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self-X Artificial Intelligence for European Process Industry digital transformation

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D4.1 Autonomic Managers for Data in Motion and Humans Support in Al solutions – Initial Version

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List of Acronyms

AAS	Asset Administration Sheel
AM	Autonomic Manager
DAG	Directed Acyclic Graph
DaR	Data at Rest
DiM	Data in Motion
DPP	Digital Product Passport
EAF	Electric arc furnace
HITL	Human in the Loop
IDSS	Intelligent Decision Support System
MAPE-K	Monitor, Analyse, Plan, Execute - Knowledge
MAE	Mean Absolute Error
OCB	Orion Context Broker – FIWARE Generic Enabler
OSS	Open Source Software
PU	Public
RMSE	Root Mean Squared Error
SEN	Sensitive

Abstract

The Deliverable 4.1 "Autonomic Managers for Data in Motion and Humans support in AI solutions" represents the initial version of the development of the s-X-AIPI Autonomic Managers at M18.

It demonstrates the domain-agnostic infrastructure of the Autonomic manager in charge of coordinating different self X AI components, developed by the s-X-AIPI use cases. It furtherly demonstrates the effective integration of raw data flow from industrial data sources and the preliminary concept of the Human in the Loop.

Despite the D4.1 is of Type "Other", a deepen effort has been made by the project consortium to provide a comprehensive analysis on the adopted methodology to design the four Autonomic Managers. The AMs' roles and tailored actions, the connection with AI Data Pipelines and self-X components and, the measures devoted to analyse the human support and develop the related User Interfaces have been described in the current report.

The document foresees five main Sections:

- *Introduction*, which provides the Deliverable's context, its scope and the relation with other project Deliverables;
- *Background and Vision*, which supports the definition of the s-X-AIPI project ambition, the main concepts and metadata sharing practices among the self-X components, the AI Data Pipelines and the information flow with the Autonomic Manager;
- Autonomic Manager for Data in Motion, which describes its role and range of actions, its preliminary development and the rule-based engine defined per Use Case in the four domains of application, namely Asphalt, Steel, Pharma and Aluminum. It furtherly provides scalability and replicability preliminary considerations, and an initial analysis of the Autonomic Managers' Key performance Indicators;
- *Human Support in AI solutions*, which provides the adopted methodology to identify the Use Cases's requirements devoted to ensure the Human-in-the-Loop, shares the first demonstration of the HITL concept, provides the requirements collection relevant for Work Package 4 to identify the specific components to be developed for HITL purposes and, shows main commonalities for the development of the User Interfaces.
- Lastly the *Conclusions* describe the next steps on Autonomic Manager development and future deployment.

Introduction

I.I Context and scope of deliverable

The Deliverable 4.1 "Autonomic Managers for Data in Motion and Humans support in AI solutions" represents the initial version of the development of the Autonomic Managers at M18, at the middle of s-X-AIPI project implementation.

The D4.1 has a dissemination level which is Public and it includes information concerning the different activities performed in the following Tasks:

- Task 4.1 Development of autonomic managers for New Data in self-X AI solutions;
- Task 4.2 Integration of New Data for AI solutions into use cases infrastructures;
- Task 4.3 Improvement of Autonomic Managers for human in the loop feedback;
- Task 4.4 Preliminary intergration of human in the loop into AI solutions.

Despite the D4.1 is of Type "Other", a deepen effort has been made by the project consortium to ensure a comprehensive analysis on the adopted methodology designed to:

- define the Autonomic Manager's requirements, role and main actions;
- design the information flow with the AI Data Pipelines and self-X components as developed under Work Package 3 and with the Human-in-the-loop;
- identify the rule-based engine of the Autonomic Managers per Use Case, as a necessary information to tailor the Autonomic Managers on the basis of the Use Cases's specific requirements, including human support and its interaction with the Autonomic Manager;
- design its engine and component selection;
- implement the Autonomic Managers' common preliminary development;
- identify key scalability and replicability purposes and measures to be undertaken;
- establish the following steps on Autonomic Managers' development to be tailored in the next months on the basis of the Use Cases's needs and the first validation at M24;
- ensure the connection with Task 4.5 and Work Package 5 via the preliminary definition's of Autonomic Managers's Key Performance Indicators and the methodology on its monitoring.

Therefore, the current D4.1 represents a domain-agnostic initial version of the Autonomic Manager' development, to be furtherly tailored in four different Autonomic Managers on the basis of the four Use Cases's needs in the s-X-AIPI selected domains. In line with the DevOps life cycle, we can identify our current status at M18 in the first iteration related to the development of the Autonomic Manager's coding phase, as depicted in Figure 1.



Figure 1. Autonomic Manager life cycle

I.2 Relationship with other tasks and deliverables

The D4.1 represents a key cornerstone of the implemented activities performed during the project lifetime.

It provides the initial version of the Autonomic Manager' infrastructure, ensuring a tight connection with the Work Package 2 "Design and Architecture of self-X AI solutions integration in process industry plants" and especially with the following:

- D2.1 "Scenarios and Requirements for Self-X AI adoption in Process Industry" (R, PU), which aimed at analysing the industrial scenarios of the selected Use Cases and identifying the preliminary requirements –functional and non-functional for the adoption of the self-X AI solutions and the connection with the Autonomic Manager. In this context, the current D4.1 enlarges the D2.1 analysis, envisaging the collection of additional human-in-the-loop requirements to ensure the development of dedicated components under T4.3 and the User Interfaces for human feedback under T4.4.
- D2.2 "AI for Process Industry Reference Architecture and implementation" (R, PU), where the flexible and general-purpose Reference Architecture has been designed to ensure a smooth and easy integration of the Autonomic Manager with the developed AI pipelines. In this context, the D4.1 furtherly supports the definition of the s-X-AIPI Information Flow and the relation among the AM, the Data Pipelines and the Human-in-the-loop applications. It furtherly extends the Autonomic Manager range of actions and the definition of rule-based engine per Use Case, supported under T4.1.

A deepen connection within WP3 "Self-X abilities in AI Data pipeline components for human support" has been also ensured since:

- The D3.4 "Initial version of self-X components and AI procedures for pipeline integration with Data-at-Rest" (Dem, SEN) provided an initial instance of the Orion Context Broker. In this context, the current D4.1 furtherly extends the interaction between the Autonomic Manager and the AI Data Pipelines via the metadata sharing on Orion Context Broker, supported under T4.2.

Furthermore, the future D3.1 "Validation of human collaboration concept in use cases relevant environment" (Dem – SEN) and D3.3 "Testing of self-X abilities of pipeline components into industrial use cases" (Dem – SEN) will benefit from the effort made during the past implemented activities, specifically concerning the AM's preliminary development and the Human Support in AI solution dedicated activities.

The D4.2 "Validation report for Data in Motion and HITL in IT/OT use cases' infrastructure" (R - PU) will represent the validation phase of the Autonomic Manager and the established information flow. Additionally, the Task 4.5 "Technology Requirements validation" will benefit from the initial effort made to identify the preliminary steps on the Autonomic Manager' KPIs definition.

Lastly, the WP5 "Self-X AI Apps prototype demo, user training and performance improvement in process industry" will be enabled by the Autonomic Manager's baseline developed in the current D4.1. Furthermore, the preliminary analysis on potential KPIs related to the Autonomic Manager is setting the basis for the future validation reports of the proposed technology, namely "D5.1 "Commissioning Report of AI solutions for use cases" (R - SEN), D5.2 "Validation report of AI solutions for use cases" and D5.3 "User acceptance assessment of AI solutions into process industries".

2 Background and Vision

2.1 Project Objectives

The overarching project objective of s-X-AIPI is to engage in research, development, testing, and experimentation to create an innovative toolkit comprising custom, reliable self-X AI technologies and applications. These tools are intended to empower process industries workers to effectively address both external and internal influences, facilitating agile and resilient responses within the European process industry's processes and product lifecycle. This initiative aims to achieve genuine integration into the circular economy ecosystem by delivering agility of operation and performance enhancements across various key indicators. Additionally, it aspires to provide state-of-the-art AI-based sustainability tools for the design, development, engineering, operation, and monitoring of plants, products, and value chains within existing process industries and their workforce.



Figure 2. s-X-AIPI Reference Architecture

The Autonomic Manager with MAPE-K methodology is a concept in the field of autonomic computing, which aims to create *self-managing systems* capable of *adapting to changing conditions* and optimizing their performance. MAPE-K is an acronym that stands *for Monitor, Analyze, Plan, Execute, and Knowledge*. It is a powerful approach to building self-managing systems that can adapt to changing conditions, optimize

performance, and maintain system health. It is commonly applied in areas like cloud computing, network management, and distributed systems¹.

The innovative aspect of s-X-AIPI project approach lies in the integration of self-X AI, which combines AI as the intelligent processing system with an Autonomic Manager rooted in the MAPE-K model (representing continuous Monitoring, Analysing, Planning, and Execution, based on the knowledge of the AI system under control). This integration is designed to facilitate the development of self-improving AI systems.

The s-X-AIPI proposed infrastructural solution is based on the Reference Architecture, depicted in Figure 2, already outlined in D2.2, titled "*AI for Process Industry Reference Architecture and Implementation*." In this framework, the Autonomic Manager assumes a central role, functioning as an *autonomous AI data pipeline coordinator and decision-maker*. It operates by adopting the MAPE-K framework and implementing self-X capabilities. The primary objective is to empower the Autonomic Manager to engage in real-time problem-solving, detect issues during routing processing, devise solutions for these problems, perform repairs, and consolidate strategies for learning and supporting the reuse of these solutions.

This functionality is made through the combination and analysis of metadata and information sourced from various components. These components include the edge, where metadata from the physical layer and AI Data applications are situated, as well as the metadata processing layer, where AI pipelines consume the information. The ultimate goal is to apply rule-based actions and reactions to implement and improve the named self-X abilities.

It is important to remark that the Autonomic Manager occupies a central position within the infrastructure and is both scalable and extensible, capable of accommodating numerous requests simultaneously, thus enabling it to effectively serve and coordinate the entire dataflow. Basic role integration of the Autonomic Manager has already been described in D3.4 "Initial version self-X components and AI procedures for pipeline integration with Data-at-Rest". The Autonomic Manager integration via a Rule-based Engine capable to implement the event-based coordination features is more deeply described in this current deliverable in its initial state.

2.2 s-X-AIPI Autonomic Manager design

According to the s-X-AIPI Reference Architecture described in D2.2, the Autonomic Manager has to coordinate autonomously AI Data pipeline, work as a decision maker adopting MAPE-K framework, support the implementation of the Self-X abilities and interact with the applications layer to improve its functionalities. Therefore, the Autonomic Manager (AM) aim is to design a toolset of technologies envisaging innovative AI solutions with autonomic computing capabilities.

S-X-AIPI project identifies its Autonomic Manager at the centre of the infrastructure, as depicted in Figure 3, involving a Rule-based Engine with event-based coordination capabilities.

To implement these coordination capabilities for the whole AI system, the Autonomic Manager mainly interacts with the AI pipelines and the AI Methods developed to enable the pipelines of their self X abilities. This is achieved by analysing metadata from different components, including the edge where physical layer and AI Data apps metadata reside, and the metadata processing layer where AI pipelines consume data. The Autonomic Manager is also enabled via the interaction with the Operator (Figure 3), represented by the Data Scientist, the IT Operator or the Plant Operator, whenever necessary, ensuring Human-in-the-Loop principles.

The main central component capable to ensure the integration among the edge, the AI Methods, the Autonomic Manager and ensuring human-in-the-loop is the Orion Context Broker, demonstrated in its deployment in D3.4 "Initial Version of self-X components and AI procedures for pipeline integration with Data-at-Rest".

The Information Flow depicted below is in line with the Reference Architecture designed in D2.2 "AI for Process Industry Reference Architecture and implementation" where the Autonomic Manager has been conceived with a central role as an autonomous AI Data pipeline coordinator and decision maker, who adopts MAPE-K framework and implements the Self-X abilities.

