Data-driven method based on a process mining approach for Automated Digital Twin generation, operations, and maintenance in circular value chains

Deliverable

D1.1 Consolidated specifications

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1.0	29/05/2023	TTS,TUE,POLIMI	Final revision

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2 Definitions and acronyms

CA	Consortium Agreement
EC	European Commission
EU	European Union
GA	Grant Agreement
PC	Project Coordinator
TC	Technical Coordinator
WP	Work Package
CSD	Central Sterilization Department
SDU	Service Department User
ITS	Information Tracking System
CDC	Centers for Disease Control
CPM	Centre's procedures manual
OWD	Organization of work document
MD	Medical device
ETO	ethylene oxide
IAP	inspection, assembly and packing
WHO	World Health Organization
ED	Emergency Department
ICU	Intensive Care Unit
OR	Operating Room
WIP	Work in process

Disclaimer

3 Executive Summary

AUTO-TWIN addresses the technological shortcoming and economic liability of the current system-engineering model by 1) introducing a breakthrough method for automated process-aware discovery towards autonomous digital twin generation, to support trustworthy business processes in circular economies; 2) adopting an (International Data Space) IDS-based common data space, to promote and facilitate the secure and seamless exchange of manufacturing/product/business data within value-networks in a circular-economy ecosystem; 3) integrating novel hardware technologies into the digital thread, to create smart Green Gateways, empowering companies to perform data and digital twin enabled green decisions, and to unleash their full potential for actual zero-waste Circular Economy and reduced dependency from raw materials.

The project is articulated in 3 phases as indicated in Figure 1, at the moment of release of this deliverable, the project is currently in phase one, and D1.1 represent the first result for the use-case definition phase.

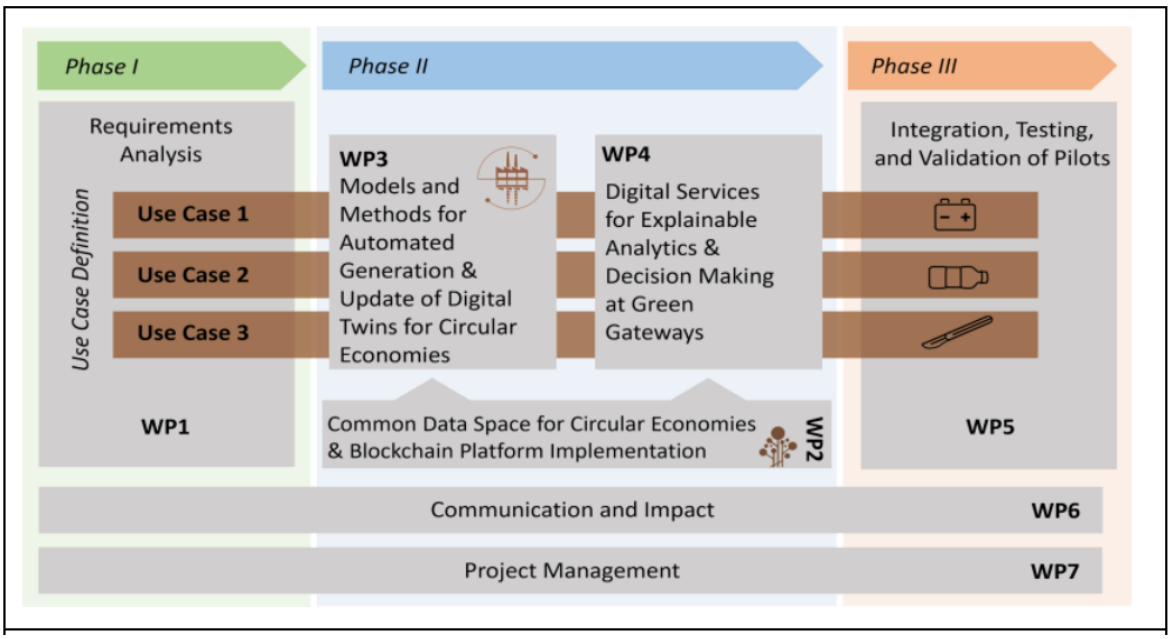

Figure 1 AUTO-TWIN project phases

This deliverable analyses three different industrial pilots:

- CROMA, a surgical instrument supplying and management company
- GR3N, a company which developed a process for breaking down any type of PET and polyester into its two core components which can be then re-assembled to obtain virgin-like plastics enabling endless recycling loops.
- Libattion, a company which manufactures battery systems reusing cells coming from used batteries.

In this document, the value chain of the end users is analysed to contextualize the actors in the market and to put in evidence the circular aspects, with a particular emphasis on the data that are already traced by existing systems, their availability, and possible additional information that could be tracked in the future adding additional sensors or data collection systems.

Each process of the industrial pilots is then inspected, detailing the process steps and the flows between them. Also in the process description, particular attention has been paid to the data that are already tracked or could be of particular interest for the next work packages.

An iterative work with the end-users has been conducted to understand their current needs, derive potential developments and to match each development with the project objectives indicated in Figure 2, to ensure a solid link between the technical requirements and the global scope of the project.

