AI·PROFICIENT

Artificial intelligence for improved production efficiency, quality and maintenance

Deliverable 3.1

D3.1: AI-PROFICIENT hybrid models and digital twins first version (state of the art, designing and specification)

WP3: Platform AI analytics and decision-making support.

T3.1: Hybrid models of production processes and digital twins.

Version: 1.0

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Executive Summary

The Deliverable 3.1 is a public document of AI-PROFICIENT project delivered in the context of WP3 (Platform AI analytics and decision-making support), and more precisely T3.1: (Hybrid models of production processes and digital twins), regarding state of the art of the technology and the specification of two use cases related to the different pilot sites. These use cases were initially described and reported in deliverable D1.1 (Report on the pilot characterizations and operation scenarios) and their demonstration scenarios were described and reported in deliverable D1.3 (Pilot-specific demonstration scenarios).

This deliverable D3.1 presents the state of the art of hybrid modelling and digital twins, covering the techniques from first principles modelling to fully data based surrogate models and digital twins based on these approaches. On that basis, designing of the approach for selected use cases and the specifications in each case are described.

A second deliverable associated to task 3.1, namely deliverable 3.6 “AI-PROFICIENT hybrid models and digital twins (final version)”, is due in M30. This second deliverable will consist of the digital twins.

1 Introduction

In AI-PROFICIENT, digital twins are linked to a range of AI services, such as predictive production quality assurance and process optimization. The goal of this deliverable is to first describe the links to AI-PROFICIENT services and then give an overview of the state of the art of the modelling methods that are used as a basis for deriving digital twins for these, covering the techniques from first principles modelling to hybrids and surrogate models. On that basis, designing of the approach for selected use cases and the specifications in each case are described, keeping in mind the requirements of the necessary functionalities to AI-PROFICIENT to provide the S_HYB service detailed in the deliverable D1.5:

Table 1: Services to be provided by the AI-PROFICIENT project (from D1.5).

Service ID	S_HYB
Service input and dependency on other services:	Service input consists of process data and user experience. Process online data including but not limited to flow rates, compositions, temperatures, physical measures and pressures is required. In addition, laboratory data is needed. User experience of process operation, effects of process conditions and raw materials is also used as input. The service is linked to several other services. Inputs it may get from component level data acquisition and pre-processing (T2.2). Several services will utilize results that are based on the digital twin either directly or indirectly via another service. Both predictive AI analytics for production quality assurance (T3.2) and generative optimization (T3.4) will be able to directly utilize results of the service.
Service output:	The developed hybrid models will provide the information on how the manipulated process variables and disturbances affect process outputs. Digital twins will be fast adaptive versions of hybrid models that provide the same information on-line while they continuously improve the match of the model to reality.
High level service description:	Hybrid models, and digital twins based on the hybrid models, will be constructed by combining first principles modelling of the production processes with data driven modelling and human feedback. Depending on the use case, different model combinations will be developed. For first principles modelling, state of the art modelling tools will be exploited (such as ChemSheet for equilibrium chemistry and OpenFOAM for CFD). For Ineos UC1 the chosen solution approach is a hybrid model that combines first principles modelling, data driven modelling and human feedback. For Conti UC2 the solution will be based on integration of a feedback system with a databased model. In case of INEOS UC3, the approach will be chosen after data analysis is carried out and the part of the process that causes rheology drift is identified. Depending on the modelling requirements, simplified linear/nonlinear/one-dimensional forms will be considered and developed to achieve the required computational speed of a digital twin. For this purpose, any physical models will be hybridized using ML techniques that will exploit and combine the operation data from the process (enabled by WP2), and human feedback whenever feasible (WP4), with modelling results.

The service is linked to other services, especially S_PRE (Predictive Production quality assurance service) and S_GEN (Generative holistic optimization) and indirectly through these services possibly to other services.

This service will cover the _HYB requirements identified and detailed in the deliverable D1.4 as result of T1.4., shown in Table 2.

Table 2: Functionalities to be provided by the AI-PROFICIENT project (from D1.4).

AI-PROFICIENT Functionalities	***ID***
Monitoring	_MON
Diagnostic and anomaly detection	_DIA
Health state evaluation	_HEA
Component prognostics	_PRO
Hybrid models of production processes and digital twins	_HYB
Predictive Production quality assurance	_PRE
Root-cause identification	_ROO
Early anomaly detection	_EAR
Opportunistic maintenance decision-making	_OPP
Generative holistic optimization	_GEN
Future scenario based Lifelong self-learning system	_LSL
Human feedback	_HUM
Explainable and transparent decision making	_ETD

The _HYB functionality will be included in two or three use cases as is shown in Table 3 that shows an excerpt of the synthesis table that was included in the end of D1.3 to provide an overview of the expected components to be part of the solution of each use case.

Table 3: Excerpt of expected partners' involvement in T3.1 for each use case (from D1.3).