¹ IBM Research. "MAPE-K: A Reference Model for Self-Aware and Self-Adaptive Computing Systems." [PDF] https://www.research.ibm.com/haifa/dept/vst/papers/2010/MAPE-K.pdf





Figure 3. s-X-AIPI Infrastructure Information Flow

Through autonomic computing system concepts, s-X-AIPI project would support the development of the Autonomic Manager enabled by its capability to control AI pipelines thanks to high-level policies implemented following the MAPE-K framework abovementioned. This will lead to a continuous Monitor-Analyze-Plan-Execute flow based on Knowledge of the AI system under control. AI pipelines are then able to self-regulate and self-improve through a range of capabilities denoted as *Self-X abilities* which are enabled under the Autonomic Manager control policies. The goal is to empower the Autonomic Manager for real-time issue resolution, detecting and addressing problems during pipeline execution. The Autonomic Manager is able to support the implementation and in case even develop the self-X abilities in terms of:

- Self-Configuration: ability to self-configure components to integrate new systems and adapt to changes in the working environment.
- **Self-Optimization:** enables automatic monitoring and management of resources to ensure an optimal functioning with respect to the defined needs.
- **Self-Healing:** ability to monitor the system health, detecting failures and planning a set of actions to correct errors and recover automatically.
- Self-Protection: Ability in identifying and protecting from arbitrary attacks in proactive manner.

The AM design phase considered autonomic computing discipline and the already existing independent coordinators and decision makers. It's expected that during the development and the deployment of a component like the AM will arise the need to continuous monitoring and tuning the selected technologies.

2.3 The role of Metadata in the Autonomic Manager

This current deliverable describes the initial version of the integration and implementation of the Autonomic Managers in charge of coordinating the different self-X AI components of the s-X-AIPI project use cases. Despite the Autonomic Managers should integrate appropriately the flow of "*New RAW data*" from industrial data sources and the human support according to the particularly available self-X abilities, the current approach has been slightly adapted to ensure an effective monitoring of the execution of the AI pipelines, with the goal of detecting any issue which will require self-management.





Figure 4. s-X-AIPI project AI data pipeline

In the context of the s-X-AIPI proposed AI data pipeline (see Figure 4), "New Raw Data" refers to the latest or most recently collected data that has not yet been processed or transformed for use in the artificial intelligence (AI) system. New raw data originates from various sources such as sensors, logs, databases or any other data collection mechanism used in the AI data pipeline system that can include the labelling to give context awareness and eventually, even the generation of Artificial Data for improving trained models. Raw data consists of typically unstructured or minimally processed information that requires processing within the AI pipeline. As depicted in Figure 4, this involves passing it through the Data Ingestion block, where it undergoes cleaning, pre-processing, and preparation within the Data Transform block. Only after these steps it can be utilized for training machine learning models in the Model Training block or be directly applied in the Real-World Usage block. The latter is responsible for addressing the pertinent real-world operational task at hand. In certain scenarios, Human-In-The-Loop interaction, facilitated through labelling or real-life feedback, may become necessary.

It is important to note that the functionality of these blocks, and their degree of self-adaptation, varies depending on the specific AI application and use case. This adaptation aims to minimize human intervention.

As better explained in D3.4 "Initial version self-X components and AI procedures for pipeline integration with Data-at-Rest", the self-X AI components will be monitored via the analysis of the **metadata** previously collected in the same deliverable. Since the model training phases and real-time anomaly detection methodologies can be conducted in a similar manner, under D3.4 it has been concluded that AI-based industrial systems require a more sophisticated maintenance approach based on self-adaptive AI systems capable to collect and support advanced processing of the metadata related to the execution of selected modules.

Therefore, the Autonomic Manager plays a pivotal role in coordinating the selected models and the components of the AI pipeline. This will be done via the execution rule-based engines which will support the analysis of the metadata previously collected in D3.4 "Initial version self-X components and AI procedures for pipeline integration with Data-at-Rest", and which will ensure the interaction with the AI Data Pipelines and the relative services used to ingest, store, manage data.

It also supports Human-in-the-Loop roles in diverse circumstances, recalling recommended action such as the mentioned labelling training data, or enhancing models through context awareness, giving feedback for the runtime operation based on environment-derived context, and generating artificial or labelled data for model improvement, and optimizing the user interface and overall user experience.

In summary, despite "New Raw Data" within the s-X-AIPI project AI data pipeline represents freshly acquired, unprocessed data from diverse sources and the critical stages of pre-processing and transformation seems to be essential for converting this raw data into a suitable format for training AI models and/or making real-time predictions or decisions of the "Real-World Usage", the role of the metadata in the Autonomic Managers become the essential baseline to ensure the monitoring and maintenance of the developed AI Pipelines.

3 Autonomic Manager for Data in Motion

The Chapter 3 identifies the adopted measures to support the "Design about the Autonomic managers in charge of coordinate different self X AI components of use cases to integrate appropriately the flow of "New RAW data" from industrial data sources and the human support according to self-X abilities available".

Since the proposed infrastructure is designed to be domain-agnostic, the Autonomic Manager's role and application-independent range of actions have been described. Furthermore, a preliminary development has been defined in order to demonstrate the infrastructure instalment, where common tasks among the four different Use Cases and the integration of the selected components have been implemented. Lastly, the related rule-based engines support in tailoring the Autonomic Managers according to the specific Use Cases' needs and the developed self-X AI components. The customization of the Autonomic Managers is an ongoing process, developed via the creation of specific DAGs in AirFlow.

The integration of data sources is demonstrated via the section on metadata sharing via Orion Context Broker.

The scalability, replicability, and preliminary analysis on KPIs definition conclude the Autonomic Manager design phase.

3.1 Automic Manager's role and range of actions

The s-X-AIPI Autonomic Manager has a central role depicted as an autonomous AI Data pipeline coordinator and decision maker, who adopts MAPE-K framework and support the implementation of the Self-X abilities, as described in Chapter 2.

It enables self-regulation of AI pipelines, based on each use case needs, promoting gradual enhancement of their performance through the self-X abilities. To achieve this, it establishes an adaptation loop, continuously observing pipeline operations and facilitating experiential learning following the MAPE-K model.

To integrate autonomic computing features across the entire AI system, the Autonomic Manager primarily engages with both the AI pipelines and the AI Methods designed to empower the pipelines with self-X abilities. Additionally, the Autonomic Manager follows the principles of Human-in-the-Loop interaction, questioning operators such as Data Scientists, IT Operators, or Plant Operators, whenever needed.

AI pipelines are complex systems that ingest and process data in several steps. Each of this step produces a set of *metadata:* performance indicators reflecting the status of the whole AI system. Hence, thanks to these metadata analysed with defined AI Methods, the Autonomic Manager can monitor the system, plan and execute tasks from a *range of actions* to meet the required self-X abilities.

The generic range of actions provided by the autonomic manager are the following ones:

- Failures:
 - Monitor failure state from metadata, for example by checking results error, execution times or exit statuses of applications
 - Analyse and categorize the failure case
 - Execute a hypothetical application rescheduling with or without different configuration parameters (i.e.: larger amount of allocated resources)
 - Applying corrective measures if possible
- System Adaption to Production Data:
 - Monitoring AI pipeline performances using defined metrics like Mean Absolute Error (MAE), Root Mean Squared Error (RMSE), MSE, F1 score, accuracy, validation accuracy, loss, etc.
 - Analyse the performance trends, detection of performance decreases
 - Generation of corrective measures such as starting a performance tuning session (i.e., following the continuous training paradigm) or the training new version of the degraded AI model based on new data, manage the CI/CD flow of the new model

• Invoking Human-in-the-Loop for feedback

- System Adaptation to Request Peaks:

- Monitoring of the AI system performances like CPU consumption, memory consumption, execution times for each AI task.
- o Monitoring available hardware performances, status and remaining computing capabilities
- Analyse possible bottlenecks, detect tasks with high impact
- o Schedule and actuate deployment of additional hardware resources to ensure scalability

- ETL Support for historical data:

- Reception of AI Pipeline data, application of data quality evaluation techniques (outlier detection, percentage of missing data), analysis of data quality over time
- Automatic cleaning, labelling, backfilling
- Human in the Loop invocation for feedback and manual tasks

- AM Task Orchestration:

- o Automatic detection for data dependencies, scheduling data requests when necessary
- Task dependencies building and scheduling based on system needs
- Automatic resource allocation for tasks
- Task status monitoring, failure detection and recover

The different actions above-mentioned have been deeply analysed with a specific overview per Use Case in the following paragraph, to ensure the definition of a scalable and replicable Rule-based Engine at the basis of the Autonomic Manager's development.

3.2 Rule-based Engine per Use Case

According to Task 4.1 " Development of autonomic managers for New Data in self-X AI solutions", specific autonomic managers should be defined, designed and implemented to coordinate self-X AI components and to integrate appropriately the flow of "New RAW data" from industrial data sources so to ensure the impact according to self-X abilities available (configuration, optimization and healing) into RealWorld models reflected in self-X AI data pipeline.

Therefore, the design of the Autonomic Managers envisaged the definition of main elements and expected actions of the Autonomic Manager's to support the self-x AI components and process the maintenance of the AI pipelines. Several iterations for collecting the information and developing the Autonomic Managers have been followed:

- 1. from the collected information under Work Package 3 on metadata and the expected AI methods to support the self-X capabilities, the analysis has been enlarged on the Autonomic Manager expected contribution, its role and the data sources to be analysed, in the case of differences from WP3 related data sources. This is represented by the so-called *rule-based engine* provided per Use Case via the subchapters below. Furthermore, the interaction via Orion Context Broker has been demonstrated.
- 2. The collection of the Rule-based engines depicted per Use Case defined a preliminary set of actions previously described in Chapter 3.1. In the case additional requirements should be identified during the Autonomic Managers' final development, potential novel actions could be analysed and envisaged.
- 3. A preliminary development of the main infrastructural components has been set to define the common baseline of the four Autonomic Managers. It has been developed and demonstrated the effective implementation of the selected components, available in Chapter 3.3.

The Autonomic Managers' *rule-based engines* are provided in the following sub-chapters, divided per domain.

3.2.1 Asphalt

Table 1. Asphalt preliminary analysis on AM's rule-based engine

UC	Self-X Solution	Which is the need/ problems to be solved	WP3 Metadata Same information collected in D3.4.	WP3 AI methods' solution Same information collected in D3.4.	WP4 - AM role and solutions (UC) Brief description	WP4 - Selected Metadata for the AM engine (NISSA/CORE, UC) If different from column D, coming as output from WP3 processing or from UCs solutions : 1. Aggregated Data from WP3 - light description 2. New Raw Data from HITL (e.g. after labelling) - light description 3. Sub-system of Column D: light description	 WP4 - AM Actions & Rule-Engine (UC, NISSA/CORE) Please describe them with reference to the AM Range of Actions (sheet 3 -AM Actions): Failures - descr. of the specific action Monitoring - descr. of the specific action Orchestrator - invoke HITL for labelling dataset in Column D or Column G Other - descr. of the specific action (If different from the provided actions) How to use Data from Column G to define a rule or action More Range of Actions can be described (see the example) Please use numbers to make a prioritization of the actions (see the example)
АЅРНАГТ	Asphalt mix design	detect anomalies in the asphalt production process	data reception rate ranges of the variables of interest	"Data quality check detection"	AM will inform to the Data scientist on a the global data reception rate changes and/or if a change in the range of a variable of interest is detected. As a result of the warning, the analyst must review the data ingestion procedure and/or readjust the anomaly detection model.	na	UC: 1. Monitoring Data quality (Monitor) 2. Failures - Retry if global data reception rate changes (Analyse & Plan) 3. Orchestrator - Invoke HITL for validation & Return feedback to readjust the anomaly detection AI model within WP3 (Execute)
	Plant elements diagnosis	Detect anomalies regarding the efficiency of the factory motors	Data reception rate Ranges of the variables of interest Model accuracy Model execution time	"Data quality check detection" "Quality of the model"	AM will inform to the Data scientist on a the global data reception rate changes and/or if a change in the range of a variable of interest is detected. As a result of the warning, the analyst must review the data ingestion procedure and/or readjust the anomaly detection model. AM will inform to the Data scientist on a change in the prediction error.	na	UC: 1. Orchestrator - Invoke HITL for validation 2. Orchestrator - Return feedback to AI Methods (WP3) 3. Failures - Retry if failure happens or apply corrective measures 4. Monitoring – Success or failure status
	Paving conditions and parameters	 predict asphalt paving temperature at job site 	model accuracy model execution time	"Quality of the model"	AM will inform to the Data scientist on a change in the prediction error. After validation, the "Autonomic feature selection" & "Autonomic algorithm selection" procedures [with Self-X abilities to minimize Data Scientist involvement] will be launched.	na	UC: 1. Monitoring Model Quality (Monitor) 2. Failures - Retry if global model accuracy changes (Analyse & Plan) 3. Orchestrator - Invoke HITL for validation & Return feedback to retrain the prediction AI model (Autonomic feature selection OR/AND Autonomic algorithm selection) within WP3 (Execute)
	Quailty traceability at lab level	predict mechanical/volumetric properties within asphalt mix detect anomalies in the granulometry	data reception rate ranges of the variables of interest model accuracy model execution time	"Data quality check detection" "Quality of the model"	AM will inform to the Data scientist on a the global data reception rate changes and/or if a change in the range of a variable of interest is detected. As a result of the warning, the analyst must review the data ingestion procedure and/or readjust the anomaly detection model. AM will inform to the Data scientist on a change in the prediction error. After validation, the "Autonomic feature selection" & "Autonomic algorithm selection" procedures [with Self-X abilities to minimize Data Scientist involvement] will be launched.	na	UC: 1. Monitoring Data quality and Model Quality (Monitor) 2. Failures - Retry if global data reception rate or model accuracy changes (Analyse & Plan) 3. Orchestrator - Invoke HITL for validation & Return feedback to readjust/retrain the AI model within WP3 (Execute)