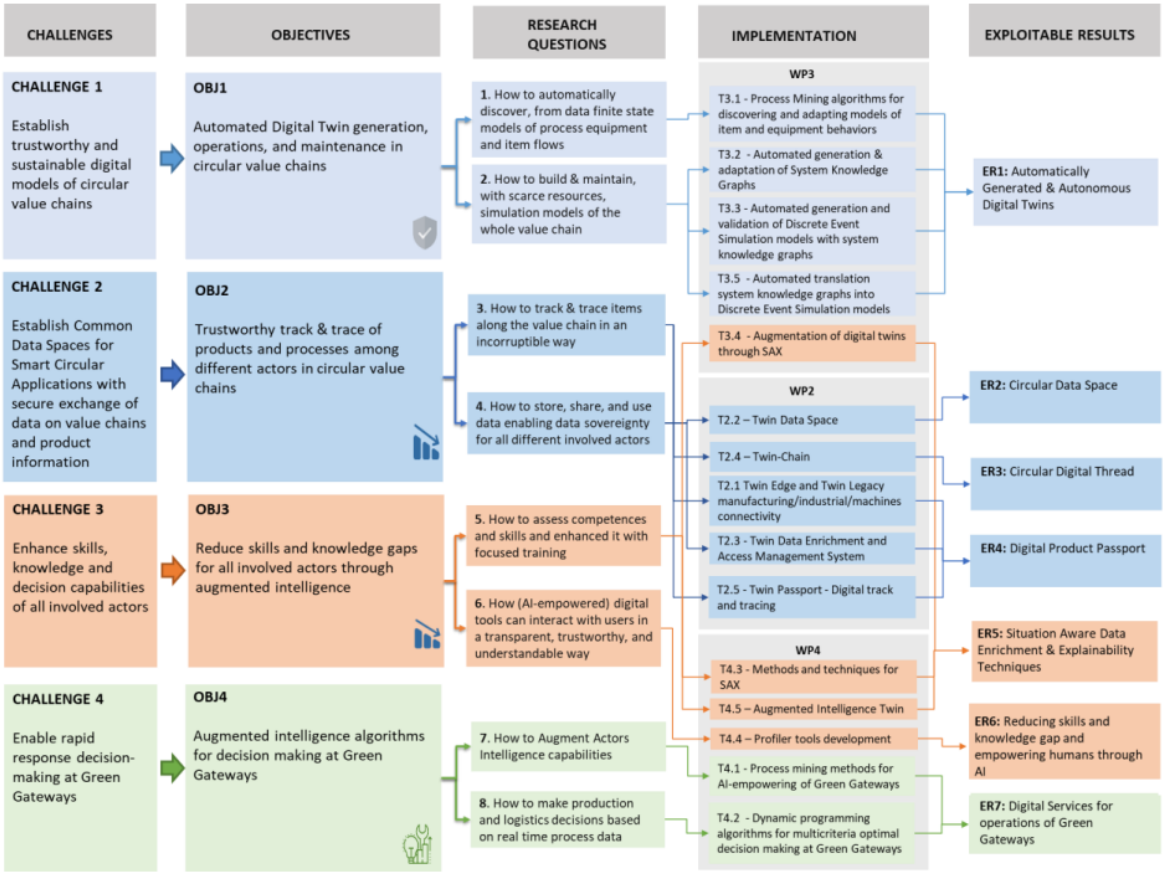

Figure 2 AUTO-TWIN methodology, from challenges to exploitable results

Finally, for each use case the decisions which can be taken by the user to influence the process have been mapped, to state which actors can take a decision, the moment in time and the steps of the process which are influenced by that decision. The objective is ensuring that the results of the project will provide value to the right people, at the right time, and above all, will determine real impacts improving industrial processes or parts of them.

To measure the effect of the aforementioned decisions and the application of potential developments, the KPIs that will be used to evaluate improvements in the process have been defined. The identified measures represent the most reasonable set according to the outcomes of the elicitation phase, and they will represent a solid ground to carry on both the development and the validation phase. Nevertheless, they are not meant to be exhaustive since the use case processes will evolve along the next project months and the potential developments will be adapted to comply as much as possible with the changes.

In the Croma use case the process is already well established, and lot of historical data are available, while the other two use-cases are either in commissioning stage (Gr3n) or in the state of switching from a prototypal phase to an industrial pilot line (Libattion), so data availability will be re-checked in the upcoming months. For this reason, it is expected that a later revision of baseline values for the quantitative impact indicators will be required.

The expected results collected during the analysis work and formalized in this document will serve as the basis to elaborate the technical requirements of the single components of the overall architecture reported in Deliverable D1,2.

4 Introduction

The deliverable is the first result of WP1," Requirements analysis and guidelines for industrial uptake" and contains the use case analysis results and collected requirements from the end users in the AUTO-TWIN project.

4.1 Description of the document

This document represents the results of the work carried in the first 6 months of WP1,

aiming to analyse the use-cases to understand their needs and expectations in order to set the ground for WP3, WP4 and WP5.

Sections 5,6 and 7 contain the analysis of the three use cases: Croma, Gr3n and Libattion.

Paragraph 5.1 contains the nomenclature and glossary for the use case, paragraph 5.2 describes the value chain for Croma use-case describing the context and actors, paragraph 5.4 describe the flows , meaning the exchanges of entities which happen between the actors, in paragraph 5.5, for each entity a table of data collected to feed the automatic digital twin generation process along which their format and availability is provided.

Paragraph 5.6 contains the description of Croma process, providing a schema of process inputs, internal steps and outputs, paragraph 5.7 lists the interna flows of the process and paragraph 5.8 describes more in detail each flow and data that could be collected, paragraph 5.9 describes more in detail each step of the process, along with collected data, required resources and control parameters.

Paragraph 5.10 contains the description of objectives and impacts for the end user in the AUTO-TWIN project which are the result of the work conducted in the first part of WP1 and will be used to derive technical requirements for the components of the architecture.

Paragraph 5.11 describes the decisions which can be taken by the end-user to influence the process, providing a set of critical decision processes which could be supported by the AUTO-TWIN project.

Paragraph 5.12 contains KPIs which can be used to measure the performances of the process and to provide a measurable impact of the project results.

Paragraph 5.13 contains some notes on the as-is state of the use case to highlight the current status of the process since the maturity level between cases is different.

The structure of chapter 5 is replicated for Gr3n use case in chapter 6 and for Libattion use case in chapter 7.

Chapter 8 contains a table which summarizes key features representing the flows and the processes of the three use-cases.

4.2 WP and Tasks related with the deliverable

This deliverable is the output of WP1," Requirements analysis and guidelines for industrial uptake". This WP sees the cooperation of scientific, technical, and industrial partners to set the scene for the development of the AUTO-TWIN solutions. Needs and expectations are collected, and technical requirements are distilled and provided to the following WPs for the design of the overall platform. Considering the nature of the project, it is of paramount importance to offer platform usage mechanisms that can be easily adopted. Main WP objectives are: (i) to define the initial status of the industrial use case pilots including KPIs to be met in to-be state; (ii) to detail hardware and software specification for Common Data Space (WP2), automated generation of digital twins (WP3) and for the Green Gateways (WP4); (iii) to define the overall AUTO-TWIN system architecture to achieve target scenarios' objectives.

The deliverable is the result of T1.1 and T1.2.

