the original design material do not represent the current behaviour of the plant. Figure 30 presents the results of the optimization during Model Adaptation for the B200 water tank level

and the F100 water flow process variables. Table 3 compares the model parameter values before and after their optimization during Model Adaptation.

Table 4 compares the NRMSE of the simulation model with that of the historical process data series before and after the model optimization. These results show that the model optimization method can successfully be applied for Model Adaptation. The model optimization is able to find a set of model parameters that significantly reduces residuals of the simulation model generated by following the proposed AMG approach. Consequently, the adapted model can be connected to the ICT system of the process to be used as a tracking simulator for the SBDT.



**Figure 29.** Tracking simulation connection diagram. The model components highlighted in dark green are those which have a parameter adjusted by the model optimization method during Model Adaptation and Offline Estimation phases.



**Figure 30.** Comparison of the automatically generated model (AGM) results before and after Model Adaptation as well as its comparison with the HPP experimental data [75].

**Table 3.** Parameter values before and after model optimization during Model Adaptation.

Model component	Parameter	Nominal parameter value	Optimized parameter value
Y102	Nominal flow rate	1.6 [kg/s]	1.33 [kg/s]
Y501	Nominal flow rate	1.6 [kg/s]	1.45 [kg/s]
P100	Head loss coef.	0.1	4.90
P200	Head loss coef.	0.1	0.11
P300	Head loss coef.	0.1	0.09

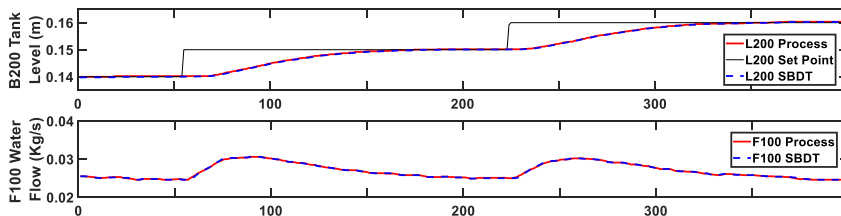
**Table 4.** Comparison of the NRMSE obtained from Figure 30 before and after optimization during Model Adaptation.

Description	NRMSE
Model before Model Adaptation	112.85
Model after Model Adaptation	17.01

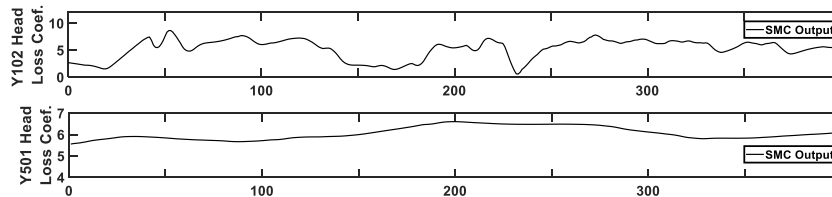
#### 4.3.2 Tracking simulation results

Model Deployment is performed by connecting the OPC UA client of the simulation system to the OPC UA server of the process CS. Next, at the Online Model Initialization phase, the deployed simulation model is controlled to the current state of the process by the CS model, as explained in Section 3 of this work and in **Publication II**. Tracking Simulation begins only after the state of the simulation model corresponds to the current plant state. Once this is achieved, the model is connected to the outputs of the plant's control application and the dynamic estimation is started. As presented in Section 3, the architecture implemented utilizes SMC controller-based implicit dynamic feedback as its dynamic estimation method.