3.2.2 Steel

Table 2. Steel preliminary analysis on AM's rule-based engine

UC+A 1:H1	Self-X Solution	Which is the need/ problems to be solved	WP3 Metadata Same information collected in D3.4.	WP3 AI methods' solution Same information collected in D3.4.	WP4 - AM role and solutions (UC) Brief description	WP4 - Selected Metadata for the AM engine (NISSA/CORE, UC) If different from column D, coming as output from WP3 processing or from UCs solutions : 1. Aggregated Data from WP3 - light description 2. New Raw Data from HITL (e.g. after Ibabellion).	 WP4 - AM Actions & Rule-Engine (UC, NISSA, CORE) Please describe them with reference to the AM Range of Actions (sheet 3 -AM Actions): Failures - descr. of the specific action Monitoring - descr. of the specific action action Orchestrator - Invoke HITL for labelling dataset in Column D or Column G Other - descr. of the specific action (If different from the provided actions) How to use Data from Column G to define a rule or action More Range of Actions can be described (see the example) Please use numbers to make a prioritization of the actions (see the example)
	Data ingestion / cleaning and transformation	To ensure integrity and quality of input data during data ingestion and data cleaning transformation process	Metadata defined: Number of heats Statistical description Number of missing data Number of zeros (implicit number os scraps)	A comprehensive set of statistical descriptions is created, including minimum, maximum, mean and standard deviation of each input variable	After the evaluation of each variable, warnings are generated if the information is incomplete or not valid.	na	 Data dependencies: e.g. upstream data is missing. Filling data with reference values (i.e mean value) Orchestrator - Return feedback about a new material being introduced into the system? If so, the HITL should interact aproving that a new material has been introduced
Steel use case	Data exploration	Statistical analysis is considered when defining the upper and lower bound	Metadata defined: Upper and lower limit of parameters Number of outlier	Outliers (anomaly) for each parameter within the dataset is calculated	In case of an anomaly detection, a warning should be generated	na	1- Orchestrator - Return feedback about anomalies detected to HITL, providing the information on: -Is a meterial chemistry out of range? i.e chart with limits
	ML modeling training	Perform the ML and statistics about retraining, performance	Metadata defined: 1 - Number of input parameters 2 - Number of heats 3 - Number of targets 4 - The R2-score 5 - MAE score 6 - RMSE score 6 - RMSE score 7 - Linear regression coefficient for all inputs 8 - The peak memory usage of the system when training the model	Calculation of the ML accuracy	Models are Re-trained and in case of a best performance the new model replaces the current model.	na	1- Failures - Retry the model if the accuracy is out of scope (wihout HITL intervention)
	ML modeling	Calculation of scrap chemistry and furnace expected temp and chemistry for posterior scrap mix optimization and EAF performance		Calculation of coefficients (chemistry) of different scraps Calulation of EAF temp + chemistry considering a Machine Learning Black Box approach	Modeling results implemented for The scrap mix optimizer For EAF status prediction	na	 Deployment: Update the scrap coefficients (scrap chemistry) Deployment: Update the EAF coefficients (liquid steel Temp and chemistry)

3.2.3 Pharma

 Table 3. Pharma preliminary analysis on AM's rule-based engine

uc	Self-X Solution	Which is the need/ problems to be solved	WP3 Metadata Same information collected in D3.4.	WP3 AI methods' solution Same information collected in D3.4.	WP4 - AM role and solutions (UC) Brief description	WP4 - Selected Metadata for the AM engine (NISSACORE, UC) If different from column D, coming as output from WP3 processing or from UCs solutions: 1. Aggregated Data from WP3 - light description 2. New Raw Data from HTI, (e.g. after fabelling) - light description 3. Sub-system of Column D: light description	WP4 - AM Actions & Rule-Engine (UC, NISSA, CORE) Please describe them with reference to the AM Range of Actions (sheet 3 -AM Actions): - Failures - descr. of the specific action - Monitoring - descr. of the specific action - Orchestrator - Invoke HITL or labelling dataset in Column D or Column G - Other - descr. of the specific action (If different from the provided actions) How to use Data from Column G to define a rule or action Morre Range of Actions can be described (see the example) Please use numbers to make a prioritization of the actions (see the example)
	Self-X OCT: OCT probe position evaluation	OCT probe position is adjusted manually, this is error prone and might vary between different operators.	Position OK or not OK. Position of electrode in image will be passed on to ORION.	Frequency can lead to systematic hardware problems such as loose screws. Positions can be compared between processes to ensure reproducibility.	AM will inform operator if the position deviates from previous processes. AM guides the operator when adjusting into the correct position. Frequency of wrong position is tracked and systematic errors are shown to operator.	NA	Monitoring - Success or failure status of OCT probe position. Z. Orchestrator - Invoke HITL for validation of position deviation. Failure - HITL to correct position. Orchestrator - Return feedback to AI Methods (WP3).
Pharma	Self-X OCT: Signal quality check	Currently, the operator has to periodically check the signal quality.	Number of good and bad signal events.	Frequency of events can be tracked.	AM will monitor the signal quality over time. Locally, the self-X solution can check if a signal is there or not. Gradual degradation over time will be tracked by the AM. The AM will keep historic records of signal quality. Locally, no historic data for signal quality will be kept.	NA	 Monitoring - quality of signal is tracked. Orchestrator - report poor signal back to HITL.
		Degradation over time is very hard to detect manually.	After every signal evaluation a quantifier for the quality (e.g. signal intensity) will be passed on to ORION.	Soon to occur faults can be found.	The AM will keep historic records of signal quality.	NA	 Monitoring - quality of signal is tracked. Orchestrator - inform HITL of possibility of signal degradation.
		Automatic monitoring of OCT signal quality with AM can detect systematic long-term degradation.		Systematic errors such as unclean fiber cable can be detected.	Locally, no historic data for signal quality will be kept.	NA	 Monitoring - quality of signal is tracked. Orchestrator - inform HITL of possibility of signal degradation.
	self-X IR data integrity check	It needs to be ensured that the IR is running, measuring at the defined intervals and that the spectra are not distorted. This is difficult to manage by the operator during an experiment.	The measurement event will be passed to ORION and the number of values to be kept by the AM.	Problems such as uncertain measurements lacking values can be detected.	The AM will keep historic records of the number of values and frequency of measurement events.	NA	 Monitoring - quality of signal is tracked. Orchestrator - Inform HITL if signal degrades or seems inappropriate.
	self-X power supply data check	The current at the power supply is set, the voltage is a consequence of that current and reflects the experimental conditions. Deviations in the voltage are very hard to check manually but can hint to critical faults.	Measurement events will be passed on to ORION.	If the measurement frequency deviates from historic records, this can be detected by the AM.	The AM will keep records of measurement event. Locally, the values are kept to be compared to past records and so that process faults can be made visible.	NA	 Monitoring - quality of signal is tracked. Orchestrator - Inform HITL if signal degrades or seems inappropriate.
	self-X model training supervision	The quality of the training of the model predicting the process outcome should be observed for degradation over time.	Training results and statistics will be passed on to the AM.	Changes in model training performance can be detected by the AM.	Training records are kept by the AM as reference.	NA	1. Monitoring - Model performance is ok or failure status. 2. Failure - Retrain/Update Model. 3. Orchestrator - Return feedback to Al Methods (WP3).

3.2.4 Aluminum

Table 4. Aluminum preliminary analysis on AM's rule-based engine

							WP4 - AM Actions & Rule-Engine (UC, NISSA, CORE)
uc	Self-X Solution	Which is the need/ problems to be solved	WP3 Metadata Same information collected in D3.4.	WP3 AI methods' solution Same information collected in D3.4.	WP4 - AM role and solutions (UC) Brief description	 WP4 - Selected Metadata for the AM engine (NISSA/CORE, UC) If different from column D, coming as output from WP3 processing or from UCs solutions: 1. Aggregated Data from WP3 - light description 2. New Raw Data from HITL (e.g. after labelling) - light description 3. Sub-system of Column D: light description 	Please describe them with reference to the AM Range of Actions (sheet 3 -AM Actions): • Failures - descr. of the specific action • Monitoring - descr. of the specific action • Orchestrator - Invoke HITL for labelling dataset in Column D or Column G • Orchestrator - Invoke HITL for labelling dataset in Column D or Column G • • Other - descr. of the specific action (If different from the provided actions) How to use Data from Column G to define a rule or action More Range of Actions can be described (see the example) Please use numbers to make a prioritization of the actions (see the example)
Aluminium	Aluminium mix recipe	Unknow/uncertain data from incoming materials - data might be missing or not representative	Data ingestion and Data transformation metadata: - Number of rows - Number of NaNs values per column	Dealing with missing information and uncertainty: fill-in values based on historial information and/or statistics of current state e.g., average of materials' composition in a silo, make inferences from the (historical) material behaviour	Based on metadata, warnings will be send to operators in case that the information given is not valid or sufficient. The operator will be able to fill missing information, try to access statistical analysis to fill them automatically based on historic data, or remove the input data sample.	ΝΑ	<u>Orchestrator:</u> - <u>Return feedback to AI methods</u> - <u>Invoke HITL to validate action)</u> <u>Execution dependencies</u> Run "data ingestion" and "data transformation" in serie (in pipeline)
		Lack of knowledge of internal patterns between feedstock/process during the aluminium production - no traceability of historical behaviour of raw materials or their combination	Data Exploration metadata: - Minimum - Maximum - Median - Standard deviation - Top 5 features with highest (Pearson) correlation score - Relative variance-based importance	Gain knowledge about the parameters of the process and their interrelations. Data is analyzed in a 1-to-1 and 1- to-many basis: outliers can be shown to operators to check the validity of data; relevant trends and relations can be shown to operators	Based on metadata analysis, warning messages will be sent to operators when one or more parameters are out-of- distribution or show uncommon behaviour	NA	Data depedencies: chek database availability. Process historic data: analysis of exploration results based on previous metadata
		Dependance on human expertise in the decision-making of raw materials for the aluminium production - there are more than 100 silos, with several raw materials stored at each of them, to consider	Model Training and Real- world usage metadata: - Mean Absolute Error,	Support the decision-making process for selecting aluminium recipes, more especifically, raw-materials	g Based on metadata (performance of models and human feedback), model re- training or change of the model being used will be executed.	Human feedback will be considered to	Process historic data: analysis for new models based on previous metadata <u>Orchestrator</u> - Invoke HITL for feedback and return feedback to AI methods
			- Mean Square Error - Root Mean Square Error - R-squared (R2)	Support the decision-making process for selecting aluminium recipes, more especifically, the alloys during the process		e assess the performance and fitness of the models	e.g., if model is worst, do not update, otherwise do so. <u>Data dependencies</u> : check database is available

3.2.5 Metadata sharing on Orion Context Broker

According to Task 4.2 " Integration of New Data for AI solutions into use case infrastructure", the integration of the AI Pipelines developed at the edge will be ensured via their connection within the FIWARE Generic Enabler Orion Context Broker. This integration represents the very preliminary and necessary step to furtherly support the communication among the AI Data Pipelines at the edge and the Autonomic Manager in the cloud.

According to s-X-AIPI Information Flow, depicted in Figure 3, the shared metadata will be consumed by the AI methods, HITL applications and the Autonomic Manager itself, supporting and triggering in the next steps the self-X capabilities. Currenty the UCs are provinding two Orion Context Broker entities in NGSI-LD format, publishing the metadata in two different intervals (greater window and smaller window).