WP/Task	CONTI-2	CONTI-3	CONTI-5	CONTI-7	CONTI-10	INEOS-1	INEOS-2	INEOS-3
WP3- Platform AI analytics & decision-making support								
3.1 Hybrid models of production processes and digital twins	TEK					VTT		VTT

The deliverable is structured as follow. In section 2, the state of the art of hybrid models and digital twin is proposed. Then, in Section 3, a detailed description of the specifications and design for digital twins in different use cases is presented.

2 State of the art of hybrid models and digital twins

2.1 Introduction

The definitions given for a digital twin somewhat vary in the literature. Here we apply the definition that a digital twin is a numerical description of the considered process or other entity and that there is a two-way synchronized relation between the physical and the digital asset so that the numerical description is continuously calibrated using real time data. To what extent the two-way relation is applied in the direction from the model to the physical object varies but is typically related e.g. to control and predictive maintenance. The application of the digital twin can be automated or rely on a human-in-the loop approach.

There are different ways to construct the digital twin and the underlying numerical model, examples of which are illustrated in Figure 1. Depending on the complexity and availability of the first-principles (based on fundamental science, e.g. physics and chemistry) description of the phenomena involved, the model can be based on a fully data-driven approach or combine data with the first-principles description in form of a hybrid model. In the following state-of-the art of data-driven and hybrid modelling approaches is summarized.

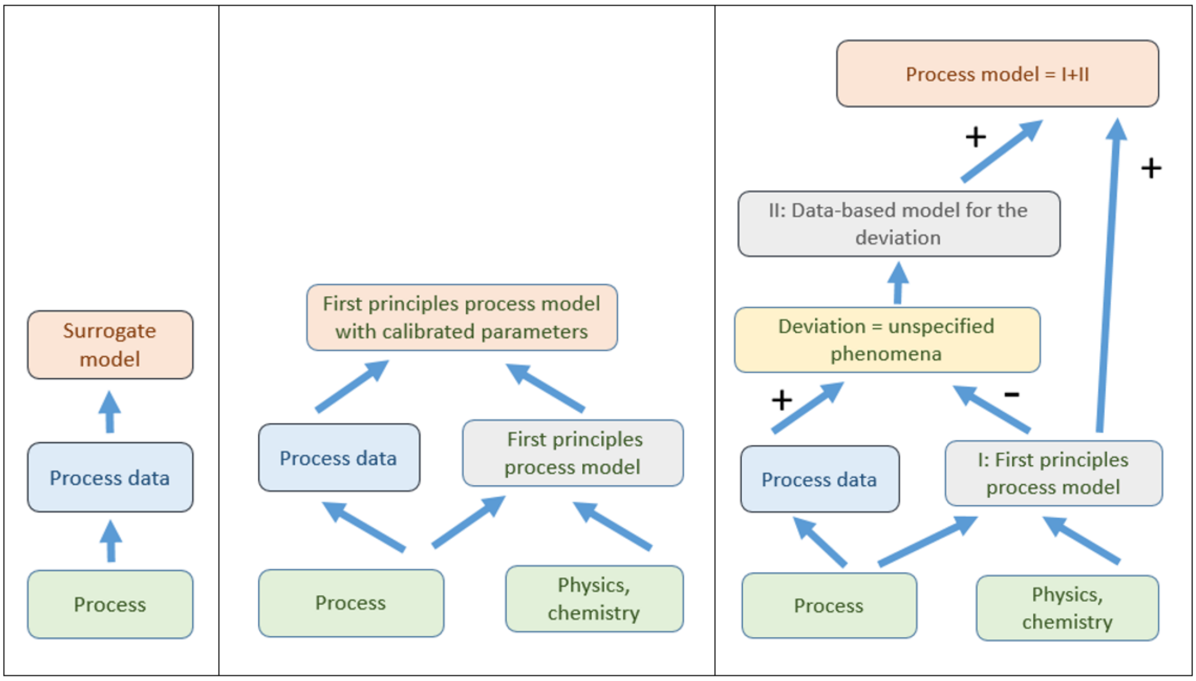

Figure 1. Examples of alternative ways to construct the mathematical model that is the core of the digital twin: a data-driven / surrogate model (left), a first-principles model with calibrated parameters (middle) and a first-principles model augmented with a da data-driven model for all unspecified phenomena (right).

2.2 Digital twins based on surrogate models

Some industrial processes are so complex that producing accurate models based on Finite Element Methods (FEM) or other demanding modelling techniques would be too expensive and time consuming or technically not feasible, due to the huge amount of data needed to develop and validate the models (Yilmaz et al., 2021). Additionally, the need to run a twin model of a plant on real time (the essence of digital twins) requires the models to be computationally fast, so that different scenarios can be simulated in real time to provide feedback to the real asset. This requirement is difficult to achieve with FEM models, and hence, other modeling approaches with faster computation times are required.