During the tracking simulation tests, two simulation variables are adjusted by two SMC parameter controllers, as shown in Figure 29. The time constant of the SMC controllers is tuned to match the behaviour of two PI parameter controllers, which are tuned following the Ziegler-Nichols tuning method [171]. One of the parameter controllers aligns the simulated flow from tank B100 to B200 with the real-time process measurement by adjusting the head loss coefficient of the modelled proportional valve Y102. The other parameter controller aligns the real and simulated B200 tank level L200 by adjusting the head loss coefficient of the modelled valve Y501. These parameters were selected following the same sensitivity analysis used for parameter adjustment during the Model Adaptation phase. Figure 31 shows the tracking simulation results. The upper trend in Figure 31 compares the simulation results against the plant data of tank level L200 during the production transients caused by changes in the L200 set point. The lower trend in Figure 31 compares the simulation results against the plant data of flow F100 during the same transients. Figure 32 shows the SMC parameter controller outputs during the tracking simulation experiments of Figure 31. The proposed architecture allows the utilization of other feedback controllers for implicit dynamic feedback estimation. **Publication VI** presents a tracking simulation comparison of the SMC and PI parameter controller approaches. The results show that automatically generated model can be successfully used for tracking simulation purposes after undergoing Model Adaptation. The variables adjusted by dynamic estimation closely match their corresponding process measurement. Curves of the parameter controller outputs during the tracking simulation experiment, shown in Figure 31, fluctuate within a bounded region of head loss coefficient values. Furthermore, the proposed dynamic estimation method performed by the SMC parameters controllers can be applied for implementing SBDTs.



**Figure 31.** Tracking simulation results of B200 tank level and F100 water flow.



**Figure 32.** Head loss coef. values for valves Y102 and Y501 calibrated by the SMC parameter controller during the tracking simulation experiment shown in Figure 31.

#### 4.3.3 Offline Estimation and Predictive Simulation results

Offline Estimation is carried out in parallel during Tracking Simulation (as shown in Fig. 4 of **Publication VI**) to continuously enhance the prediction results. Offline Estimation is also based on applying the model optimization presented in Section 3 of **Publication VI**, as was done previously during Model Adaptation. However, the optimization method evaluates model results with recent process information, instead of using historical process data. It is also possible to apply Offline Estimation based on historical data series from common operating regions or transients for improving the prediction results of those specific regions. In these experiments, Offline Estimation is carried out for demonstrating the latter case. Therefore, during Offline Estimation, the same five model parameters (see Figure 29) adjusted for Model Adaptation are adjusted utilizing historical data from HPP common operation transients. The values of the process variables that define the selected transients are described in Table 5.

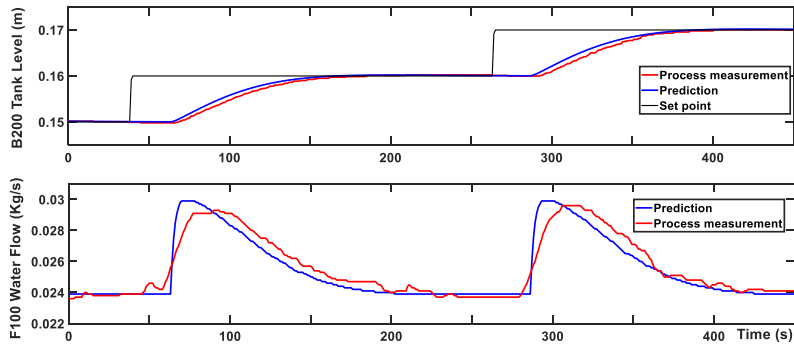
**Table 5.** Process variable values describing the production transients selected for Offline Estimation

Production [%]	Valve Y501 Position [%]	P300 [MPa]	L200 Set Point Change [m]
100	60%	0.106	0.15 - 0.16
100	60%	0.106	0.16 - 0.17