Table 5 provides the demonstration of the incurred interaction among the edge and Orion Context Broker in the four Use Cases related to the s-X-AIPI Project.

Use Case	Metadata sharing on Orion Context Broker
Asphalt	Entity with greater window; Entity with smaller window
Steel	Entity with greater window; Entity with smaller window
Pharma	Entity with greater window; Entity with smaller window
Aluminum	Entity with greater window; Entity with smaller window

Table 5. Metadata sharing on Orion Context Broker

3.3 Preliminary development

The Autonomic Manager's (AM) preliminary development relies on the necessity to coordinate self-X AI components, integrating properly the flow industrial data sources, supported by the analysis performed in the workflows under definition in WP3. The MAPE-K framework is at the base of the development phase, as well as the need to improve overall AI system and human operator intervention to support the process.

A dedicated GitHub repository has been created to include the Autonomic Manager's main functionalities, useful tools, functional requirements, and shared metadata. The instructions on how to run the Autonomic Manager and how to setup the Identity Management have been also included.

Figure 5 shows the selected components used to define the infrastructure and which will support the Autonomic Manager development, taking into account the interaction with external components like the use cases, the human in the loop (HITL) application and Metadata Processing Method from WP3.



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The FIWARE Orion Context Broker (OCB) is the star centre of the infrastructure with its implementation of the Publish/Subscribe mechanism able to manage the entire lifecycle of context information. It based on NGSI-LD data format, adopted as a standard for the communication in the entire architecture. So that, all the actors in this infrastructure (Use cases, WP3 analysis outcomes, HITL) converge the metadata produced and retrieve the results from the OCB. In this way the Autonomic Manager is aware of all the information flow from and to the different components.

The rule-based engine is represented by Apache Airflow², containing the knowledge of the AM to act in autonomous way. It's a tool for the workflow management, where there is the possibility to schedule them and implement the range of actions to be performed by the AM. It is essential to clarify that the Use Cases' Autonomic Managers might differ from each other in terms of specific actions to be performed. This will be released via the development of specific DAGs, according to the rules defined in Chapter 3.2 Rule-based Engine per Use Case.

Figure 6, Figure 7 and Figure 8 depict some examples of the DAGs already developed in Airflow to run common tasks identified among the four different Use Cases, like:

- monitoring of entities in OCB;
- decision making, based on the rules defined for each action the AM can do;
- planning and scheduling of the activities and backup procedures;
- query PostgreSQL to perform analysis and extract information from historical data;
- publishing results on OCB;
- orchestrate jobs and components.



Figure 6. Publish and Subscribe to OCB



Figure 7. Query a Database



Figure 8. Execution dependencies

FIWARE Draco together with PostgreSQL enable the archiving of information circulating, this will help to have an historical dataset from which it is possible the extraction of information and the run of analysis to

² https://airflow.apache.org/

support the AM. Keyrock, combined with Wilma Pep Proxy for Orion-LD, from FIWARE Generic Enablers catalogue is the component will act as identity manager. Its adoption is due to the necessity to have different user, roles and organizations for each component will interact with the AM. Each Use Case has its own user with the relative grants (see Figure 9, Figure 10 and Figure 11) able to interact only with the OCB entities and subscriptions connected to its domains. This is indeed valid for HITL applications and WP3 methods.

Polos	1	Pormissions		
Provider		Cot and assign only public owned rates		
Purchaser		Get and assign only public owned roles		
Jpdaters Pharma	r û	Get and assign all public application roles		
Jpdaters Asphalt	C D	Manage authorizations		
Jpdaters Steel	C D	Manage roles		
Jpdaters Aluminium	e	Manage the application		
		Get and assign all internal application roles		
		PATCH Steel	ľ	
		GET Asphalt	ľ	0
		GET Aluminium	ľ	
		✓ GET Pharma	ď	Û
		PATCH Asphalt	ď	1
		GET Steel	ľ	Û
		PATCH Aluminium	ß	1

Figure 9. Roles Management in Keyrock

PATCH Pharma

1

9	show	15 * entries	Fil	ter	Create	user Delete user
		Id	Username	Email	Enable	Actions
	4	3de9ee44-f6d2-43be-bc8b-b471d7ec47c0	Cartif Operator	operator@cartif.es		Select action 👻
	-	76a2b4c2-52e3-4bfc-be9a-493b6239d1dc	Nissatech Operator	operator@nissatech.com		Select action +
	4	78081aae-ce39-41df-823f-245c9b5cb9dd	Cartif Admin	admin@cartif.es		Select action 👻
	-	aaaaaaa-good-0000-0000-000000000000	Engineering Admin	admin@eng.it		Select action +
	4	bddec2ab-d133-4c04-a71c-a78767ba7169	Nissatech Admin	admin@nissatech.com		Select action 👻
	<u>.</u>	c93b2dc5-1d44-42fd-8d7a-7f5b5520bc8d	RCPE Operator	operator@rcpe.at		Select action +
	4	cbd66921-f6a9-43b1-ba93-5b75182b463c	BFI Admin	admin@bfi.de		Select action 👻
	۵	cecdffd7-119c-481b-b060-c20fe149d06e	RCPE Admin	admin@rcpe.at		Select action +
	2	e947d4c6-9254-43d4-bb6d-23dfb23ee00f	Aimen Admin	admin@aimen.es		Select action 👻
	-	ee6c8821-298a-4b7c-a424-af8e6a4b5560	Aimen Operator	operator@aimen.es		Select action 👻

Figure 10. Users Management in Keyrock

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All organizations	cart	Author	rized Organizations 🚱	filter	
CARTIF	+	205 000	RCPE	3 roles 🗸	×
		105	Aimen	3 roles 🗸] ,
		44	Security	12 roles 🗸	,
		쇖	Nissatech	9 roles 🗸	,
		-		Owner	-
		125	BFI	✓ Purchaser Provider	,
		-		✓ Updaters Pharma	-
		205	CARTIF	🗸 Updaters Asphalt	,
				✓ Updaters Steel	_
				 Updaters Aluminium 	
				filember	Sav
		_		Purchaser	-
	And RCPE			Provider	
	Can Manage Pharma			✓ Updaters Pharma	
	Socurity			Updaters Asphalt	
	Managers of Keyrock			 Updaters Steel Updaters Aluminium 	

Figure 11. Organization and Permissions Management in Keyrock for Orion-LD Application

The s-X-AIPI repository in GitHub related to the Autonomic Manager includes, among the others, the Identity Management (IDM) and access control mechanisms, developed to assure security and data protection on the use of the Autonomic Managers by the four different s-X-AIPI Use Cases.

The IDM setup enables the creation of the different users per organisation. The guideline is organised as the following:

- Users management
 - Creating Users
 - List all Users
 - Grouping User Accounts under Organizations
 - Create an Organization
 - List all Organizations
 - Assign users to organizations
 - o List Users within an Organization
 - Managing Roles and Permissions
 - Create an Application
 - Create a Permission
 - List Permissions
 - Create a Role
 - Assigning Permissions to each Role
 - o List Permissions of a Role
- PEP Proxy
 - Create a PEP Proxy
 - o Read PEP Proxy details
- Authorizing Application Access
 - Grant a Role to an Application
 - Grant a Role to a User
- Securing Orion Context Broker

- \circ $\;$ Access to Orion Context Broker without Access Token $\;$
- How to obtain Access Token
- o Access Orion Context Broker with an Authorization token: Alice user
- Access Orion Context Broker with an Authorization token: Managers (e.g. Bob)
- Access Orion Context Broker with an Authorization token: Users (e.g. Charlie)
- Access Orion Context Broker with an Authorization token: Data owners (e.g. Ole)
- Access Orion Context Broker with an Authorization token: Other users (e.g. Eve)

The final working environment will be put in place by an administrator user having the permission to create all the entities and subscriptions on the OCB, to facilitate the information flow among the different technologies abovementioned.

The s-X-AIPI repository will be furtherly updated during the project lifetime, describing the future developments of the s-X-AIPI Infrastructure and the Autonomic Managers developed per domain of application in the four Use Cases. The repository is available at: <u>GitHub - Engineering-Research-and-Development/s-X-AIPI-Autonomic-Manager</u>

3.4 Scalability and Replicability

The Autonomic Manager covers the core role of self-management of many deployed AI pipelines, being it in charge of constantly monitor, analyse, plan and execute corrective actions on them when necessary. The amount of work needed to fulfil its role rises a scalability requisite for this component: it should be able to manage each pipeline independently minimizing resource consumption and, by consequence, to self-recover from faults.

Apache Airflow and Kubernetes are the main support components ensuring scalability of the Autonomic Manager. Airflow is a highly scalable tool thanks to its modular architecture able to rely on a Kubernetes cluster. It has a "core" made of one or more *schedulers*, a *webserver*, an *executor* and a *metadata database* to control each workflow execution; all tasks are then executed in other places named workers.

Airflow scalability is granted by three major causes:

- The effective hardware deployed and available (number of machines for horizontal scalability, computing capabilities of each machine for vertical scalability)
- Configuration parameters set by the user while deploying the component
- The Executor

Hardware choices are self-explainable and do not need further in-depth analysis. On the other hand, the other two points need further details.

Configuration parameters influence scalability on three levels:

- **Environment-level:** parameters influencing the execution of each DAG in the same airflow environment and can be set inside the "*airflow.cfg*" file. These settings can be furtherly divided in *core settings* influencing the number of concurrent processes or processes maximum runtime and *scheduler settings* influencing how schedulers parsed DAG files and create DAG runs.
- **DAG-level:** parameters applying only to specific DAGs, defined in the DAG code itself. These configurations allow a finer control of workflow, especially when influencing external systems. Being DAG level settings finer that environmental level ones, the former ones take precedence over the latter.
- **Task-level:** parameters defined in each task operator, allowing the finest control over performances. The use of task-level settings is suggested for tasks causing performance issues

The choice of the Airflow executor influences scalability of the overall Autonomic Manager. Airflow provides four types of executors, two of which are designed for scalability. Among them, the **Kubernetes**

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Executor can leverage the scalability provided by a Kubernetes cluster, optimizing workflow scheduling and resource allocation.



Figure 12. Airflow with Kubernetes Executor Communication Schema

Its advantage is the possibility to scale from zero, meaning that no resources are wasted when the Manager has not active tasks, while if the Autonomic Manager needs to run tasks, resources are automatically allocated based on needs. Moreover, the use of a Kubernetes Executor allows also the possibility to decide the amount of resources to allocate to specific tasks. This is possible thanks to the execution of tasks in separate pods: isolated environment acting as single machine where tasks live until their completion. Last, but not least, Kubernetes pods mechanism is naturally fault-tolerant: each pod incurring in crashes is automatically re-created by Kubernetes that retries the execution of failed tasks based on its settings.

To leverage the Kubernetes Executor, Airflow must have access to a Kubernetes cluster, and in particular a multi-node one is the best option for scalability needs of the Autonomic Manager. In a multi-node Kubernetes cluster, a node is an isolated environment. Kubernetes can simulate a multi-node environment on a single machine via docker containers (virtual horizontal scaling) or can leverage both the power of a physical multi-node machine or of a cluster of physical machines (physical horizontal scaling). The first node is defined as *master node*, runs the Kubernetes control panel and can control the whole cluster, while the other ones are named *worker nodes* and execute the workload.

In particular, the master node includes an API server, a database to hold the state of the cluster, a control manager, a scheduler and other components to make the master able to manage the whole cluster. Each worker node, instead, has the containerized workload which is controlled from the master thanks to *kubelets* (Kubernetes servlet): an agent inside each worker node allowing the control panel to have control on worker nodes.

Using this deployment schema, main components (webserver, schedulers and metadata database) of Airflow are loaded in one worker node if its resources are sufficient. Otherwise, the Kubernetes cluster tries to balance the load among multiple nodes. Thanks to the Kubernetes APIs running on the master node, the schedulers are enabled to launch tasks in separate pods among the other nodes of the cluster based on the decision taken from the Kubernetes control panel.



Figure 13. Example of Airflow deployed on a local Kubernetes cluster using Kind³

The Autonomic Manager's replicability and easy adoption in domain-agnostic use cases is ensured via the promotion of standardised and efficient approach to AI pipeline management.

All the tools selected for the Autonomic Manager, including Orion-LD and Airflow, are open-source and provided with easily deployable methods like docker-composes and/or helm charts. These installation methods ensure simplicity and platform independence when deploying the Autonomic Manager on various hardware setups. Regarding AI pipeline management, the tool's flexibility lies in its ability to customize workflows for specific use-cases using a variety of basic operators offered by the Airflow tool.