Surrogate models are interesting alternatives as their computation times are minimal in comparison to FEM models and, depending on their simplicity, can cope well with small samples of data. Essentially, surrogate models are data-based models that represent the relation among the inputs of a system and its outputs (Zhang et al., 1012). They are also known as metamodels or emulators, and their purpose is to represent the behavior of the system as closely as possible with a reduced computational cost. Generally, they are built to compute the output of different input scenarios with the surrogate model and can be applied in different kinds of problems such as: model approximation, design space exploration, problem formulation, reliability, sensitivity analysis, digital twin, or optimization (Fuhg et al., 2021 & Bárkányi et al., 2021).

The development of a surrogate model has three main aspects to be considered:

- The sampling
- The modelling
- The management strategy

2.2.1 The Sampling

Sampling consists of the identification of scenarios (observations) that will provide valuable information to build the surrogate model. In general, it is preferred to build a rich set of scenarios instead of repeating similar situations so that the final model shows a greater generalization capability (Suhas Garud et al., 2017). Usually, these scenarios are generated following a design of experiments, and, in general, observations are generated via real experiment or via costly simulation. Sampling can be carried out in two different ways. Firstly, it can be based on grid methods, geometry-based methods or other stochastic methods which are known as **non-adaptive sampling strategies**. Secondly, in some cases it is possible to start from a small sample of points and use some criteria or procedure (such a partial surrogate model itself) to add points sequentially (**adaptive sampling methods**) which tend to be more robust and reduce the cost of the experimentations. Some important aspects that affect the sampling are the amount of input variables to consider, the size of the sample (i.e. the amount of observations) and the deterministic behavior of the experiments (their repeatability or the amount of noise in each iteration) (Liu et al., 2018).

2.2.2 The modelling

Modelling consists of creating a model that maps a set of inputs with a single or more target variables, generally, at the cost of having some error. The choice of model is critical, as there are many models that can be used with different hyperparameters, and they will impact the final accuracy of the model. Many different models are used for building surrogates, most commonly: gaussian processes, linear regression, support vector machines, decision trees and random forests, artificial neural networks, etc.

The following work by Gary Wang & Shan (2007) shows an interesting summary of modelling (or metamodeling as it is somehow mentioned in surrogate modeling literature) methods:

- Kriging methods: Accurate for nonlinear problems but difficult to obtain due to a global optimization process. Capable of interpolating sample points or filtering data that is noisy.
- Polynomial models: Even though less accurate than Kriging models, they are easy to construct, clear on parameter sensitivity and computationally inexpensive. However, they do not interpolate sample point and are restricted the function type chosen. There are some variants, Least Interpolating Polynomials, that use polynomial basis functions but also interpolate the responses, for that purpose they are bases on a polynomial basis function of “minimal degree”.
- Support vector regression methods: Tend to achieve higher accuracy than the rest of methods, Additionally, they can be extended with radial basis functions to increase their flexibility.
- Artificial Neural Networks (ANN): Are known to be stable in comparison to other methods such as Kriging for large sample points. At the same time, they are able to provide accurate surrogates with reasonable computational time (Bamdad et al., 2020). In general, Kriging and Radial Basis Functions are more sensitive to physical or computational noise than polynomial and linear approaches. There are however methods to modify Kriging, RBF or ANN algorithms to handle noise under acceptable signal to noise ratio conditions.

2.2.3 The management strategy

The management strategy consists of the balance of the sampling technique and modelling along with the objective of the surrogate model (model approximation, optimization, reliability…). This aspect is dependent on the sampling technique employed. If the sampling technique is classical (DoE) the management strategy is one-step strategy, whereas if the sampling technique is adaptive, the management strategy is adaptive. In one-step strategy, the aim is to fit the model not only for being as accurate as possible, but also for being the most suitable as possible to achieve the objective of the surrogate. In adaptive strategy, the samples are selected in order to improve the performance of the model and achieve the objective of the surrogate (Ghassemi et al. 2019).

A typical exploitation of surrogate models is the case of the **surrogate-based optimization**, that is, when the objective of the surrogate is to find an optimal solution of the problem that is modelled. Once a surrogate model is built, an **optimization process** that creates sets of observations and **determines which input combinations reach the most desired outcomes** is launched. The fact that the model that is being used for optimization is surrogated one allows to run tens of thousands of fast simulations that compare a variety of scenarios while considering the trade-offs among variables. The optimization process iterates until the scenarios with the most desired conditions are reached. Depending on the employed management strategy two procedures can be distinguished: in one-step sampling the model is build based on a set of fixed data, and after that, optimization is launched; otherwise, if an adaptive management strategy is employed, new samples are selected based on the model's ability to approximate the search space and the interesting regions for the optimization that are found, so that the modelling and the optimization are carried out at the same time (Fuhg et.al. 2021).