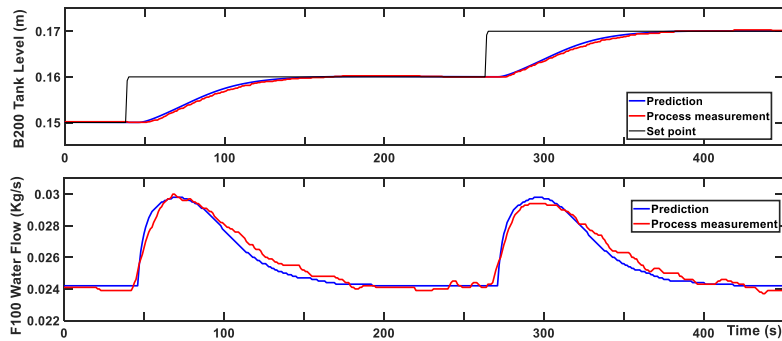
During Offline Estimation, the model optimization is executed in the Optimization Simulator. The common operation transients were manually selected by a process expert. Upon request, the Optimization Manager retrieves the process data of these regions from the historian. This is done using OPC UA historical access functions. The historical data is then used to iteratively evaluate the model results. Once the model optimization finds an optimal set of model parameters that best represent the behaviour of the HPP at the transients selected,

the parameters are provided to the tracking simulation model. As shown in Figure 31, the dynamic estimation performed by the SMC controllers produces accurate tracking simulation results even before carrying out offline estimation. Offline Estimation is mostly beneficial in the Predictive Simulation stage, where model optimization can further reduce the residuals of the predictions.

During Predictive Simulation experiments, the Predictive Simulator takes a snapshot of the Online Simulator and runs it faster than real time through the transients selected for Offline Estimation. Figure 33 shows the B200 water tank level and the F100 flow predictions obtained before Offline Estimation as well as compares these with process measurements during production transients corresponding to the regions selected for Offline Estimation. As described in Table 5, transients are caused by a change in the L200 set point. Figure 34 shows the B200 water tank level and the F100 flow predictions obtained after Offline Estimation as well as compares these with process measurements during production transients corresponding to the regions selected for Offline Estimation. The predictions are obtained using the average parameter values calculated by the SMC parameter controllers during Tracking Simulation. Table 6 compares the NRMSE of the B200 tank level and F100 flow predictions with the process measurements before and after Offline Estimation. These results show that the optimization method applied for Offline Estimation significantly improves the accuracy of the predictions obtained by the Predictive Simulator. Furthermore, applying the same optimization procedure for Model Adaptation and Offline estimation reduces the integration time of the architecture with other simulation methods.



**Figure 33.** Comparison of the predicted B200 tank level (L200) and the F100 water flow with their respective process measurements during production transients caused by a change in the L200 set point. These predictions were obtained before the Offline Estimation phase.



**Figure 34.** Comparison of the predicted B200 tank level (L200) and the F100 water flow with their respective process measurements during production transients caused by a change in the L200 set point. These predictions were obtained after the Offline Estimation phase.

**Table 6.** Comparison of the NRMSE for the predictions before and after Offline Estimation.

Description	NRMSE
Predictions before Offline Estimation (Figure 33)	38.44
Predictions after Offline Estimation (Figure 34)	<b>14.67</b>

## 5. Discussion of the results

After presenting the results of this work, there are important aspects of the proposed method that should be discussed.

Regarding the 3D plant model-based AMG method, the results of the proposed approach show that significant improvements in the model fidelity are expected by utilizing information available from the 3D plant model for AMG. The proposed approach is expected to result in improvements over state-of-the-art methods that use only equipment data sheets and P&IDs as sources of information. The degree of quantitative improvement will depend mostly, but not only, on the pipe routing of the particular case study, as the number and properties of pipe fittings significantly impact head losses. Precise calculation of head loss coefficients is vital for accurate modelling of transient behaviour.

A drawback of the proposed AMG method is its dependence on information access options, which can vary according to the 3D modelling tool utilized. This can limit the applicability of the proposed AMG method to only those 3D modelling tools that provide access to their 3D model databases. 3D model information exchange formats would significantly increase the applicability of AMG methods. However, standards supported by some commercial 3D modelling tools, such as IFC, should also be extended for data exchange between industrial process systems.