Additionally, it enables the reuse of tasks or DAGs with modified configuration parameters, allowing the same processes to be applied to different situations, like it happens following the AI pipeline approach. To ensure replicability also with what concerns the rule-base engine, commonly used DAGs are available in a code repository along with a configuration manual.

This facilitates a quick setup of the Autonomic Manager with a pre-configured set of actions for common use-cases.

3.5 Preliminary identification of Autonomic Managers' key performance indicators

After the considerations on scalability, another important aspect to consider is monitoring the Autonomic Manager's efficiency via its performance indexes, since it is at the centre of the architecture and responsible for the orchestration of the self-X components.

Despite the Autonomic Managers' development is still in its preliminary phase, an initial analysis capable to identify the main possible implications of deploying the declared tools and, which concepts and timely KPIs should be considered when evaluating the Autonomic Manager' effectiveness, should be considered.

Four main focus areas, where specific, timely and measurable KPIs will be identified, have been detected during the Autonomic Managers' preliminary development:

Overall Autonomic Manager Performance: it is important to monitor the tool performance, such as the service response times and service availability, considering them under the orchestration perspective. This could reflect in measurements of Airflow DAG execution delays, Airflow DAG execution failure over success ratio, intra-component response times, external services availability time or components failure and recover. This field of analysis ensures the robustness of the tool.

Resources Allocation and Load Balancing: it includes the hardware utilisation rates for the Autonomic Manager, as well as its ability to strategically allocate hardware resources according to the varying load of requests. This performance indexes ensures scalability requirements to be optimally satisfied.

³ kind is a tool for running local Kubernetes clusters using Docker container "nodes". kind was primarily designed for testing Kubernetes itself but may be used for local development or CI.

Data Management: it foresees the monitoring of both real time data and historical data exchange volumes, by evaluating indicators such as the evolution of Orion Context Broker response times over data exchange ratio, or the database query performances. Monitoring data exchange can help identifying potential areas of improvement.

Autonomic Manager usability: it includes the evaluation of the ease of interaction between the Autonomic Manager with external services, easiness of installation, maintenance, and operability. It also foresees the evaluation of the human-in-the-loop feedback and the tool usability. This field of analysis wants to ensure both ease of use and replicability requirements.

This analysis will be made in the context of T4.5 "Technology requirements validation" to ensure a coherent approach among WP4 and WP5. The proposed approach will be validated in the next project activities so to identify additional KPIs to monitor the quality of the Autonomic Managers via the efficacy of the AI Pipelines maintenance measures, potential gaps or barriers in the identification and measuring of Key Performance Indicators per Focus Area, as well as to tailor the identified KPIs to the needs and requirements of the selected use cases and extend them to the relevant domain of application where the Autonomic Manager and the s-X-AIPI concepts might be replicable.

4 Human Support in AI solution

The Chapter 4 identifies the adopted measures to support the "Design about the Autonomic managers in charge of coordinate different self X AI components of use cases to integrate appropriately the flow of "New RAW data" from industrial data sources and the human support according to self-X abilities available".

Therefore, a preliminary analysis of the findings from the revised version of D2.1 "Scenarios and Requirements for self-X AI adoption in Process Industry", which included the User Stories and has been submitted in July 2023 (M14), has been proposed. The Human-in-the-Loop has been deeply analysed identifying the Users and related scenarios with the Autonomic Managers' interaction.

Lastly, an analysis of the specific Infrastructure requirements for adopting the human-in-the-loop and a preliminary investigation on commonalities for the development of User Interfaces have been proposed.

4.1 HITL's Role in User Stories

In the proposed AI solution, the HITL is a central figure. The role of the HITL is diverse and arranges many different activities. About the four different use cases, two larger groups can be determined: (i) HITL that interact in real-time with the production process, usually the "operator", and (ii) HITL that interact in planning, modelling and remote monitoring of the process, ranging from the role "data scientist" to "manager" and "maintenance technician".

The interest of the role "operator" can be separated into two principal stories:(i) the operator needs the status information of the process or the plant to detect and prevent malfunctioning or perform necessary maintenance operations, and (ii) the operator requests a process forecast to work efficiently as possible related to overall cost and resources.

The "data scientist" role differs in term of the human interaction taken, the following principles are common over the use cases: (i) the data scientist needs to obtain clean and useful data from the production plant; (ii) the data scientist wants to develop accurate and reliable models helping other HITL and the AI solution to cooperate and to perform and (iii) the data scientist requires real-time information to regularly review and necessarily revise the developed models.

These introductory descriptions will be discussed very detailed for each of the use cases in the following Chapter. A comprehensive description of the user roles, their tasks and their involvement with the developed self-X solutions is performed to efficiently integrate the HITL in the overall solution.

4.1.1 HITL demonstration

CORE's AI solution is designed to cater to the diverse needs and responsibilities of the various user roles, each contributing uniquely to the operational efficiency and success of the system. In this section, we delve into the HITL (Human-in-the-Loop) interactions of three distinct user levels, which serve as the baseline and will be further tailored and adjusted to align with the unique requirements of each specific use case:

- 1. Operator Level: This level encompasses operators, supervisors, and technicians. Operators primarily rely on real-time data feedback such as graphs and warnings, enabling them to make immediate adjustments to their work to maintain process stability and productivity.
- 2. Manager Level: Managers hold the authority to trigger substantial changes, including decisions related to machine maintenance and production rate adjustments. They play a pivotal role in strategic decision-making for process optimization.
- 3. Data Scientist Level: Data Scientists operate at a higher level, equipped with comprehensive access to historical information. They not only monitor key metrics and explanations of deployed models but also possess the authority to reinforce AI models through actions like data relabeling and retraining.

Envisioning the role of a Data Scientist and their diverse interactions, CORE has developed a demonstration to showcase one of these interactions involving data and the model. In this demonstration, the Data Scientist possesses the capability to review the metrics of the current model in production, delving into its explainability by leveraging SHAP values (values that explain the significance of each feature toward

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Human In The Loop Conc Simple app to showcase our hit lideas built with an open source diabete	ept Demo
Current Model Metrics:	
Initial Metrics:	*
Explaining Predictions:	
Explain	~
Relabel and Retrain:	
Show Labeling Instances	

Figure 14. HITL demonstration - Landing page

Moreover, users can explore new data originating from a recent 'experiment' and determine whether relabelling is necessary. After making this pivotal decision, the Data Scientist can proceed to retrain the model while tracking its metrics, employing the technique of Transfer Learning. Finally, they can choose whether to update the model or maintain its current configuration. As depicted in Figure 15, it is possible to select "Show Labelling Instances" to see incoming data and choose if it is necessary a re-labelling procedure.



Figure 15. Labelling Function

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4.2 Mapping of the s-x-AIPI HITL Requirements

4.2.1 Asphalt

4.2.1.1 Description of user roles

In the case of asphalt use case, the Human-in-the-loop is envisaged for the following roles (Table 6):

- Plant Operator_(AS-USR1)
- Maintenance Technician (AS-USR2)
- Plant Supervisor_(AS-USR3)
- **Operators and laboratory responsible, QC engineers**(AS-USR4)
- Data Scientist_(AS-USR5)

 Table 6. Asphalt User Roles

User role	Role ID	Description and tasks
Plant Operator	AS-USR1	The plant operator is responsible for overseeing and operating the machinery in the plant. Their primary role is to ensure workplace safety and contribute to the quality control of the final product. This involves closely monitoring the manufacturing process and taking measures to maintain safety and product quality at all times. They will interact with all the self-X solutions to be developed.
Maintenance Technician	AS-USR2	They play a crucial role in maintaining and repairing the various machines used in the asphalt manufacturing process. Their responsibility is to ensure that all industrial equipment operates optimally and safely. This includes conducting regular inspections, performing necessary repairs, and verifying the proper functioning of the machinery. They will interact mainly with the self-X solution "Plant elements diagnosis".
Plant Supervisor	AS-USR3	The plant supervisor shares similar responsibilities with the previous role in terms of machinery maintenance and safety. However, the main difference is that the plant supervisor has a higher level of authority and decision-making responsibility. Their role involves overall process supervision and resource management to ensure efficient and safe plant operation. They will interact with all the self-X solutions to be developed.
Operators and laboratory responsible, QC engineers	AS-USR4	Person in charge of supervising the performance of the analyses and transferring the specifications of the mixtures to the plant supervisor. He will be the main user of the self-X solution "Quality traceability at lab level".



Data Scientist AS-USR5	The role of a data scientist is to turn data into actionable insights to help an organization make informed decisions and solve complex problems. They will be in charge of reviewing the performance of the AI pipeline, in order to fine- tune or retrain the existing AI models when necessary. Additionally this role must be able to manage the software used in the asphalt plant such as SCADA, databases, and device communication. The Data Scientist is a mandatory profile for various project solutions. Among their competencies, we can find complete database management, reading, visualization, exploration, and transformation of data; statistical and mathematical understanding for designing machine learning models, the use and creation of artificial intelligences; automation algorithms, and more.
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Therefore, HITL are all those operators, supervisors, or anyone involved in the production process who can and have the capabilities to interact with the planned AI tool, whether it be actively or passively. Besides, the people in charge of maintaining the developed self-X applications (dashboards, labelling apps, SCADA, etc..) must also be considered. It actively interacts with the solution by inputting new data, providing feedback, and/or validating the information provided by the self-X solutions. HITL individuals passively (and actively depending on the role) engage with the self-X solutions to observe trends and acquire relevant information from historical data.

4.2.1.2 Mapping of user roles to user scenarios

Table 7. Asphalt	User Stories	associated with	the	User Roles ⁴	
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Role ID	Associated user stories
AS-USR1	AS-US1.1, AS-US1.2, AS-US1.3
	AS-US2.1, AS-US2.2
	AS-US3.1
	AS-US4.1
AS-USR2	AS-US2.2
AS-USR3	AS-US1.1, AS-US1.2, AS-US1.3
	AS-US2.1, AS-US2.2, AS-US2.3
	AS-US3.1
	AS-US4.1
AS-USR4	AS-US4.2
AS-USR5	AS-US1.4
	AS-US3.2

⁴ Asphalt Use Case User Stories can be found in more detail in deliverable D2.1 "Scenarios and Requirements for Self-X AI adoption in Process Industry" section 3.1.

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	AS-US4.3, AS-US4.4
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4.2.1.3 HITL/AM involvement scenarios

The HITL will get involved in the following scenarios (Table 8) and data management phases:

- DATA INGESTION → In this stage, the only HITL involved is the data scientist. They are responsible for collecting and gathering raw data with the aim of using it later for data analysis, reading, visualization, and modelling. This data is collected in its raw form and stored in the database. Here the Data Scientist need to know when the data reception rate changes.
- DATA TRANSFORMATION → In this second stage, once again, the data scientist is the only HITL involved. They oversee the process of modifying and restructuring the collected data to make it more suitable for analysis, modelling, and presentation. Actions performed in this stage include data cleaning, normalization, aggregation, and visualization, as well as studying different variables and format changes. Here the Data Scientist need to know when the range of the variables of interest is outside the normal nominal variables.
- DATA EXPLORATION → This stage is responsible for acquiring and understanding the information contained in the data set. This process involves data visualization, review, and analysis to extract knowledge, identify patterns, trends, and relationships, and make decisions based on available information. All HITL individuals (plant operator, maintenance technician, plant supervisor, and data scientist) are involved in this stage, since all the users are able to interact with the data visualization screens (web dashboards and SCADA screens). A clear need is identified by the availability of data visualization graphs for all the users involved.
- MODEL TRAINING → The stage of AI model training involves only the data scientist. They are responsible for supervising all created algorithms and their testing, adjusting various parameters in our solution to make predictions and ensure the efficient operation of different processes and aid in the detection of future failures or anomalies. In this case we can find two possible situations depending on the solution developed: (1) Data Scientist need to have access to the results of retraining AI models (2) No human interfaces are needed since the Data Scientist interacts directly with the AI models through its code.
- REAL-WORLD USAGE → In this final stage, all HITL individuals are involved in the self-X solutions, but each performs a different function. (1) The plant operator only has read and data visualization permissions. They can also receive alerts for malfunctions and failures but cannot make decisions regarding them. (2) The maintenance technician and the plant supervisor can make decisions such as changing or cleaning a bearing based on a sensor alert. Additionally, they could label the different variables involved or anomalous detected in the process. (3) Finally, the data scientist also has decision-making power. In their case, they can take actions to adjust the model, add or modify parameters, and relabel data. Data Scientist need to know when the model accuracy changes. Plant supervisor must be able to obtain predictions related to laying temperature and mechanical/volumetric properties.