Regarding the different methods that can be employed for the optimization, heuristic algorithms, that can deal with nonconvex problems, are the more common type of optimization algorithm. There are different families of heuristic algorithms that follow various criteria to create new populations, for instance, local search, tabu search, simulated annealing or some other genetic algorithms that mimic the behavior of certain animals, such as the swarm optimization algorithms.

In the case of the **surrogate-based digital twin**, the benefits of a computationally simple and robust model with a fast execution are used by running the model in parallel to a real process/system and stablishing a bidirectional flow of the data: data from the model is used to assist on the control of the system, whereas the real sensory data is used to re-train and update the surrogate model. This way the model can better adapt to the changes on the real system and provide more accurate outputs.

2.3 Digital twins based on first principles modelling and hybrid models

In the development of digital twins based on first principles models two steps are required: 1) development of a first principles model that describes the target entity with sufficient accuracy and 2) development of the digital twin based on the model. These two steps are described in the following.

2.3.1 Entity model and its development

First principles modelling

A first principles model expresses the connections between process variables by means of mathematical description of the phenomena occurring in the considered target entity. Different numerical methods are involved when the models are applied. To what degree the details of the physics and chemistry are described in the model depends on

- the goal of the modelling and the details that are relevant for achieving the target
- availability of phenomenological models and required parameters (reaction rates, transfer rates, material properties etc.)
- computational capacity required and availability of such capacity at reasonable cost

Thus all first principles models are simplifications and limited in the extent to which they describe details.

For description of a production process consisting of several unit processes, **a system modelling approach** is required. A system model describes a production process by means of interlinked models for unit operations. Several commercial and some open source software are available for system modelling and thus it is common to apply one of the existing software instead of writing models from scratch. The background of a software is typically in a specific industrial branch and thus they have varying ready-made submodels and databases available. Some of the tools allow only steady state modeling while others describe process dynamics, including process control. Typically the tools allow core calculations of chemical engineering, including those concerned with mass balance, energy balance, vapor-liquid equilibrium, heat transfer, mass transfer, chemical kinetics, fractionation, and pressure drop. The most popular software for system modelling is ASPEN PLUS that has built-in capabilities for modeling of a wide range of chemical processes including polymers, electrolytes and solids and large materials databases. An extensive list of commercial and open-source process modeling software is presented in Wikipedia at https://en.wikipedia.org/wiki/List_of_chemical_process_simulators.

For unit processes such as e.g. chemical reactors and for hydrodynamics and aerodynamics, **3D computational fluid dynamics (CFD) modelling** is used, utilizing numerical discretization such as e.g. FEM and Finite Volume Method FVM. However, in many simple reactors, plug flow, stirred tank or other simple reactor models suffice and such models are easily written and also available in system modelling software. For situations where mixing inside a reactor is more complicated and there are large variations in condition, a 3D CFD model is necessary.

The core of CFD is discretized equations for

- mass transfer
- energy transfer
- transfer of chemical compounds

In many reactor modes, chemistry, in addition to energy balances, is the main phenomenon to be modelled. Hundreds of reactions and tens of chemical components may be required and chemistry may include e.g. catalytic or heterogeneous reactions. For multiphase systems, additionally interaction between the phases (transfer of heat, mass, momentum, chemical components) needs to be accounted for and there may be mechanical submodels required for e.g. fragmentation, attrition, bubble growth and split etc. Particle size distribution for the dispersed phase is often used to describe dispersions and the chemical and physical phenomena in those. A large number of commercial and open source software are available for generation of the geometry and computational mesh and for solution of the equation. The most widely used commercial solver is Ansys Fluent and the most popular open source solver is OpenFOAM. Software for grid generation and solvers are listed e.g., in https://www.cfd-online.com/Wiki/Codes.

There are limitations for where and how CFD modelling can be used. Such limitations are e.g.

- lack of first principles sub models for some phenomena, e.g. chemistry, materials description
- complexity of the phenomena which leads to excessive computation time in each computational cell
- large and/or complicated geometry that leads to too large number of computational cells and unreasonable simulation times

Lack of sub models can be often compensated by experimenting and describing the phenomena by means of a data-based or semi-empirical sub model. Similarly, if some phenomena are too time-consuming to model in each cell, such phenomena can be modelled separately in the required range of conditions and a data-driven description can be derived on basis of the modelling data and implemented in the CFD code, see e.g., Niemi & Kallio (2018). Alternatively, the flow field can be described in a fine mesh and a multiblock approach can be used in which the mesh cells with similar conditions are grouped in blocks in which the complicated chemistry and particle size distribution calculations are performed (Ojaniemi et. al, 2014).

Fine computational mesh and long computation times are required in direct simulation where turbulent flow structures are resolved by the simulation. Similarly, for multiphase flows, fine flow structures such as particle clusters and strands and bubble boundaries need to be described. To facilitate faster simulation and coarse mesh resolution, turbulence models and other filtered modelling approaches have been developed.