T1.1 “Investigation of the use case and related KPIs”, aims to conduct comprehensive analysis of the pilot use cases, to examine the industrial needs and requirements for the developments to be done in the ensuing AUTO-TWIN WPs. The pilots will be described both at plant level and value chain level in terms of process inputs, outputs, characteristics, and constraints, with emphasis on sustainability indexed and analysis of imported raw/harmful critical materials. Since data availability is at the base of process mining for automatic digital twin deployment, a special focus will be given in describing data-based interactions and needs at the sensor-network layer. Once the baseline situation is examined, this task will define clear and measurable goals for each pilot use case. Such goals will be used as targets in WP5.

In T1.2 “Requirements definition”, the expectations collected in T1.1 are analysed from a technical perspective and from a skill-needed perspective, to define business and engineering requirements for automatic generation of digital twins in production systems. Detailed requirements are mapped to concisely present and correlate all the elicited needs and elements to ensure the AUTO-TWIN solution is developed according to the best-in-class research activities and to the actual necessities of manufacturing companies. Requirements are structured, analysed, refined, and validated.

4.3 Note on the evolution of potential developments and impacts

It is important underlying that the potential developments and the impacts identified at this stage of the project and reported in this document represent the best mapping between the current status of the end user processes and the technological targets of AUTO-TWIN project. Nevertheless, they are not meant to be exhaustive since the use case processes are expected to evolve along the next project months and the potential developments will be adapted to comply as much as possible with the changes. In particular, a further process of assessment of feasibility and generalization of the potential developments will follow this first analysis and will be reported in Deliverable D1.2 to clearly identify the application scenarios for the technologies developed in WP2, WP3 and WP4. Further improvements are expected in the context of WP5 during the actual adoption of the chosen solutions and their final customizations.

5 Croma use case

5.1 Nomenclature and glossary

Autoclave	An autoclave or sterilizer is a device used to sterilize equipment and supplies by subjecting them to high pressure and steam at 121ÆC or above. For the purposes of this document, the term autoclave refers to a large industrial sterilizer used in a central sterile services department. (World Health Organization, 2016)
Cart / chariot	Support for transport kits from SDU to CSD, i.e., batch of kits arriving at CSD.
Cleaning	The first step required to physically remove contamination by foreign material, e.g., dust, soil. It will also remove organic material, such as blood, secretions, excretions and microorganisms, to prepare a medical device for disinfection or sterilization. (World Health Organization, 2016)
Container	Kit type. Recipient containing a set of MDs used for a specific type of surgery. The container includes the tray with the set of medical devices, the container box and the container cover. Each element of the container kit is identified with the same code and is not interchangeable with other container kits. In addition, each container kit presents a maximum number of reconditioning cycles, mainly based on the container cover filter.
Contamination	The soiling of inanimate objects or living material with harmful, potentially infectious or unwanted matter. (World Health Organization, 2016)
Decontamination	Removes soil and pathogenic microorganisms from objects so they are safe to handle, subject to further processing, use or discard. (Centers for Disease Control, 2008)
Disinfection	A process to reduce the number of viable microorganisms to a less harmful level. This process may not inactivate bacterial spores, prions and some viruses. (World Health Organization, 2016)
Kit	Set of MDs used for a specific type of surgery. Generally, it refers to a container, i.e., set of MDs, or a pouch, i.e., single MD or small set of MDs.
Medical device (MD)	Any instrument, apparatus, appliance, material or other article, whether used alone or in combination, intended by the manufacturer to be used in humans for the purpose of the diagnosis, prevention, monitoring, treatment or alleviation of - or compensation for - an injury or handicap. (World Health Organization, 2016)
Original device	A new, unused single-use device. (World Health Organization, 2016)
Pouch	Kit type. Single-use bag, used to contain one MD or a small set of MDs.
Rack	Support for kits (separated in trays mainly) used during Disinfection and Sterilisation steps.

Reprocessing	All steps that are necessary to make a contaminated reusable medical device ready for its intended use. These steps may include cleaning, functional testing, packaging, labelling, disinfection and sterilization. (World Health Organization, 2016)
Reprocessed single-use device	A reprocessed single-use device is an original device that has previously been used on a patient and has been subjected to additional processing and manufacturing for the purpose of an additional single use on a patient. (World Health Organization, 2016)
Single-use device	A device intended for one use only or on a single patient during a single procedure. (World Health Organization, 2016)
Sterilisation	A validated process used to render an object free from viable microorganisms, including viruses and bacterial spores, but not prions. (World Health Organization, 2016)
Tray / Basin	Support used to contain a set of MD. Element inside containers. Also related to pouches kits.
Automated washers / Washer-disinfectors	Washing machines used for Disinfection.
Cart washer	Equipment used in the Disinfection stage for containers and carts/chariots/trolleys.
Pass-box	Equipment used for transport, from clean to dirty area, empty racks and racks needing to reprocess the Disinfection stage due to failure of the quality test results.

5.2 Value chain analysis

CROMA, founded in 1935, deals with the selling and the maintenance of surgical instruments, as well as the realization of operating rooms and sterilization centres. In the Spanish market, the Sterilization Centre of the Burgos Hospital is managed directly by CROMA and accredited ISO 9001, ISO 13485 and ISO 14001. This centre has become a reference model for the organization and for the qualitative system in all the Spanish territories and so has been selected as the pilot plant for the AUTO-TWIN project.

Figure 3 illustrates the value chain of the use case.

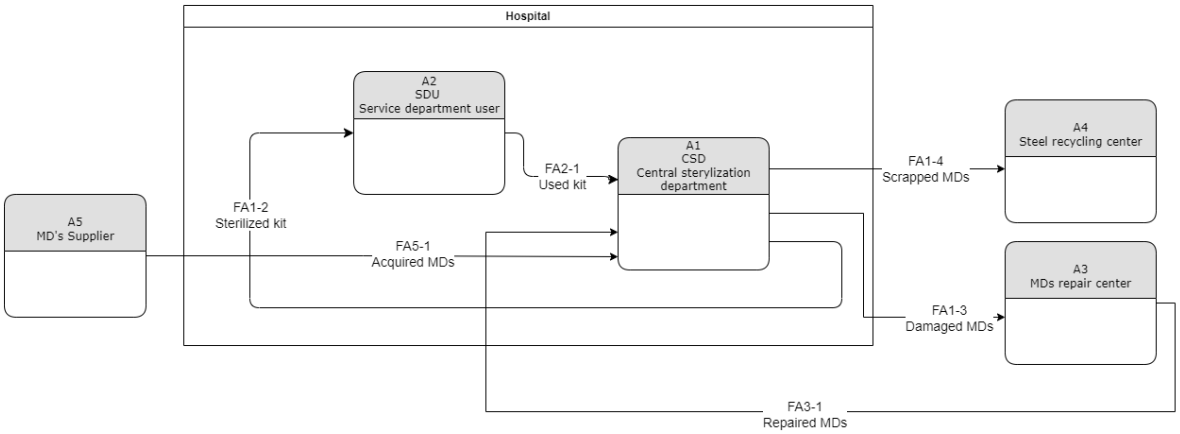

Figure 3 Croma Value Chain Overview

The Actor A1 “CSD Central Sterilization Department” is the core of CROMA operation, it receives surgical kits from users, which are mainly operating theatres, but also all other locations in which tools are used inside the hospital. During the process MDs kits are washed, inspected and sterilised, MDs which needs repairing are sent to an external repairing centre and MDs which are beyond repair are wasted and replaced with new ones purchased on the market.