If the analysis is carried out at the user profile level the following scenarios that do not involve interactions with the Autonomic Manager, will be defined:

Scenario ID	AS-HITLSC-1.1
Short description	Graph visualization
Detailed description of interaction	The user will be able to access any of the developed dashboards and view the available graphs, being able to filter by dates.

Table 8. Asphalt HITL involvement scenarios

Interaction with AM	This user does not interact with the AM
Feedback-loop to AM	This user does not interact with the AM
Technical requirements	The user needs to have access to a computer connected to the internet. The way to access the dashboards will be through a web browser

Scenario ID	AS-HITLSC-1.2
Short description	View and label unsupervised detected anomalies in the manufacturing process
Detailed description of interaction	The user will be able to access a web application developed ad-hoc to label unusual situations detected in an unsupervised way. He/she will be able to indicate whether it is really an anomaly, as well as make any comments he/she consider appropriate.
Interaction with AM	This user does not interact with the AM
Feedback-loop to AM	This user does not interact with the AM
Technical requirements	The user needs to have access to a computer connected to the internet. The way to access the apps will be through a web browser

Scenario ID	AS-HITLSC-1.3
Short description	Obtain laying temperature or volumetric/mechanical properties predictions
Detailed description of interaction	The user will be able to access a web application through which he/she will obtain in advance (1) the laying temperature at which the asphalt mix will arrive at job site and/or (2) the mechanical/volumetric properties of the asphalt mix
Interaction with AM	This user does not interact with the AM
Feedback-loop to AM	This user does not interact with the AM
Technical requirements	The user needs to have access to a computer connected to the internet. The way to access the apps will be through a web browser

Scenario ID	AS-HITLSC-2.1
Short description	SCADA interaction
Detailed description of interaction	The user will be able to access any of the developed dashboards and view the available graphs, being able to filter by dates.

Interaction with AM	This user does not interact with the AM
Feedback-loop to AM	This user does not interact with the AM
Technical requirements	The user needs to have access to a computer connected to the internet. The way to access the dashboards will be through a SCADA system.

Scenario ID	AS-HITLSC-3.1
Short description	Graph visualization
Detailed description of interaction	The user will be able to access any of the developed dashboards and view the available graphs, being able to filter by dates.
	The user will be able to access a web application developed ad-hoc to label unusual situations detected in an unsupervised way. He/she will be able to indicate whether or not it is really an anomaly, as well as make any comments he/she consider appropriate.
Interaction with AM	This user does not interact with the AM
Feedback-loop to AM	This user does not interact with the AM
Technical requirements	The user needs to have access to a computer connected to the internet. The way to access the dashboards will be through a web browser

Scenario ID	AS-HITLSC-3.2
Short description	SCADA interaction
Detailed description of interaction	The user will be able to access any of the developed dashboards and view the available graphs, being able to filter by dates.
	The user will be able to access a web application developed ad-hoc to label unusual situations detected in an unsupervised way. He/she will be able to decide whether or not it is really an anomaly, as well as make any comments he/she consider appropriate.
Interaction with AM	This user does not interact with the AM
Feedback-loop to AM	This user does not interact with the AM
Technical requirements	The user needs to have access to a computer connected to the internet. The way to access the dashboards will be through a SCADA system.

Scenario ID	AS-HITLSC-3.3
Short description	View and label unsupervised detected anomalies in the manufacturing process

Detailed description of interaction	The user will be able to access a web application developed ad-hoc to label unusual situations detected in an unsupervised way. He/she will be able to indicate whether or not it is really an anomaly, as well as make any comments he/she consider appropriate.
Interaction with AM	This user does not interact with the AM
Feedback-loop to AM	This user does not interact with the AM
Technical requirements	The user needs to have access to a computer connected to the internet. The way to access the apps will be through a web browser

Scenario ID	AS-HITLSC-3.4
Short description	Obtain laying temperature or volumetric/mechanical properties predictions
Detailed description of interaction	The user will be able to access a web application through which he/she will obtain in advance (1) the laying temperature at which the asphalt mix will arrive at job site and/or (2) the mechanical/volumetric properties of the asphalt mix
Interaction with AM	This user does not interact with the AM
Feedback-loop to AM	This user does not interact with the AM
Technical requirements	The user needs to have access to a computer connected to the internet. The way to access the apps will be through a web browser

Scenario ID	AS-HITLSC-4.1
Short description	Obtain volumetric/mechanical properties predictions
Detailed description of interaction	The user will be able to access a web application through which he/she will obtain in advance the mechanical/volumetric properties of the asphalt mix
Interaction with AM	This user does not interact with the AM
Feedback-loop to AM	This user does not interact with the AM
Technical requirements	The user needs to have access to a computer connected to the internet.

Scenario ID	AS-HITLSC-5.1
Short description	Graph management
Detailed description of interaction	The user will be able to access any of the developed dashboards and manage the developed graphs, being able to modify them

Interaction with AM	This user does not interact with the AM in this scenario
Feedback-loop to AM	This user does not interact with the AM in this scenario
Technical requirements	The user needs to have access to a computer connected to the internet. The way to access the dashboards will be through a web browser.

Besides, the following scenarios will involve the interaction with the Autonomic Manager:

Scenario ID	AS-HITLSC-5.2
Short description	Data Ingestion and Data Transform management
Detailed description of interaction	The user will be able to access the Docker systems that manage the ingestion and transformation of data in order to detect possible failures in computer processes and correct them.
Interaction with AM	The user (data scientist) receives an alarm generated by the AM indicating if it has detected changes in the reception rate or in the range of any of the variables
Feedback-loop to AM	Acknowledgement feedback signal
Technical requirements	The user needs to have access to a computer connected to the internet and with high calculation capabilities

Scenario ID	AS-HITLSC-5.3
Short description	AI models training management
Detailed description of interaction	The user will be able to access a web application and re-train the AI models used within the self-X solutions, both classification and/or predictive models.
Interaction with AM	The user (data scientist) receives an alarm generated by the AM indicating changes in the AI models accuracy
Feedback-loop to AM	Acknowledgement feedback signal
Technical requirements	The user needs to have access to a computer connected to the internet and with high calculation capabilities

4.2.1.4 Technical implementation details

Table 9. Technical requirements for Asphalt User Interface

Role ID	Mode of interaction
AS-USR1	This user will interact with the system in twofold: using a computer connected to the internet or through the SCADA system

AS-USR2	This user will interact with the system through the SCADA system
AS-USR3	This user will interact with the system in twofold: using a computer connected to the internet or through the SCADA system
AS-USR4	This user will interact with the system using a computer connected to the internet
AS-USR5	This user will interact with the system using a computer connected to the internet and through the SCADA system

4.2.2 Steel

4.2.2.1 Description of user roles

What user roles do I have for the human-in-the-loop

- In the context of the steel use case, various user roles engage with the human-in-the-loop (HITL) system to optimize the scrap management and the electric arc furnace operations (Table 10):
 - Scrap Yard Operator
 - Furnace Operator
 - Data Scientist
- Should we include data scientist?

Data scientists can significantly contribute to enhancing the efficiency and productivity of the overall process.

- Data scientists' rule is crucial for modelling and therefore, identifying any irregularities or anomalies in the scrap chemistry. These anomalies can prevent from mismatches in the final liquid steel composition.
- Data scientists can also develop and fine-tune predictive models. These models can
 provide insights into critical furnace parameters such as temperature, chemistry, and
 performance, allowing for proactive adjustments and process optimization.
- The analysis of historical and data in motion, will allow to identify trends and patterns can lead to process improvements and informed decision-making, ultimately optimizing resources in terms of scrap utilization and the overall efficiency electric arc furnace.
- Data scientists can aid in continuous process improvement by identifying areas for enhancement and fine-tuning existing models.
- Who is a HITL and who is not?
- Scrap Yard Operator, Furnace Operator and Data scientists are defined as HITL.

User role	Role ID	Description and tasks
Scrap Yard Operator	ST-USR1	This operator plays a crucial role in having a better control on the characterization of scraps in terms of chemical composition. Their responsibility is to ensure that the scraps' chemical makeup aligns with the desired final chemistry of the produced steel, maintaining control over residual elements like copper (Cu). Additionally, the scrap yard operator benefits from a tool that calculates the

Table 10. Steel User Roles



		optimal scrap mix based on the calculated chemistry of the scraps. This enables them to efficiently fill the furnace while minimizing costs and resource usage.
Furnace Operator	ST-USR2	The furnace operator relies on the expected information about the predictions of temperature and chemical composition at the end of the melting process. These predictions allow them to anticipate and address any anomalies that may arise during the melting process, ensuring the smooth operation of the furnace.
Data Scientist	ST-USR3	For data scientists involved in the process, simplicity and efficiency are key. They need tools that enable them to easily train predictive models. This facilitates quick model retraining when necessary, minimizing downtime and ensuring that the system remains up to date.

4.2.2.2 Mapping of user roles to user scenarios

The scrap yard operator's expertise (ST-USR1), built upon a profound understanding of the steelmaking process and extensive knowledge, guides them in selecting the recipe. To maintain control over the final chemistry of steel and the levels of residual elements, it is imperative that the scraps loaded into the furnace are meticulously characterized in terms of their chemical composition (ST-US1.1).

In the pursuit of efficiency, scrap yard operators undertake the task of calculating the optimal scrap mix. Their objective is clear: to load the furnace in a manner that minimizes overall costs while conserving valuable resources. This delicate balance ensures the operations are both cost-effective and sustainable (ST-US1.2).

In collaboration with data scientists, the scrap yard operators harness the power of data and AI-driven insights to diagnose anomalies. This dynamic module empowers the operators to delve deeper into any deviations they encounter, evaluating the significance of these anomalies. Furthermore, it offers invaluable support in updating scrap properties through AI-enhanced scrap supervision (ST-US1.4)

Furnace operators (ST-USR2) are at the forefront of ensuring the desired chemistry and temperature at the end of the furnace process. To achieve this, they need to constantly fine-tune both the static and dynamic AI furnace models, adapting them to the real-time conditions of the process. This agile approach enables them to maintain control over the chemistry and temperature of the steel throughout the melting process. By working closely with data scientists, furnace operators can anticipate and effectively address potential anomalies that may occur during the melting process.

Data scientists involve in data analysis and predictive model training related to the scrap yards and electric arc furnace.

Role ID	Associated user stories
ST-USR1	ST-US1.1, ST-US1.2, ST-US1.4
ST-USR2	ST-US1.3, ST-US1.4

Table 11. Steel User Stories associated with the User Roles⁵

⁵ Steel Use Case User Stories can be found in more detail in deliverable D2.1 "Scenarios and Requirements for Self-X AI adoption in Process Industry"

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ST-USR3 ST-US	31.1, ST-US1.3
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4.2.2.3 HITL/AM involvement scenarios

- At what stages in the process does the HITL get involved?
 - The HITL is involved from scrap yard operations, through charging and melting, to data analysis, anomaly detection, and continuous improvement. More precisely:
 - Scrap Yard Operations: HITL, such as scrap yard operators, can be involved in the well-characterized scrap in terms of chemical composition. Scrap yard operators can actively participate in deciding the optimal scrap mix for charging the furnace. They may utilize the mix optimizer to calculate the most cost-effective and resource-efficient mix of scrap materials. The mix optimisation will be based on the ML regressions carried out by the Data scientist.
 - **Furnace Operations**: During the melting process, the AI models can provide them with predictions about temperature and chemical composition at the end of the process, allowing them to anticipate any anomalies or deviations.
 - **Data Analysis and Model Training**: Data scientists, who are considered HITL, may be involved in data analysis and predictive model training. They actively work on improving AI models by analysing historical data and training machine learning models. They use the AI to detect anomalies, deviations, or unusual patterns during the overall operation, and pass through this info to the Scrap yard and furnace operators. Also, they will seek for continuous improvement. They may analyse trends and insights generated by the system to make informed decisions for optimizing the process.
- What information does each HITL role need at each stage?

• Scrap Yard Operator:

Stage: Scrap Yard Operations

Information Needs:

- Chemical composition data for incoming scrap materials.
- Suitability assessments of scrap materials for EAF.
- Recommendations for optimizing scrap selection based on cost and resource efficiency.
- Alerts and notifications regarding anomalies or deviations on the scrap chemistry

• Furnace Operator:

Stage: Furnace operation

Information Needs:

Temperature and chemistry predictions for the end of the melting process.