Hybrid modelling

Data-driven and first principles modelling approaches both have advantages and drawbacks. A compromise that tries to find a good balance between theory and data is hybrid modelling. The main advantages and drawbacks of the approaches are summarized in Table 4.

Table 4: Advantages of the modelling approaches.

Advantage	Data-driven modeling	Hybrid modeling	First principles modeling
Ease and speed of development	High	Medium-low	Low
Reliability of obtained results	Low - medium	Medium	Medium - high
Capability of producing unexpected new insight	High	Medium	Low - medium
Independency of quality of data	High	Medium	Low
Ease of modelling multivariate nonlinearities	Low	High	High
Insensitivity to validity of assumptions and accuracy of theories	High	High	Low
Requirement only a limited amount of data	Low	Medium-high	High

The term hybrid model covers all approaches that combine theory with process data. First principles models usually contain empirical data-based sub models, such as models of reaction rates, mixing rates, transport rates and material properties. To make them true hybrid models, these data-based submodels should, however, be based on data from the actual process or entity that is modelled instead of literature sources. The way data and theories are combined can vary in a wide range, e.g.

- data-driven models with functional forms limited applying theoretical knowledge
- data-driven models where input variables are constructed using theoretical knowledge (e.g. Reynolds number instead of velocity, dimension and viscosity separately)
- data-driven models with constraints based on theoretical knowledge (e.g. we know that the predicted variable is always positive)
- theory-based functional forms with data-driven parameters
- partial model, e.g. one submodel fully based on data-driven approach and others based on physics
- first principles model with data-driven correction (deviation model)

2.3.2 Development of the digital twin based on the model

First principles models and even hybrid models can be too heavy for on-line use. To reduce computation time, special methods such as **model order reduction techniques** have been developed (e.g. Chinestaet al., 2018). They require that either plenty of data from accurate simulations or measurement data are available. Other options are to use simplified first principles models or to use a heavy first-principles model to produce a set of systemically sampled data on basis of which a data-driven model is derived.

Since first principles models are of practical reasons only approximations of the reality, a data-driven part is always needed when a first-principles model is used in a digital twin. Compared to surrogate models, a smaller amount of process data is required as basis of the data-driven models since only the unexplained phenomena need to be modeled on basis of observations. The main ways to account for data are **deviation modelling** and **parameter calibration**.

3 Hybrid models and digital twins: Detailed description for each use case

3.1 CONTI2: Restart set

The CONTINENTAL production line produces many different types of tires. The extrusion is a fundamental part of the production line, and it consists of combining several compounds that are heated in different extruders and fused into a single tread.

For a variety of reasons (such as needing to change the input compounds) the extrusion process needs to be stopped and relaunched later. This restart is a critical part of the process as many rework is created and the quality of the final product can be compromised if the adequate extrusion conditions are not reached.

3.1.1 Solution

The surrogate model of UC2 mimics the behavior of an extrusion process where various extruders are used to produce tire recipes.

The extrusion process is complex to model as many physical phenomena occur and are influenced by the environment and the large number of different compounds that are used on the production. For that reason, building an accurate physical model of the extrusion is technically complex, which turns this UC more appropriate to be tackled with data-based surrogate models.

According to the requirements defined by CONTINENTAL on D1.4 - Project requirements and performance assessment KPIs, the AI system would need to satisfy the following requests:

A) Ensure fastest setup of the restart of the machine (UR1_CONTI2): Meaning the proposed speed setpoints must focus on reducing the time required to reach production stability.

B) Ensure less rework (UR2_CONTI2): Meaning that the proposed parameters need to also consider the amount of rework that will be created as a consequence of the extrusion settings.

A surrogate model is built so that the previous requisites are fulfilled. In this particular Use Case sampling is not of great importance, as the CONTINTENAL historic database is large, and experiments (real extrusions) occur very frequently.

Taking the database containing signal records of the last 3 years, extrusions are identified, and some statistical features are extracted from the extrusions. At the same time, other features that represent the quality of each extrusion are extracted, i.e. the quality indicators.

A surrogate model that maps the extrusion features with the extrusion quality indicators is built. This model is later used by the optimization system, that provides various populations to the surrogate model