In this work, equipment nominal data from their technical data sheets was manually organized and provided to the AMG method as a CSV file. In this respect, approaches followed by some of the existing AMG methods [28], [65], [91], in which nominal data is automatically extracted from plant design systems, could be also applied to completely automate this process. In the proposed AMG method, the control application required to control the generated model is developed manually. One possible approach for automating this step could be to utilize IEC 62424 descriptions for generating the control application model, as these descriptions are already available during early plant design. Alternatively, it would be possible to utilize the information of the process control loops available from the P&IDs.

Concerning the proposed tracking simulation architecture, utilizing OPC UA industrial interoperability standard reduces implementation and configuration effort required to interface the architecture components. This is necessary for reducing integration effort throughout the architecture lifecycle. OPC UA client-server communication between the architecture components was implanted utilizing the OPC UA subscription service. While OPC UA communication could

also have been achieved utilizing OPC UA Write and Read services, the information flow in the proposed implementation only required OPC UA servers to provide data to the subscribed clients. Information exchange based on OPC UA subscriptions enables a more efficient exchange of information between servers and clients, compared to the OPC UA Write and Read services [166], [172]. This is required for maintaining continuous synchronization during the tracking simulation lifecycle.

An important aspect to be considered is the OPC UA communication overheads that can cause communication delays, as this interoperability standard has limitations for interfacing complex processes with real-time requirements. Although communication delays could negatively impact results of more complex and faster processes, in the HPP process, this aspect did not have a significant effect in the experimental results. OPC UA is currently being extended in order to support real-time capabilities. This extension to the OPC UA standard includes the development of a publish-subscribe information exchange model that can be utilized over an Ethernet time-sensitive network [56], enabling OPC UA-based communication over real-time networks.

Regarding dynamic estimation, both PI and sliding mode control-based methods are suitable for the example implementation. However, single-input-single-output dynamic parameter estimation may cause fluctuation around the target value when using overly aggressive feedback controllers. Multiple-input-multiple-output (MIMO) control methods could be applied to dynamically align simulated variables with process measurements.

## 6. Conclusions and future work

This work has proposed and tested an integrated method for implementing a SBDT from an FPM generated automatically utilizing 3D plant model information. A crucial first step in the proposed implementation is the automatic generation of the underlying plant simulation model from the 3D plant model. Overall results show that the model generated using the proposed AMG approach can be successfully applied for implementing SBDTs after its integration into the physical plant. This integration is enabled by the proposed tracking simulation architecture as well as by the application of the proposed tracking simulation methodology. The SBDT developed can be utilized for a number of important applications during plant operation, including virtual sensor and predictive simulation of production transients. This is a significant improvement compared to the current state-of-the-art for AMG, in which the achieved fidelity of the resulting model limits its application to only factory acceptance tests and virtual commissioning. Furthermore, this approach should result on a reduction of implementation effort for developing SBDTs, thereby increasing industrial adoption of these systems.

The hypothesis and research questions presented in Chapter I are discussed as follows:

Regarding Hypothesis 1, the results show that it is possible to automatically generate and configure a thermal-hydraulic simulation model from information available in the 3D plant model. An AMG method was developed which utilizes 3D plant model information for generating and configuring a dynamic simulation model. Since nominal information of the process is not always included in the 3D plant model, the proposed method configures modelled equipment nominal data based on information from equipment data sheets. A key step in this method, which has not been considered in previous works, is the utilization of the pipeline structure information included in the 3D plant model to configure the model pipeline network lengths and elevations. In addition, geometrical information on pipe fittings is utilized for calculating the head loss coefficients of the model pipeline network. This information cannot be obtained from other data sources previously explored for AMG. Simulation results for the model generated using the proposed AMG method closely correspond to the process measurements, even during process transients.

The results of the proposed AMG method show that this work addressed Research Goal 1, described in Section 1.2, as the proposed method enables more rapid, efficient model development compared to manual modelling approaches. Additionally, it utilizes design data available during early stages of the plant

lifecycle. This enables early application of simulation models not only for the implementation of SBDTS but also for other important applications even before constructing the plant.