ID	Actor Name	Description
A1	CSD	CROMA sterilization process inside the hospital
A2	SDU	Service department user
A3	MDs repairing centre	External supplier which repairs damaged MDs
A4	Steel recycling centre	Unrepairable MDs are recycled as steel
A5	MDs supplier	Supplies new MDs to replace unrepairable ones

5.3 Value chain flows

ID	Flow Name	Description	Entity	Trace
FA2-1	Used kit	Used Kit coming from SDU	Kit	YES
FA1-2	Sterilised kit	Requested kit by SDU	Kit	YES
FA3-1	Repaired MDs	Repaired MD returns to stock	MD	YES
FA5-1	Acquired MDs	MDs are purchased to replace non repairable MDs	MD	YES
FA1-3	Damaged MDs	Damaged MDs are sent to repairing facility	MD	YES
FA1-4	Scrapped MDs	Non repairable MD is treated as recyclable steel	MD	NO

5.4 Value chain entity data

Each paragraph of this chapter reports the data related to a certain entity flowing in the value chain (mandatory for entities marked with trace=Yes in the flows table). The objective is capturing the information that could be useful for:

1. Tracking of the entity in the value chain and automated process-aware discovery towards autonomous digital twin generation
2. Association of the digital passport to the entity

5.4.1 FA2-1: Used kit

Data name	Description/Availability/Format
Kit ID	Kit identifier/Database/String
MDs list	List of MD composing the kit/Database/List<String>
Kit type	Type of container/Database/String [container/pouch]
Kit size	Size of the container[length/width/height]/ Database/[double/double/double]
SDU	Identifier of the origin service user (OR, ED, clinics)/Database/String

5.4.2 FA1-2: Sterilised kit

Data name	Description/Availability/Format
Kit ID	Kit identifier/Database/String
MDs list	List of MD composing the kit/Database/List<String>
Kit size	Size of the container[length/width/height]/ Database/String enumerarion [double/double/double]
SDU	Identifier of the origin service user (OR, ED, clinics)/Database/String

5.4.3 FA3-1: Repaired MD

Data name	Description/Availability/Format

MD ID	MD identifier/Repair order/String

5.4.4 FA5-1: Acquired MD

Data name	Description/Availability/Format
MD ID	MD identifier/Purchase-loan orders/String

5.4.5 FA1-3: Damaged MD

Data name	Description/Availability/Format
MD ID	MD identifier/Repair order/String

5.5 Process analysis

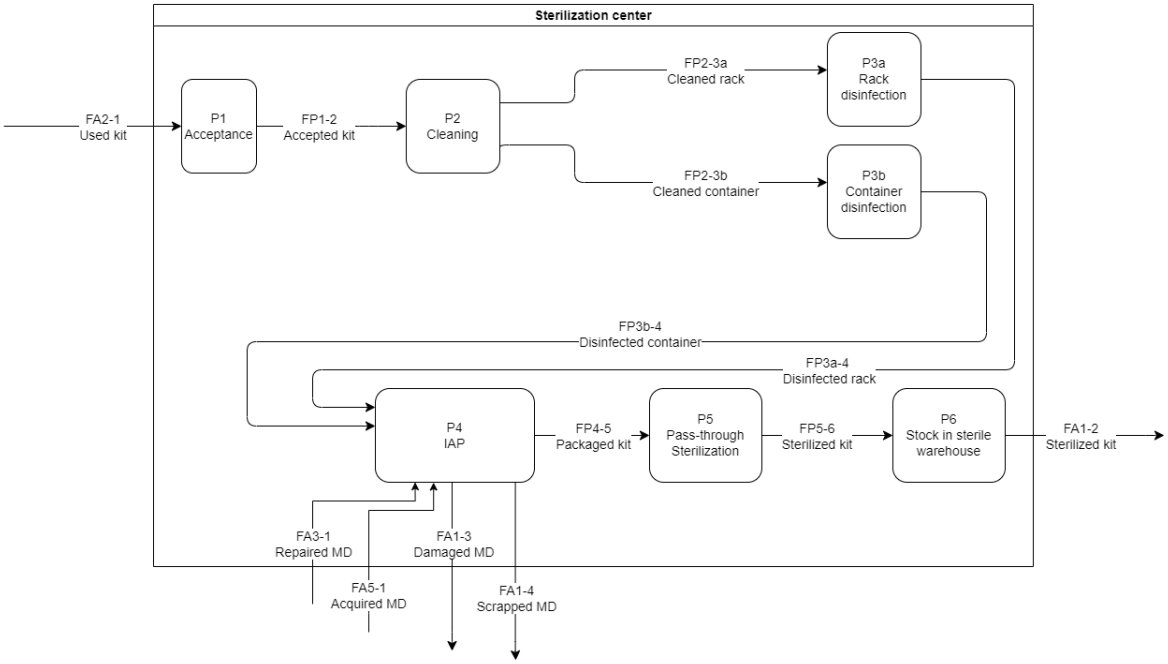

Figure 4. Croma processes overview

5.6 Process flows

The table below reports the short description of the main entity flows of the process.