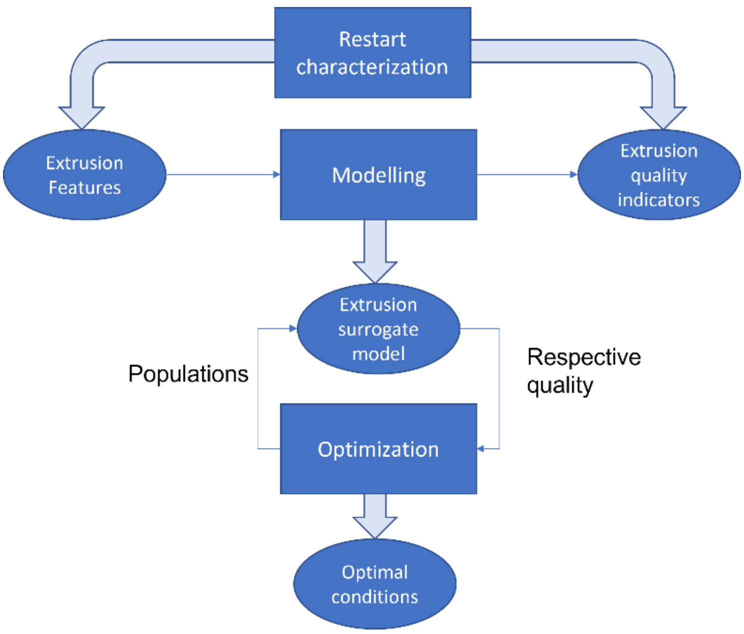

Figure 2. Schema of the surrogate modelling building process.

and the extrusion surrogate returns the quality associated to each of these populations. The optimization process will iterate on this process until the optimal conditions that satisfy CONTINENTAL's requirements are met. The process is depicted in the following Figure 2.

Taking a closer look on the specific surrogate model used to mimic the extrusion, the inputs and outputs used by the model are depicted in the following Figure 3. Note that the specific signal indicators and processing techniques are not disclosed due to the public nature of the deliverable, however, this schema gives a general idea of how the inputs and outputs of the surrogate model work.

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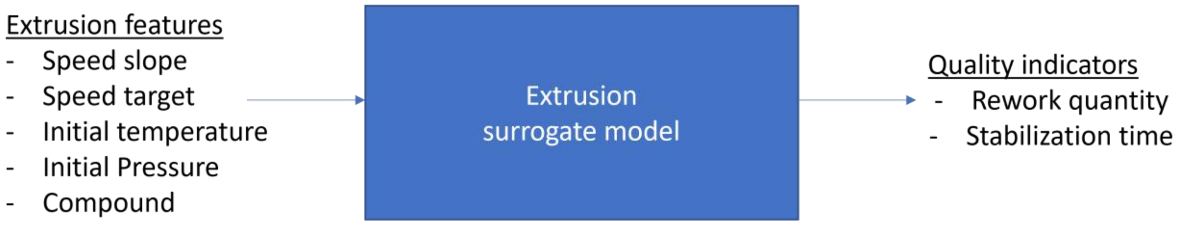

Figure 3. Surrogate model and inputs and outputs.

Due to the complex nature of the extruder system, it is reasonable to assume that the surrogate model will not be a perfect surrogate and it will incur in some error. In order to consider this fact during the optimization, including some uncertainty measure together with the estimated output value would be of great interest. In that sense, Kriging methods (a.k.a Gaussian process regression) are good modelling candidates as they are widely known for providing confidence estimates of the outputs (Jung et al, 2021). However, as the volume of available data is considerably large, and the set of input variable and indicator combinations is also wide, this kind of algorithms could be inefficient due to their computational cost and stability (Bamdad et al., 2020). If this is the case for UC2 alternative approaches such as radial basis support vector machines or non-parametric artificial neural networks will be used, as there are already precedents of works that suggest methods to quantify the uncertainty of these methods (Gal et al., 2016).

Once the surrogate model is available a data flow needs to be established. This flow of data is in charge of providing the outputs of the model to the final users so that they can use the suggestions to govern the production line. At the same time, the real data generated on the extruders can be used to update the parameters of the surrogate model and improve the fidelity of the model, which turns the surrogate model a complete digital-twin of the plant.

3.1.2 Ethical aspects

Considering the ethical issues related to CONTI2, identified in D1.3, Table 5 shows the ones related to this use case and task and the measures planned to address them.

Table 5: Ethical issues related to utilization of digital twins in CONTI2 use case.

D1.3 – Ethics code	Description	Measures	Responsible
ETHICS 2 (3)	A protocol should be created to deal with the situation when the AI makes an error	Besides the HMI to allow users to introduce error feedback, this feedback will be used to retrain the DT so that it improves from the real data and from the bad predictions in particular.	TEK/CONTI
ETHICS 3 (4)	The operator will be expected to adjust all extruders if AI is integrated, it is necessary to consider the extra effort required from the operator.	During the development of the digital-twin of the extrusion process, special emphasis will be place on identifying the best conditions be only manually setting a single extruder so that no additional overhead is caused to the operator.	TEK

3.2 INEOS1: Reactor stability at Geel plant

The case and proposed solution are described in D1.3 and the following is based on that description, with emphasis on development of the model that will be the basis of a digital twin.