• Data Scientist:

Stage: Data Analysis and Model Training

Information Needs:

- Access to historical process data.
- Data preprocessing and cleaning for model training.
- Model performance metrics and results for continuous improvement.

- Feedback on model accuracy and areas for enhancement.
- What input comes from the HITL?
 - Data scientist can provide feedback on the predictions or recommendations generated by AI models. This feedback helps validate the accuracy and reliability of AI-generated insights.
 - Data scientist can actively participate in data quality assurance by identifying data discrepancies, missing data, or data that require cleaning. This input helps maintain the integrity of the AI pipeline.
 - Scarp operator and EAF operator can make informed decisions and strategic choices based on AI recommendations and insights. This contributes to process optimization and resource allocation.
 - Data scientist can signal when model recalibration or retraining is necessary. This can be triggered by changes in the production environment, shifts in material properties, or evolving process conditions.

Scenario ID	ST-HITLSC-1.1
Short description	Mix scrap recipe
Detailed description of interaction	Scrap yard operators can actively participate in deciding the optimal scrap mix for charging the furnace. They utilize the scrap characterization to get the scrap types and amount of scrap loaded to the furnace and mix optimizer to calculate the most cost-effective and resource-efficient mix of scrap materials. The scrap characterization will be based on the ML regressions carried out by the Data scientist.
Interaction with AM	This user does not interact with the AM
Feedback-loop to AM	This user does not interact with the AM
Technical requirements	Computer with the internal Internet with access to the dashboard

Table 12. Steel HITL involvement scenarios

Scenario ID	ST-HITLSC-1.2
Short description	EAF adjustment
Detailed description of interaction	The Furnace Operators can monitor the current heat state of the EAF process more precisely and adjust electrical energy, natural gas, oxygen or injected lime to achieve the desired steel quality.
Interaction with AM	This user does not interact with the AM
Feedback-loop to AM	This user does not interact with the AM
Technical requirements	Computer with the internal Internet with access to the dashboard

Scenario ID	ST-HITLSC-1.3
Short description	Data Ingestion and Data Transform
Detailed description of interaction	A comprehensive set of statistical descriptions is sent to the AM to detect the invalid and incomplete data.
Interaction with AM	Data scientist receives an alarm by the AM indicating when it has detected changes in the data
Feedback-loop to AM	The HITL can provide its feedback, for example, on the acceptance of new scrap types.
Technical requirements	Computer with the Internet and connection between AI pipeline and AM

Scenario ID	ST-HITLSC-1.4
Short description	Data Exploration
Detailed description of interaction	A set data about outliers send to the AM
Interaction with AM	Data scientist receives an alarm generated by the AM indicating when it has detected anomalies
Feedback-loop to AM	The HITL will provide feedback upon request to confirm the anomaly.
Technical requirements	Computer with the Internet and connection between AI pipeline and AM

Scenario ID	ST-HITLSC-1.5
Short description	ML modelling and scrap supervision
Detailed description of interaction	The results of the ML models are transferred to the AM
Interaction with AM	Data scientist receives an alarm generated by the AM indicating when the scrap compositions change, or the accuracy of the ML model changes
Feedback-loop to AM	The HITL can provide feedback that confirms the need to train models.
Technical requirements	Computer with the Internet and connection between AI pipeline and AM

4.2.2.4 Technical implementation details

The interfaces to be implemented in the steel use case will be of web type integrated in the process data visualization system. Therefore, each agent involved as a HITL will have at its disposal the specific interfaces for interaction with the automatic manager and also the necessary information to evaluate the situation and make the appropriate decisions.

Table 1	3. Technica	l requiremen	ts for Stee	l User	Interface
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Role ID	Mode of interaction
ST-USR1	Internal Wi-Fi net to connect to the scrap supervising system and mix optimizer tool, by means of a shared computer among Operators and private computer of Managers.
ST-USR2	Internal Wi-Fi net to connect to the EAF predicting tool, by means of a shared computer among Operators and private computer of Managers

4.2.3 Pharma

In the pharmaceutical use case, an electrochemical reaction occurs within a quartz glass cell, facilitated by three real-time analytical tools. The OCT offers microscopic images of the electrode's surface, the IR provides insight into the chemical composition of the solution through a spectrum, and the power supply maintains constant voltage and current settings for continuous monitoring. The primary objective is to optimize this electrochemical reaction with the self-X solution by reducing overall power consumption, minimizing irreversible electrode damage due to corrosion, and maximizing API production throughput in a shorter time frame.

4.2.3.1 Description of user roles

What user roles do I have for the human-in-the-loop?

In the pharma use case two different HITL cooperate with the self-X solution as shown in Figure 16. The HITL "Process operator" interacts in real-time with the AM to setup and perform the experiment. The HITL "Data scientist" does not directly interacting with the overall setup, but is involved via the data acquisition, the developed models, and other feedback from the self-X solution.



Figure 16. Schematic HITL workflow in Pharma use case

- In the context of the pharma use case, two user roles engage with the human-in-the-loop (HITL) system to optimize the yield of the electrochemical reaction process:
 - Process operator: The operator relies on real-time information about the status of the electrode, positioning and functionality of sensors, as well as on the prediction of the conversion rate trajectory. The status information allows the operator to readjust sensors or intervene in case of sensor malfunction. Based on the predictions, the operator can anticipate the end of the process and receives information about a potential discrepancy between prediction and the recorded process data.
 - **Data scientist:** The involved data scientist wants to obtain clean data from the sensors. Based on the data and model development the conversion rate trajectory is predicted. Further the model predictions are passed to the control strategy in the next self-X solution.
- Should we include data scientist?
 - Data scientists can significantly contribute to increasing the efficiency and productivity of the entire process.
 - Data scientists' rule is crucial for collecting and preparing the data, which is the foundation of the modelling.
 - Data scientist develop models to forecast the conversion rate trajectory.
 - Analysis of historical and moving data allows the data scientist to identify trends and patterns that can lead to process improvements and optimization of resources in the electrochemical process.
- Who is a HITL and who is not?
 - Only the process operator and data scientist are identified as HITL. 0

able 14. Pharma User Roles		
User role	Role ID	Description and tasks
Process operator	PH-USR1	The process operator sets up the process equipment required for the electrochemical reaction. The process operator starts and monitors the process.
		case of malfunction.
Data scientist	PH-USR2	The data scientist collects and prepares the sensor data.
		The data scientist develops and trains the forecast model.

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Mapping of user roles to user scenarios 4.2.3.2

The tasks of a process operator include real-time monitoring of electrode condition for corrosion and fouling via OCT, managing OCT probe positioning as suggested by the autonomous manager, tracking the predicted conversion rate trajectory, addressing sensor malfunctions, monitoring the process surrogate model and responding to unexpected scenarios.

The role of a data scientist involves obtaining and processing relevant data, such as periodic OCT images of electrodes and corrosion/fouling percentages, to develop process models and predictive conversion rate

trajectories. Data scientists also ensure the cleanliness and reliability of sensor data for modeling purposes and use their models' predictions to inform data-driven control strategies in self-X solutions.

Table 15. Pharma	a User Storie	s associated with	the User Roles ⁶
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Role ID	Associated user stories
PH-USR1	PH-US1.1, PH-US1.2 PH-US2.1, PH-US2.2, PH-US2.3, PH-US2.4 PH-US3.1
PH-USR2	PH-US1.3, PH-US1.4 PH-US2.5, PH-US2.6

4.2.3.3 HITL/AM involvement scenarios

- At what stages in the process does the HITL get involved?
 - The HITL is involved from process setup, through starting and monitoring the process, to data collection, model development and continuous model improvement. More precisely:
 - **Process operator:** setting up the process, i.e., filling the liquid into the reactor, starting the process, checking the process setup based on the given information, monitoring the process and intervening in a possible situation.
 - **Data scientist:** development of data collection, data pipeline as well as model training.
- What information does each HITL role need at each stage?

• **Process operator:**

- Stage: Process start
 - Information needs: status of OCT positioning, alerts and notifications about further reactor setup.
- Stage: During process
 - Information needs: predicted trajectory, expected end time and conversion rate of the process, as well as potential failure alerts.
- Data scientist:
 - Stage: Data analysis and Model development
 - Access to historical process data.
 - Data pre-processing and cleaning for model training.
 - Model performance metrics and results for continuous improvement.
 - Feedback on model accuracy and areas for enhancement.
- What input comes from the HITL?

⁶ Pharma Use Case User Stories can be found in more detail in deliverable D2.1 "Scenarios and Requirements for Self-X AI adoption in Process Industry"

- Process operator can readjust OCT, change the current as suggested by the control strategy in scenarios where the change was deemed too large to be undertaken automatically.
- The data scientist retrains the model when necessary, i.e., when a significant difference occurs between the projected and actual process trajectories.

Table 16. Pharma HITL involvement scenarios

Scenario ID	PH-HITLSC-1.1
Short description	Adjustment of OCT probe position
Detailed description of interaction	The HITL (operator) has adjusted the position of the OCT probe incorrectly. The AM has a historic record of successful positions and advices the HITL.
Interaction with AM	The operator receives a message on the screen.
Feedback-loop to AM	The system automatically evaluates the new position of the probe and reports it to the AM.
Technical requirements	The lab system where the script runs needs to be connected to the system where the AM runs. The operator needs to have access to the screen and OCT probe.

Scenario ID	PH-HITLSC-1.2
Short description	Change of current in extreme situations
Detailed description of interaction	The model control suggests an extreme change of the current value, which is deemed to be unsafe if undertaken automatically. The HITL reacts and performs the changes on the power supply device.
Interaction with AM	The operator receives a message on the screen.
Feedback-loop to AM	The system automatically evaluates the new current value.
Technical requirements	The lab system where the script runs needs to be connected to the system where the AM runs. The operator needs to have access to the screen and the power supply device.

Scenario ID	PH-HITLSC-2.1
Short description	Retraining or change of forecasting model
Detailed description of interaction	The HITL (data scientist) retrains or changes the forecasting model. The AM has a historic record of the models used.

Interaction with AM	The data scientist receives a message from the AM.	
Feedback-loop to AM	The system automatically evaluates the new forecasting trajectory and reports it to the AM.	
Technical requirements	The lab system where the script runs needs to be connected to the system where the AM runs. The data scientist needs a connection to the AM.	

4.2.3.4 Technical implementation details

- What technical possibilities exist in the plant?
 - In the pharma use case the operator will interact with the system via a laptop placed next to the experimental setup in the laborator.

Table 17. Technical requirements for Pharma User Interface

Role ID	Mode of interaction
PH-USR1	The operator will interact with the system via a laptop that is placed next to the experimental setup. This laptop is connected to all sensors and to the public internet for communication with the AM.
PH-USR2	The data scientist works on a separate computer for modell developing. The data scientist transfers updated models to the operator laptop offline.

4.2.4 Aluminum

4.2.4.1 Description of user roles

There are several HITL in the aluminium use-case. At the industrial plant level, the potential users of the Intelligent Decision Support System (IDSS) include the "scrap yard" operator, two "furnace" operators, and the "alloy" operator. Figure 17 summarizes the plant operators considered in the aluminium use-case and the corresponding part of the aluminium making-process in which they participate.



Figure 17. User roles considered at the plant level and their corresponding participation in the process

In different levels of management, the **production manager**, the **R&D manager**, and the General Manager, are also considered users of the IDSS. The specific roles and the task of each user is described in more detail in Table 18.

- Should we include data scientist? IDALSA counts with an R&D department for the aluminium process, but data scientists *per se* are not considered users of the tool as the Department has a strong industrial focus on the aluminium-making process.
- Who is a HITL and who is not? In the Aluminium use-case, HITL are those experts and operators that can use and interact with the envisaged IDSS tool either actively or passively. HITL actively interact with the solution by introducing new data, providing feedback and/or validating information provided by the IDSS. On the other hand, HITL passively interact with the IDSS by using the app to learn about trends and/or relevant information from the process and historical data, but do not provide direct feedback to it.