ID	Flow Name	Description	Entity	Trace
FA2-1	Used kit	Kit that has been used in an SDU, mainly OR.	Kit	YES
FP1-2	Accepted kit	Received kit in the CSD, inside the cart which in turn is waiting in the dirty area.	Kit	YES
FP2-3a	Cleaned rack	Manual cleaned kit (containers and trays separated) and waiting in dirty area shelves or in racks for disinfection	Rack	YES
FP2-3b	Cleaned container	Kit container	Container	YES
FP3a-4	Disinfected rack	Disinfected racks in automated washers are sent to IAP stations.	Rack	YES
FP3b-4	Disinfected container	Disinfected containers in cart washer are sent to IAP stations.	Container	YES
FP4-5	Packaged kit	Kit already inspected, assembled and packaged ready for sterilisation process and waiting in clean area shelves	Kit	YES
FP5-6	Sterilised kit	After completing sterilisation kits are located in the sterile storage area	Kit	YES
FA1-2	Sterilised kit	Requested kit by a service department user	Kit	YES

FA3-1	Repaired MDs	Repaired MD returns to stock	MD	YES
FA5-1	Acquired MDs	MDs are purchased to replace non repairable MDs	MD	YES
FA1-3	Damaged MDs	Repairable damaged MDs are sent to repairing facility	MD	YES
FA1-4	Scrapped MDs	Non repairable MD is treated as recyclable steel	MD	NO

5.7 Entity data

Each paragraph of this chapter reports the data related to a certain entity flowing in the value chain (mandatory for entities marked with trace=Yes in the flows table). The objective is capturing the information that could be useful for:

1. Tracking of the entity in the value chain and automatic derivation of DES model
2. Association of the digital passport to the entity

5.7.1 FA2-1: Used Kit

Data name	Description/Availability/Format
Kit ID	Identifier of the kit/Database/String
MDs list	List of MD types composing the kit/Database/List<String>
Kit type	Type of container or pouch/Database/String
Kit size	Size of the container[length/width/height]/ Database/[double/double/double]
SDU origin	Identifier of the origin service user (OR, ED, clinics)/Database/string

5.7.2 FP1-2: Accepted Kit

Data name	Description/Availability/Format
Kit ID	Identifier of the kit/Database/String
MDs list	List of MD types composing the kit/Database/String
Cleaning method	Kit manual cleaning method/CPM/String

5.7.3 FP2-3a: Cleaned rack

Data name	Description/Availability/Format
Kit ID	Identifier of the Kit associated to the rack/Database/String
MDs list	List of MD types composing the kit/Database/List<String>
Rack ID	Identifier of the rack/Database/String
Disinfection method	Kit disinfection cleaning method/Database/String

5.7.4 FP2-3b: Cleaned container

Data name	Description/Availability/Format
Kit ID	Identifier of the Kit associated to the container/Database/String
Container ID	Identifier of the container/Database/String

5.7.5 FP3a-4: Disinfected rack

Data name	Description/Availability/Format
Kit ID	Identifier of the Kit associated to the rack/Database/String
MDs list	List of MD types composing the kit/Database/List<String>
Rack ID	Identifier of the rack/Database/String
Quality tests	Results of test/Database/String enumeration(OK/Repair/Replace)
Unloading datetime	Timestamp ending of automated washing/Database/String

5.7.6 FP3b-4: Disinfected container

Data name	Description/Availability/Format
Kit ID	Identifier of the Kit associated to the container/Database/String
Container ID	Identifier of the container/Database/String

5.7.7 FP4-5: Packaged Kit

Data name	Description/Availability/Format
Kit ID	Identifier of the Kit associated to the container/Database/String
MDs list	List of MD types composing the kit/Database/ List<String>
Missing MDs list	List of missing MDs which need replacement/Database/ List<String> *Note: there is no formal list of mandatory MDs*
Inspection/Assembly info	List of MDs not included in the kits for maintenance / replacement/Database/String
Sterilisation method	Technique to use in the next step/ITS/String (Autoclave/low temperature/peroxide)

5.7.8 FP5-6: Sterilised kit

Data name	Description/Availability/Format
Kit ID	Identifier of the Kit associated to the container/Database/String
MDs list	List of MD types composing the kit/Database/ List<String>
Sterilisation info	Sterilization cycle identifier/Database/String

5.7.9 FA1-2: Sterilised kit

Data name	Description/Availability/Format
Kit ID	Kit identifier/Database/String
MDs list	List of MD composing the kit/Database/List<String>

5.7.10 FA3-1: Repaired MD

Data name	Description/Availability/Format
MD ID	MD identifier/Repair order/String

5.7.11 FA5-1: Acquired MD

Data name	Description/Availability/Format
MD ID	MD identifier/Purchase-loan orders/String

5.7.12 FA1-3: Damaged MD

Data name	Description/Availability/Format
MD ID	MD identifier/Repair order/String

5.7.13 FA1-4: Scrapped MD

Data name	Description/Availability/Format
MD ID	MD identifier/Database/String

5.8 Process steps

The table below reports the short description of the main steps of the process.

ID	Step Name	Description
P1	Reception	Reception of the kit at CSD.
P2	Cleaning	Manual cleaning of tools
P3a	Rack Disinfection	Automated washing for different MDs/kits in trays batched in racks. Passage stage between dirty and clean area.
P3b	Container Disinfection	Automated washed for containers, and carts/chariots/trolleys). Passage stage between dirty and clean area.
P4	Inspection, assembly and packaging (IAP)	MDs are inspected and packaged in kits
P5	Pass-through sterilization	Passage stage between clean and sterile area.
P6	Stock in sterile warehouse	Stocking sterilised kits in sterile warehouse.

5.8.1 P1 – Acceptance

Activity ID	Activity type	Activity description
P1.1	Input Buffer	Cart arrival with used kits from different SDU, mainly from OR, clinics, or hospitalization. Cart waits till worker is free.
P1.2	Before processing	Tracking. Scanning barcode of each kit for the correct reception in the ITS
P1.3	Processing	Open kit. Enzymatic product manual spray in each kit (security reasons).
P1.4	After processing	Close kits.
P1.5	Output Buffer	Place the cart in the dirty/soiled/decontamination area before manual cleaning.

5.8.1.1 Involved resources

ID	Resource	Capacity	Task/Use
M10	Operator	*1*	*Operator scans container barcode*

5.8.1.2 Main process control parameters

The table below reports the control parameters that affect the execution of the process tasks.

ID	Parameter	Impact on process
C00	ITS	Ability to verify the history, location, or application of an item by means of documented recorded identification
C10	Arrival schedule	Planned arrivals (next meeting interview with Maria and CPM) From different SDU already a schedule: Each 30-40 min from 10:30, CSD workers are in charge of transporting carts from OR to CSD Clinics and hospitalization: Hospital internal logistics department in charge of transporting to CSD. At noon and another time.