The target process in Geel plant is a continuous-flow stirred-bed reactor in gas-phase polypropylene polymerization. The polymerization reaction is exothermic and for that reason cooling is provided by feeding liquid propylene to the reactor. Cooling takes place as the liquid vaporizes. Temperature is measured in several locations at reactor walls. Cooling is controlled by adjusting propylene feed rates.

The temperature control loop of the polymerization reactor is the key to allow normal run rates (production capacity). There are sometimes unwanted fluctuations in temperatures and in some cases the local temperature has even exceeded the melting temperature of the polymer. To bring the temperatures back to stable conditions the operator may need to reduce the production rate and hence production capacity is lost. Thus the temperature profile stability has a direct influence on maximum production rate. The goal of digital twin development is to improve understanding of what causes the oscillations and to develop an algorithm which helps to avoid oscillations.

3.2.1 Solution

Observations from the process indicate that higher temperatures occur inside the reactor than what is measured close to reactor walls. To describe also phenomena that are not measured, an approach that utilizes a first principles model was selected.

Phenomena to be considered

The main phenomena that affect the process and should be accounted for in first principles modelling are:

- Polymerization chemistry
  - The general kinetic scheme for polymerization using a Ziegler–Natta catalyst comprises a series of elementary reactions including the following:
  - Polymerization chemistry
  - Activation of potential sites, the reaction through which a potential site is converted into a reactive vacant site.
  - Chain initiation, a new polymer chain is being built.
  - Chain propagation, the mechanism step in which the polymer chain grows.
  - Chain transfer, a type of reaction that terminates a ‘‘live’’ chain, producing ‘‘dead’’ polymer and a vacant site (hydrogen as transfer agent).
  - Site transformation, produces an empty ‘‘live’’ site (of a different type), unlike the previous chain-transfer reactions that produce an initiated site, and a ‘‘dead’’ polymer chain.
  - Site deactivation, the reaction step generally accepted as the explanation for the activity loss experienced during polymerization. Both occupied and vacant sites are assumed to deactivate

- Other phase change rates
  - Rate of evaporation
  - Rate of melting of polymers

- Heat transfer and energy balance
  - Heat transfer from gas to droplets in the spray
  - Heat transfer from polymer particles to droplets in the spray
  - Heat transfer from gas to polymer particles
  - Heat transfer between polymer particles
  - Heat transfer inside polymer particles
  - Wall-gas heat transfer

    - Wall-particle heat transfer
    - Wall-liquid heat transfer
    - Heat generation in reactions
    - Consumption of thermal energy in evaporation

- Fluid dynamics
    - Flow of gas phase
    - Flow of solids
    - Flow of liquid
    - Gas-liquid interaction force
    - Gas-solid interaction force
    - Liquid-solid interaction force
    - Particle-particle interaction force
    - Particle size distribution

- System model of the process units outside the reactor
    - Submodels for the other process units and their connections
    - Time delays in the process and controls

The listed phenomena can be modeled based on existing knowledge of physics, chemistry and models for separate process units with acceptable accuracy.

Proposed solution

The proposed solution is described in D1.3 and summarized here as regards to the DT solution. This procedure is illustrated in Figure 4.

For that reason, the following complementary approaches that combine first principles modelling with data driven modelling as basis of the solution are proposed (as illustrated in Figure 4):

1. **Collection of data and assessment of the quality** of the data to determine the suitability of the different signals for data driven modelling and as inputs for first-principles modelling. Pre-processing options are also considered.

2. **First principles modelling with CFD**. Computational fluid dynamic (CFD) modelling of different sections of the reactor is carried out with OpenFOAM software to analyze heat and mass transfer effects on the temperature distribution. The CFD model will describe by means of transport equations and phenomenological submodels the transport of gas phase and its components, transport of solid particles, transport of the liquid in the spays, evaporation of the liquid, polymerization reactions, particle size distribution of the polymer particles, and energy transport phenomena (heat transfer between the different phases, inside the phases and between reactor surfaces and the different phases). Fluid dynamic description is based on a Eulerian approach with the kinetic theory of granular flow and a model of frictional forces. The general kinetic scheme for polymerization using a Ziegler–Natta catalyst comprises a series of elementary reactions. Even simplified reaction descriptions are considered.

Results from analysis of the process data will be used to validate the CFD model. Adjustments to submodels may be also done based on comparison to measurements and on basis of observed correlations.

3 A **simplified first principles dynamic model** for the reactor is developed by describing the reactor as interconnected stirred tank reactors. In each numerical reactor, reactions are modelled with the detailed kinetic mechanisms describing the catalytic polymerization reactions. The results from the CFD analysis will determine how the reactor will be split into separate numerical reactors and how mixing is described between these reactors through convection and diffusion. The goal is that this simplified dynamic model is fast enough to be run online so that it can serve as the basis for a digital twin.