User role	Role ID	Description and tasks
" Scrap Yard" operator	AL-USR1	The "Scrap Yard" operator is responsible for sorting, inspecting, and categorizing incoming scraps based on their chemical composition and characteristics. These operators are also responsible for selecting the aluminium recipes i.e., combination of scraps for the aluminium- making process.
"Furnace" operator	AL-USR2	The "Furnace" operators are responsible for introducing the materials in the furnace, providing the final, real-world recipe of scraps, as well as controlling the overall melting process i.e., maintaining operative conditions in the furnace and ensuring efficiency and safety of the process.
"Alloy" operator	AL-USR3	The "Alloy" operator is responsible for the alloying adjustment after primary melting required to ensure that the aluminium mixture meets the expected performance and quality requirements (norms). These operators provide the final, real-world "alloys recipe".
Production Manager	AL-USR4	The Production Manager oversees the overall aluminium-making process and determines the corrective actions needed to adjust the volume of production according to the composition of the mixture.
R&D Manager	AL-USR5	The R&D Manager defines, implements, and monitors new strategies to improve the current process, establishing standardized operative procedures to achieve the optimization of resources and increase productivity.
General Manager	AL-USR6	The General Manager oversees all different departments to ensure that all day-to-day

Table 18. Aluminium User Roles



	operations are successfully accomplished, while maintaining business policies and meeting business strategic goals.
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4.2.4.2 Mapping of user roles to user scenarios

As described in section 4.2.4.1, the aluminium recipes are selected by the "scrap yard" operator (AL-USR1) based on its knowledge of the process and information regarding the availability of materials, their prices, and the expected chemical composition of mixtures. The "scrap yard" operator provides the initial recipe for the aluminium-making process to the "furnace" operators, which might adapt the recipes as needed in the real-world. For this reason, "scrap yard" operators are especially interested in obtaining estimations of the chemical composition of recipes given a combination of materials (AL-US1.1), as well as suggestions for new recipes and their expected characteristics based on the current status of the plant and the desired product (AL-US1.2). In addition, information about the behaviour of materials (AL-US1.3.), as well as trends and relevant parameters-related information will also be provided by the IDSS to enhance the knowledge of the operator for their decision-making i.e., information from the Data Exploration component.

The "furnace" operators (AL-USR2) and the "alloy" operator (AL-USR3) are specially interested in the estimation of the final chemical composition of a given recipe (AL-US1.1), as they might need to adapt the initial recipe according to the real-world outcome. The behaviour of scraps during melting might vary from the initial expectations due to unrepresentative estimations of the chemical composition of scraps during their collection and storage, or due to other operational factors. Hence, the IDSS can be advantageous for operational estimations during the aluminium-making process.

On the other hand, the Production Manager (AL-USR4) might be interested in evaluating different recipes in a multi-criteria basis to supervise and contribute with their expertise and knowledge in the decision-making of materials (AL-US1.2). In addition, information about deviations in scraps (AL-US1.3) can contribute to a more adaptive production, and even allow to translate potential issues to other departments e.g., to notify that certain materials show consistent deviations over time to adjust production accordingly.

The R&D Group (AL-USR5) is interested in gaining knowledge of the process to better comprehend and improve the production and its processes. Hence, learning about deviations in the process (AL-US1.3) is especially useful for this Group, as well as expanding their knowledge on trends and relevant information that will be given by the Data Exploration component. Besides that, the estimation of the chemical composition of a given recipe (AL-USR1) can also be of special interest for R&D with the aim of being able to evaluate different paths of production to optimize the process.

Finally, the General Manager (AL-USR6) is responsible for supervising all the processes for the aluminiummaking production and, thus, is especially interested in the short- and medium- term planning of recipes (AL-US1.4) to estimate production in larger time windows. Apart from that, the Manager will be also able to access all the information of the components of the AI Data Pipeline at all times.

Role ID	Associated user stories
AL-USR1	AL-US1.1, AL-US1.2, AL-US1.3
AL-USR2	AL-US1.1
AL-USR3	AL-US1.1

 Table 19. Aluminium User Stories associated with the User Roles⁷

⁷ Aluminium Use Case User Stories can be found in more detail in deliverable D2.1 "Scenarios and Requirements for Self-X AI adoption in Process Industry"

AL-USR4	AL-US1.2, AL-US1.3
AL-USR5	AL-US1.1, AL-US1.3
AL-USR6	AL-US1.4

4.2.4.3 HITL/AM involvement scenarios

As depicted in Figure 17, the "scrap yard" operator is responsible for selecting the aluminium recipe before its production, while the "furnace" operators and "alloying" operator contribute to the aluminium-making process adapting the original recipe to the real-world scenario regarding the scraps and the alloys, respectively. Other HITL, such as the Managers, might interact at different stages of the process in a more transversal basis, as described in Table 18. Considering the AI Data Pipeline, Figure 18 shows the envisaged interaction of the different users with respect to the components of the architecture.



Figure 18. User roles and their interaction with the AI Data Pipeline.

The furnace operators, or, in its place, the Production Manager, update and validate the information of each heat in the database when a process is finished, including the quantity and type of scraps and alloys used, as well as the final chemical composition obtained from the mixture, among others. In case that newly introduced data is incomplete or out-of-the-expected-distribution, the HITL will be invoked to either discard the data sample, provide more information about it, or select an action to be executed by the app e.g., complete the empty fields exploiting data statistics.

Table 20	. Aluminium	HITL	involvement	scenarios
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Scenario ID	AL-HITLSC-1.1
Short description	Data Ingestion and Transformation Management: Introduction and validation of new data
Detailed description of interaction	The HITL introduces and validates new data from the aluminium-making process that will be further integrated in the database for future analysis and usage.
Interaction with AM	The operator introduces new data i.e., batch reference, scraps and alloys, chemical composition, etc. Based on the metadata analysis, the IDSS will

	raise a warning message if the data is not valid according to pre-defined rules e.g., number of missing parameters allowed, or out-of-the-distribution samples.
Feedback-loop to AM	The HITL will be able to provide feedback, when requested, in order to confirm the deletion of a data sample, complete missing fields, or continue with auto-filling options based on data statistics, when possible, at the pipeline level.
Technical requirements	Connection between the pipeline components (Data Ingestion, Data Transformation, and Database -optional-), and the AM.

Besides that, users will be able to exploit data statistics and analysis by means of the Data Exploration component in a passive way. For instance, the "quality" operator could be interested in having a list of materials in the plant with similar chemical composition for the recipes (clustering of materials, correlations), while the R&D Group can use the information provided by the component for a detailed analysis of the different factors that might affect the process. The R&D Group will also have access to information about the Model Training component to get information about the models trained and their performance.

Scenario ID	AL-HITLSC-1.2
Short description	Exploration of data
Detailed description of interaction	The HITL can delve into data with a set of pre-defined options. The HITL can select a parameter to learn about its statistics and/or a set of pre-defined analyses that can be performed on data e.g., regression between two parameters. The results will be shown in the UI.
Interaction with AM	Upon use, metadata will be uploaded to the AM and pre-defined rules will trigger warning notifications at the pipeline level, if activated.
Feedback-loop to AM	None
Technical requirements	Connection between the pipeline components (Database and Data Exploration), and the AM.

Focusing again on the aluminium-making process itself, there will be two main actions that will be performed by the IDSS: i) the estimation of the final chemical composition of a recipe, and ii) the suggestion of new recipes based on the current status of the factory. For the first action, the user will obtain the expected chemical composition of a recipe given the combination of materials to be considered. For the second action, the user will obtain a number of suggested recipes based on the current status of the factory given the desired product. In the latter case, users will be able to provide feedback on the proposed recipes to adapt the system in future fine-tuning phases of development.

Scenario ID	AL-HITLSC-1.3
Short description	Estimation of the final chemical composition of recipes
Detailed description of interaction	The HITL can request the expected final chemical composition of a desired recipe to ensure it satisfies the norm before production. The operator introduces the set of materials to be evaluated from the available materials

	at the plant and the AI model will provide a report of the characteristics of the expected mixture.
Interaction with AM	When re-training of AI model occurs, metadata is sent to the AM and, according to the pre-defined rules and analysis, a trigger is activated to update the model or discard the newly trained, if needed.
Feedback-loop to AM	If the recipe is produced, the real-world information will be provided by the HITL to update the IDSS in the future.
Technical requirements	Connection between the pipeline components (Database and AI model), and the AM.

Scenario ID	AL-HITLSC-1.4
Short description	Aluminium recipe suggestions
Detailed description of interaction	The HITL can request suggestions about aluminium recipes based on the current status of the plant given a desired product and its quantity (order).
Interaction with AM	The HITL introduces the product and the quantity to be produced and the AM returns a set of suggested recipes based on the current status of the factory.
Feedback-loop to AM	The HITL can provide its feedback on the suggestions e.g., acceptability, as well as the real recipe used for production, in case it differs.
Technical requirements	Connection between the pipeline components (Database, AI model), and the AM.

Finally, there will be an option for the Real-World Usage of the IDSS to access the Digital Product Passport (DPP) of products based on their heat reference. This option will allow users access standardised information of products based on the AAS and it can be considered a passive interaction with the application (no feedback expected).

Scenario ID	AL-HITLSC-1.5
Short description	Aluminium Digital Product Passport
Detailed description of interaction	The HITL can request access to the Aluminium DPP based on the AAS.
Interaction with AM	The HITL introduces the heat reference of the product and the DPP will be facilitated to the user via the UI.
Feedback-loop to AM	None
Technical requirements	Connection between the pipeline components (Database, scripts), and the AM.

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4.2.4.4 Technical implementation details

Role ID	Mode of interaction
PC The mode of interaction is equal for all Role IDs.	A (public) web-interface that can be accessed by any PC in the plant with Internet connection will be developed. Access will be controlled with specific user rights according to the user role. The AI solutions will be stored in a private server, and communication will done following client-server protocols.

 Table 21. Technical requirements for Aluminium User Interface

4.3 HITL Commonalities for common UI architecture

The UI architecture can differ due to the type of interaction. A typical distinction can be made between interaction on the level of the production plant or the process control system and interaction on the level of databases, process models, model or AI pipelines and the AM. For the latter the common UI architecture in the present use cases and moreover is the web interface. The web interface is typically accessed via a computer connected to the internet or intranet (see Figure 19). The shown structure is common for all use cases and typically addresses the HITL user role "Data Scientist". A big advantage of this UI architecture is remote access. For the interaction with the production plant or its process control system the common structure is different. The used UI architecture is typically of web type, but often further specialized, e.g., the SCADA system in the Asphalt use case. The addressed HITL is directly operating in the production plant or laboratory with user role "Operator" or "Technician".



Figure 19. Common interaction with AM and AI pipeline

However, in the field of human-in-the-loop (HITL) systems, the design and architecture of user interfaces (UI) have commonalities that go beyond the application domains. A fundamental principle is a consistent focus on the user experience, i.e., user interfaces must be intuitive, efficient, and responsive to user needs. In addition, real-time data processing and analysis are commonplace in HITL systems, necessitating UI features such as real-time data visualizations to present information in easy-to-understand formats. Collaborative teamwork and decision-making are inherent in HITL, driving UI architectures to facilitate communication and collaboration among team members through tools that suit for teamwork in the environment. These can be, for instance, views visible to multiple users and roles, chat capabilities, and collaborative tools. It is equally important to build robust error-handling mechanisms into the UI to guide the user to provide suitable input and to enable the software to recover from unexpected situations. Additionally, the user should receive clear information about any process-related anomalies to enable appropriate, timely reactions.

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To ensure that the described principles are incorporated in the end product, a collaborative approach over all HITL user roles is necessary. Pleasant and goal-oriented user interfaces, informative visualizations and clear working and feedback instructions can be achieved if, e.g., the HITL "operator" is incorporated already in the development phase. Communication channels between all HITL's are integrated in each computer.

Conclusions

The Deliverable 4.1 "Autonomic Managers for Data in Motion and Humans support in AI solutions" represents the initial version of the development of the s-X-AIPI Autonomic Managers at M18.

It identifies the adopted measures to support the "Design about the Autonomic managers in charge of coordinate different self X AI components of use cases to integrate appropriately the flow of "New RAW data" from industrial data sources and the human support according to self-X abilities available".

The design principles have been fixed and identified. Therefore, the development of a domain-agnostic infrastructure at the basis of the customized Autonomic Managers' development has been demonstrated.

The upcoming project activities will be devoted to providing tailored rule-based engines to the Autonomic Managers, which will be developed based on Use Cases' needs, the adopted AI components and related available self-X abilities.

The development and integration with the Autonomic Managers of specific components for human-in-theloop feedback will be also ensured.

Lastly, a validated set of Key Performance Indicators relevant to ensure Autonomic Managers monitoring and demonstration phases will be identified.