5.8.1.3 Process monitoring

The table below reports the process data which is currently monitored and made available.

Data name	Description/Availability/Format
Cart ID	Identification of the cart/Database/String
Kit ID	Identification of the kit/Database/String
Accepted datetime	Date and time of the reception (bar scanning) /Database/Datetime
SDU	Source department that used the kit/Database/String
Operator ID	Employee who did the activity/Database/String

5.8.2 P2 – Cleaning

Activity ID	Activity type	Activity description
P2.1	Input buffer	Kit selection and pick up from cart.
P2.2	Before processing	Kit-container: Separate container-tray and container-box. If there is a big volume of MDs, add a new tray to contain all MDs of this kit. Tracking: Assign this tray to kit-container. Kit-pouch: Discard pouch. Tracking: in case of pouches several pouches could be mixed in a tray
P2.3	Processing	Each MD from kit-tray(s) is cleaned manually.
P2.4	After processing	MDs are placed in the washing machine tray
P2.5	Output buffer	Trays wait on the workbench before being loaded in washing machine

5.8.2.1 Involved resources

ID	Resource	Capacity	Task/Use
M00	Operator	1 kit at time	Employee who performed separation and cleaning
M20	Cleaning stations	3 big basins, 2 small basins and 2 ultrasonics washing machine	Manual wash workplace

5.8.2.2 Main process control parameters

ID	Parameter	Impact on process
C00	ITS	Ability to verify the history, location, or application of an item by means of documented recorded identification
C20	Cleaning prioritisation rules	Precedence rule determines precedence of serving for manual washing: FIFO, top-bottom from cart or *urgent* (non-formally)
C21	Cleaning method	Kit manual cleaning method: standard (basins) or careful treatment due to fragility or composition, so with ultrasonics.
C22	Cleaning time	Activity duration, depending on the kit (number of medical devices and particular specifications).

5.8.2.3 Process monitoring

The table below reports the process data which is currently monitored and made available.

Data name	Description/Availability/Format
Kit ID	Identification of the kit/Database/String
Operator ID	Assign kits-rack/ Database/String

Cleaned datetime	Date and time of assignment of the tray to the rack, end of the cleaning stage/Database/DateTime
Rack ID	Identification of the rack/Database/String

5.8.3 P3a – Rack Disinfection

Activity ID	Activity type	Activity description
P3a.1	Input buffer	Tracking. Assign trays (kits) to racks via barcode scanning. Loading trays on racks of the washing machine, keeping trays of same kit together. When rack is full, rack waits near the washing machines for one of them to be released. Place the quality control tests in the rack.
P3a.2	Before processing	Tracking. Assign rack to automated washing machine via code bar scanning. Load racks on the washing machine in the dirty area. FIFO rule followed.
P3a.3	Processing	Select automatic wash program depending on the kits supported, indicated in ITS. Starts the automatic wash cycle. End the automatic wash cycle.
P3a.4	After processing	Unload racks of the washing machine in the clean area. Wait for the temperature of the rack to drop before treating it. Tracking. Visual inspection, check quality tests and the washing machine ticket. The washing machine ticket extracted on paper is stored and sorted. If the test result is unsatisfactory, “reprocess” the Disinfection step of the whole rack. The complete rack is sent to the soiled area through the passage-lock. Go back to step P3a.1. Otherwise, the load is released.
P3a.5	Output buffer	Let rack waiting in the clean area for IAP.

5.8.3.1 Involved resources

ID	Resource	Capacity	Task/Use
M00	Operator	1	Employee who did the activity
M30a	Automated washer	4 machines 1 rack/machine	Automatic washing cycle
M31a	Rack	How many MDs can be loaded?	See glossary. 3 different types of racks, different sizes: 3, 4, and 5-storey

5.8.3.2 Main process control parameters

ID	Parameter	Impact on process
C00	ITS	Ability to verify the history, location, or application of an item by means of documented recorded identification
C30a	Rack Disinfection prioritisation rules	Precedence rule determines precedence of serving for disinfection automated washing: FIFO and urgent?
C31a	Rack Disinfection method	Washing machine cycle for the rack. Normal/delicate/new tools/prions.

C32a	Rack Disinfection time	Duration of the process depends on washing machine cycle.

5.8.3.3 Process monitoring

The table below reports the process data which is currently monitored and made available.

Data name	Description/Availability/Format
Rack ID	Identification of the rack/Database/String
Kit list	List with identification of the kits being loaded/Database/List<String>
Load Operator ID	Loading rack to machine. Assign rack-washing machine
Load datetime	Date and time of load step/Database/DateTime
Disinfection datetime	Date and time of the disinfection step (start and end)/ Database/DateTime
Disinfection method	Washing cycle (3 different)/Database/String
Disinfection time	Wash programme cycle duration/Database//Double
Quality tests	Final status of the activity, controlling that all requirements are achieved/Database/String[ok/fail]
Automated-washer ticket	Machine printed report/Only paper format/TBD
Unload Operator ID	ID of the unloading operator/Database/String
Unload datetime	Date and time of unload step/Database/DateTime

5.8.4 P3b – Container Disinfection

Activity ID	Activity type	Activity description
P3b.1	Input Buffer	Containers are placed on shelf and then into racks for loading into the washing machine
P3b.2	Before processing	Containers are batched on racks
P3b.3	Processing	Containers go through the tunnel washing machine
P3b.4	After processing	Containers are put on shelves in the clean area
P3b.5	Output Buffer	Containers are picked from shelves

5.8.4.1 Involved resources

ID	Resource	Capacity	Task/Use
M00	Operator	1	Operator loading/unloading machines
M30b	Cart-washer	1 tunnel X support/tunnel	See glossary.
M31b	Cart-washer support	TBD	See glossary. 3 different types of racks, different sizes: 3, 4, and 5-storey

5.8.4.2 Main process control parameters

ID	Parameter	Impact on process
C00	ITS	Ability to verify the history, location, or application of an item by means of documented recorded identification
C30b	Container Disinfection prioritisation rules	Precedence rule determines precedence of serving for disinfection container washing: Rule: urgent than FIFO
C31b	Container Disinfection method	Cart washer machine cycle for the rack.
C3b.2	Container Disinfection time	Duration of the process depends on cart-washer cycle.