4. **Data driven modelling**. Multivariate regression analysis is carried out to evaluate correlations between measured reactor temperatures or temperature stability and process inputs. Main process inputs in this analysis are flow rates and properties of inflows to the reactor and conditions in adjacent process units that can influence the reactor. Data analysis will also include assessment of periodicity of measured fluctuations. Even clustering analysis is considered to find effects of non-continuous variables such as varying catalysts and other chemicals.

5. CFD results and results from data analysis will be used to derive closures to improve the submodels of the simplified reactor model. Specifically, CFD results will be used to correlate temperatures at the walls with internal temperatures. This should allow the model to predict temperature distribution inside the reactor in different process conditions. Data analysis results will be used to modify the reaction models. As a result, this development step will produce a **hybrid model** that combines correlations derived from 3D CFD modelling results and data analysis with the simplified reactor model.

6. The hybrid model constitutes the basis of the **digital twin.** The digital twin will include either a deviation model or adaptive parameters. Adaptive parameters in this case are mainly reaction parameters that may be continuously adjusted to fit the model prediction to measured data, especially measured temperatures.

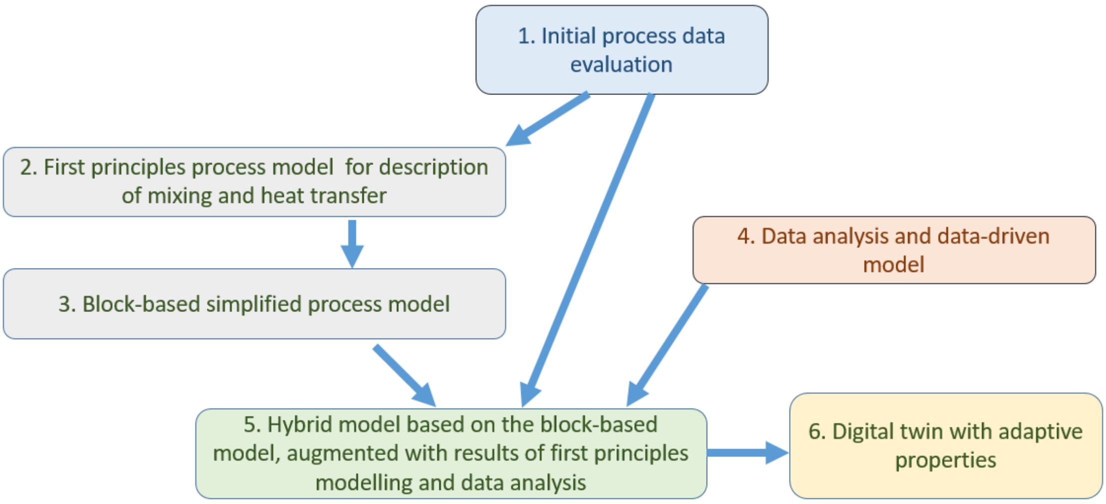

Figure 4. Path to a digital twin of INEOS UC1.

3.2.2 Ethical aspects

Ethical issues related to INEOS1 were identified in D1.3. Table 6 shows the ones related to digital twins and the measures that are planned to address them.

Table 6: Ethical issues related to utilization of digital twins in INEOS1 use case

Human Feedback Component	Description	Measures	Responsible
ETHICS 1 (1.3-3)	Limits need to be defined for the range inside which the prediction of the digital twin can be considered reliable.	Operator feedback is collected during off-line testing phase and during operation. Based on collected feedback, process engineers and operators define together limits outside which the recommendations by AI should be ignored.	INEOS, VTT
ETHICS 3 (1.3-4)	Extra workload related to offline testing of the digital twin needs to be identified and minimized.	Offline testing of the AI tools is carried out to gain experience. The DT tool will be constructed such that this testing will require about one full working day of each operator.	VTT

3.3 INEOS3: Rheology drift at Cologne plant

Whether a digital twin will be developed for INEOS UC3 depends on the results of analysis of process data. Data analysis is ongoing and so far sufficient results to make the decision have not been obtained. Thus the decision will be made later.

4 Conclusions

This report summarizes the state of the art of digital twin development. This is the first deliverable of task 3.1. A second deliverable associated to this task, namely deliverable 3.6 “AI-PROFICIENT hybrid models and digital twins (final version)”, is due in M30. This second deliverable will consist of the digital twins.

In this report, both surrogate and first-principles modelling are covered and application of the methods in the UCs of AI-PROFICIENT is presented. Depending on the availability of data and first principles models and theories, different modeling approaches are preferred in the derivation of a digital twin. Surrogate modelling requires either a large data set that covers the considered conditions or a possibility to carry out designed experiments. First principles modeling requires that the relevant phenomena can be described in sufficient details and with acceptable accuracy by mathematical formulations. In first principles modelling, it is common that the models need to be reformulated and simplified to achieve sufficient accuracy required for on-line use in the digital twin. In many cases hybrid modelling approaches that combine data-driven and first principles modelling can be the optimal method.

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