Regarding Hypothesis 2, an integrated methodology for implementing lifecycle-tracking simulation systems enabled reduction of the engineering effort required to develop SBDTs, thereby addressing Research Goal 2. The proposed approach integrates various simulation methods into a tracking simulation architecture. This architecture is designed for implementing SBDTs from FPMs generated either using AMG or from existing models developed manually during process design. The presented tracking simulation methodology consists of a model optimization method, used for Model Adaptation and Offline Estimation, as well as other methods for model initialization, dynamic estimation and predictive simulation. The proposed Model Adaptation method leverages the information availability offered by OPC UA to seamlessly retrieve historical process data. The results of this method show that the developed model optimization successfully reduces the residuals of models generated automatically from 3D plant model information. Similar results are obtained after applying the model optimization methods for adapting existing models created during process design. During Model Deployment, use of the OPC UA standard solved the problem of integrating the tracking simulation architecture with the physical plant and its ICT infrastructure. In this work, the proposed model initialization procedure is performed by a model of the real process control system (CS) that can be run faster than real time to enable faster initialization. The tracking simulation is successfully carried out using the proposed SMC-based implicit dynamic feedback estimation. Finally, Offline Estimation experiments show that the model optimization method used for Model Adaptation but applied for offline parameter estimation using recent process information or information from specific operation regions, significantly improves the prediction results during the Predictive Simulation stage.

Finally, the described approach also addresses Research Goal 3 by presenting a tracking simulation architecture that manages the proposed methodology across the tracking simulation lifecycle. The proposed architecture is comprised of a historical data repository and three independent simulators, which can be instantiated according to the application. This system applies the described model optimization method for Model Adaptation and Offline Estimation, reducing the time required for integrating different simulation methods for each task. Furthermore, the architecture includes a model of the real CS that has three objectives: to avoid configuration work when the process model needs to be controlled; to enable faster than real time execution of the process model; and to enable the parallel running of several simulation instances. In addition, the architecture exploits the use of OPC UA both to systematically retrieve historical process data and to reduce the configuration effort required to interface system components by avoiding the need for point-to-point connections.

As partially discussed in Section V, there are important aspects regarding the proposed method that should be addressed by future work.

Firstly, regarding the proposed AMG method, future work should focus on extending or proposing new standards for 3D process plant model information exchange. Utilizing standard formats for automating model development would increase applicability of the proposed and other AMG methods. Another aspect that should be addressed by future work is the integration of information from both, P&IDs and 3D plant models, for AMG. PI&Ds are created before 3D plant models. Therefore, in this case, AMG based on P&IDs information could be followed to generate a first version of the dynamic plant model. Later, fidelity of this model could be improved after updating the model utilizing AMG methods based on 3D plant model information. This should result in automatic generation of high-fidelity simulation models and of their corresponding control applications.

Secondly, concerning the tracking simulation methodology, in this work, the tracking simulation results show close convergence of the adjusted model variables with their corresponding plant measurements. Curves of the parameter controller outputs are shown to demonstrate that the model parameter adjustment remains bounded during Tracking Simulation. However, further analysis is required to verify full state synchronization between the tracking simulator and the plant. This is critical in order to fully rely on the SBDT results if utilized as a virtual sensor. Regarding dynamic estimation, MIMO control methods could be studied and applied to dynamically adjust multiple simulated variables. Future work should also focus on the parallelization of the developed model optimization method to test the scalability of the architecture.

Finally, the proposed SBDT implementation method is a semi-automatic approach since, as previously discussed, there are different steps in the proposed implementation method which are not completely automated. In this work, different suggestions have been proposed to achieve a fully automatic implementation method. Furthermore, the proposed implementation method was tested using a laboratory-scale heat production process that is comprised of process and automation components found in industrial plants. However, the HPP testbed is a considerably smaller and more controlled environment compared to real industrial plants. Therefore, applying the proposed methods in an industrial-scale process would raise the technology readiness level of the methods presented in this work.



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