5.8.4.3 Process monitoring

The table below reports the process data which are currently monitored and made available.

Data name	Description/Availability/Format
Process time	Process time/Database/Double

5.8.5 P4 – IAP (inspection, assembly and packaging)

Activity ID	Activity type	Activity description
P4.1	Input Buffer	MDs selection and transport from waiting area next to automated washers to packing area.
P4.2	Before processing	Kits selection.
P4.3	Processing	Start IAP, for each MD in kit inspection, assembly and packing in parallel. Inspection of each MD following ITS guidelines. Assembly MDs: container-kit, and container-pouch. Replacing damaged/missing MDs (traceability) End IAP
P4.4	After processing	End IAP, tracking.
P4.5	Output Buffer	Kit-container-box, in shelves in a waiting area for sterilisation

5.8.5.1 Involved resources

ID	Resource	Capacity	Task/Use
M00	Operator	1	Employee who did the activity
M41	Packing station	14 stations	MDs
M42	Inspection equipment	1	Mainly a magnifying lens used for inspections

5.8.5.2 Main process control parameters

ID	Parameter	Impact on process
C00	ITS	Ability to verify the history, location, or application of an item by means of documented recorded identification.
C40	IAP prioritisation rules	Precedence rule determines precedence of IAP activity. FIFO and *urgent*.
C41	Kit MDs-lists	Check list to verify when doing IAP activity.
C42	Missing/damaged MDs-list	Track of missing/damaged MDs.

5.8.5.3 Process monitoring

The table below reports the process data which is currently monitored and made available.

Data name	Description/Availability/Format
Kit ID	Identification of the kit/Database/String
Operator ID	Employee who did the activity on the kit/Database/String
IAP start datetime	Date and time of the IAP step/Database/DateTime
IAP station	Assembly position/Database/String

IAP time	Duration of IAP activity/Database/Double
Packing type	Type of packaging: container or pouch/Database/String
Inspection checklist	Final status of the kit after inspection step/Database/String[ok/not ok]
Production ID	Unique identification of the whole reconditioning process/Database/String

5.8.6 P5: Pass-through sterilization

Activity ID	Activity type	Activity description
P5.1	Input Buffer	Kits batched in sterilisation support
P5.2	Before processing	Kits grouped with same sterilisation method. Tracking. Load rack to be steam sterilised.
P5.3	Processing	Steam-sterilization cycle.
P5.4	After processing	Unload the rack. Tracking.
P5.5	Output Buffer	Let the rack cool down for a while in the sterile area

5.8.6.1 Involved resources

ID	Resource	Capacity	Task/Use
M00	Operator	1	Employee who did the activity
M50	Steriliser	4 steam-sterilisers	Equipment for sterilisation
M51	Sterilisation trolley	8 UST	Support for kits to be sterilised

5.8.6.2 Main process control parameters

ID	Parameter	Impact on process
C00	ITS	Ability to verify the history, location, or application of an item by means of documented recorded identification
C50	Sterilisation prioritisation rules	Precedence rule determines precedence of serving for sterilisation: FIFO
C51	Sterilisation method	Kit sterilisation method: steam-sterilisation or low-temperature sterilisation (EOP, HSP)
C52	Sterilisation time	Duration of the process depends on sterilisation method. Washing time influences process time

5.8.6.3 Process monitoring

The table below reports the process data which is currently monitored and made available

Data name	Description/Availability/Format
Kit ID	Identification of the kit/Database/List<String>
Operator ID	Employee who did the activity/Database/String
Sterilisation start datetime	Date and time of the sterilisation step/Database/DateTime
Steriliser	Sterilization equipment/Database/String
Sterilisation cycle	Programme selected for sterilisation/Database/String
Sterilisation time	Duration of sterilisation activity/Database/Double

Production ID	ID of the associated production/Database/String
Quality tests	Final status of the activity, controlling that all requirements are achieved/Database/String [ok, not ok]

5.8.7 P6: Stock in sterile warehouse

ID	Activity description
P6.1	Select kit from rack (top-bottom) and pick up
P6.2	Place the kits in their place on the sterile warehouse

5.8.7.1 Involved resources

ID	Resource	Capacity	Task/Use
M00	Operator	1 worker	Employee who did the activity

5.8.7.2 Main process control parameters

ID	Parameter	Impact on process
C00	ITS	Ability to verify the history, location, or application of an item by means of documented recorded identification

5.8.7.3 Process monitoring

The table below reports the process data which is currently monitored and made available.

Data name	Description/Availability/Format
Production ID	ID of the associated productions/Database/String
Quality tests	Final status of the activity, controlling that all requirements are achieved String [ok, not ok]

5.9 Objectives and impacts

The following table maps business objectives and technical objectives of the use case, assigning to each objective a priority level ranging from 1 (highest level of priority) to 3 (lowest).

Table 1 Technical objectives

ID	Business Objective	Technical Objective	Priority Level	Description
1	Predictive and prescriptive capabilities	Resources saturation prediction	1	The objective is being able to predict the saturation level of resources in relation to a specific temporal scheduling of sterilizations. Currently there's no model to predict resources (stations and automated machines) saturation. The saturation is only observed using collected data from the monitoring software.
2		Predict operators' behaviour	1	The objective is being able to predict the behaviour of the centre operators in terms of performance based on collected data.
3	Reduce production costs and environmental impact	Reduce the process energy cost	1	The objective is to improve the occupation of the machines, since sterilization lines require amounts of energy that is almost constant and only marginally affected by the level of volume occupation of the machines (i.e., number of kits/MDs). Therefore, improving the level of occupation of the machines could reduce the impact of energy cost on single MD sterilization.
4		Reduce the cost of MD reintegration	1	The objective is reducing the cost associated to the reintegration of lost medical devices. To this end, the loss condition needs to be identified as early as possible. A desirable solution would be to identify the missing MDs at the exit of the operating theatre.
5		Reduce the number of kits stopped along the process	2	The objective is to reduce the number of stopped kits. If a fundamental MD is missing in the kit, and there is no replacement MD in the warehouse, the kit must be stopped along the process and wait for the supplier to ship the replacement.
6		Reduce the process lead time	2	The objective would be to identify the best precedence rules in the queues to improve the load balancing between the

				phases/stations of sterilization in order to reduce the lead time.
7		Improve failure management, lower the cost for replacements due to breakdowns	1	The objective is reducing the cost related to replacement of MD breakdowns using predictive maintenance model capable to forecast the wear level. This requires the ability of extracting lifecycle information of each MD from tracked data.
8		Improve saturation of equipment	1	The objective would be reaching on average 50% of saturation. Currently the machine saturation is low especially in the morning.
9		Improve operator shifts organization	1	The objective would be improving the time allocation of human resources. In particular one of the main targets would be the optimal selection of the number of operators needed for each shift.
10		Optimize order for MD suppliers	3	The objective is to improve the management of the spare MD warehouse, optimizing the scheduling/forecasting of orders to the be issued to the suppliers.
11	Enable production planning	Organize daily scheduling to level workload peaks	1	The objective is to be able to schedule sterilization of kits in a way that avoids workload peaks. Currently, they don't schedule with the look ahead on the surgery scheduling, they just apply the FIFO logics is applied when kits return from operating theatres. This generates peaks in the afternoon and evening that could be levelled using a scheduling optimization model.
12		Learn and adapt DT to always represent the whole physical system	1	The objective is having models of the sterilization centre that are strictly bound to the real system and evolve their internal logics according to the collected data.
13	Improve human-twin relation	Create tools which can be used by different roles in the company without a deep knowledge of all the processes	1	The developed tools should be used by low skilled operators to manage the daily activity of the sterilization centre. The objective is to hide complexity increasing the level of acceptance of the tools by the final end user.

14	Data exchange	Provide the ability for all applications in data spaces to create, use, transfer, and effectively exchange data	2	The objective is to create an open access data space to publish process data that could be leveraged by hospital and MD suppliers.
15		Create continuous data flow report on processes and warehouses	1	The objective is having a continuous and coherent (standard) way of accessing all the process information. Currently there is not a single access point for all the process data. Some data are coming from different sources and don't have the same accessibility level. The data must be extracted on a batch basis.

The following table defines a set of potential developments to reach the technical objectives abovementioned and maps each solution to corresponding Exploitable Results (ER) and project Objectives (OBJ) declared in the proposal and reported in Figure 2.

Table 2 Potential Developments.

ID	Name	Potential Development	AUTO-TWIN	
			OBJ	ER
D1	Common data collector	Create a common data collector capable to organize and make available to Croma data generated from the different sources available in the sterilization centre (ERP software, sterilization machines with IT interfaces and operators/paper data)	OBJ2	ER2/ER3/ER4 (WP2)
D2	Saturation prediction model	Create a model capable to predict the saturation of machines and workload according to the scheduling, which could help improving the machine saturation and the organization of human personnel shifts.	OBJ1	ER1 (WP3)
D3	Operators behaviour prediction model	Create a model capable to predict the behaviour (availability, processing times, decrease of performances along the day) of human resources starting from the observations of the behaviour in the real process and of the exogenous factors in the surrounding environment.	OBJ1	ER1 (WP3)
D4	Sterilization process simulation model	Create a model capable to forecast the behaviour of the internal sterilization processes, based on the acquired	OBJ1, OBJ2	ER1 (WP3), ER3 (WP2), ER3 (WP2)

		historical data and on the specified design data		
D5	Scheduling optimization module	Create a user targeted module, based on the digital simulation model of the sterilization centre (R4), that is capable to optimize the scheduling of the sterilization process taking into consideration the surgery plans of the hospital. The module should be able to level the workload peaks.	OBJ3, OBJ4	ER5/ER6 (WP3), ER7 (WP4)
D6	Medical Device lifecycle model	Create a model that is capable to predict the MD lifecycle by tracing all the usage and sterilization cycles. In particular, the model would be learned from historical data of MD maintenance operations and be able to predict when each MD should undergo maintenance.	OBJ2	ER2/ER3/ER4 (WP2)
D7	Spare MD orders optimization	Create a user targeted module that, based on the lifecycle model of the medical device, is capable to suggest the scheduling of production orders to MD suppliers.	OBJ2, OBJ3, OBJ4	ER2 (WP2), ER5 (WP3), ER7 (WP4)
D8	Data Space connector	Find, create or adapt an existing IDS compliant data connector that is capable to publish process data related to sterilized kits.	OBJ2	ER2 (WP2)

The following table maps the potential developments on the use case technical objectives, providing a view on the level of coverage of the initial requirements.

Table 3 Objectives - Developments map

	Objective	**Requirement**							
		D1	D2	D3	D4	D5	D6	D7	D8
1	Resources saturation prediction		■						
2	Predict operators' behaviour			■					
3	Reduce the process energy cost		■		■				
4	Reduce the cost of MD reintegration								
5	Reduce the number of kits stopped along the process						■	■	
6	Reduce the process lead time				■				
7	Improve failure management, lower the cost for replacements due to breakdowns						■		
8	Improve saturation of equipment		■		■	■			
9	Improve operator shifts organization			■	■	■			
10	Optimize order for MD suppliers							■	
11	Organize daily scheduling to level workload peaks		■	■	■				
12	Learning and adaptation of DT to represent always the whole physical system						■		
13	Create tools which can be used by different roles in the company without a deep knowledge of all the processes					■		■	
14	Provide the ability for all applications in data spaces to create, use, transfer, and effectively exchange data	■							■
15	Create continuous data flow report on processes and warehouses	■							

The following table reports a set of measures that have been identified as possible indicators of the impact of applying the AUTO-TWIN results to the use case. This list has been defined with the current knowledge of the objectives and potential developments of the following research activities. Therefore, they will be adjusted during the validation phase. As stated in DoA, the baseline values for the impact measures will be defined in D1.2.

Table 4 Target impact measures

ID	Impact measure	Expected target value	Related user objective
1	**Process lead times** Average lead time from the arrival at the sterilization centre to the storage at the sterile inventory	-15%	6, 11
2	**Average saturation of washing machines** Calculated for automatic washing machines (Automated washer M30a)	50%	1,8
3	**Average saturation of sterilization machines** Calculated for sterilizing machines (Steam Sterilizers M50)	50%	1,8
4	**Workload balance** The measurement methodology will be completely defined during validation phase (e.g., the sample coefficient of variation of the saturation, the reduction of the difference between the maximum and the average value of the hourly average saturation).	-30%	8,9,11
5	**Sterilization energy costs** Average cost per kit.	-15%	3
6	**Number of kits blocked in process** Average number of kits blocked in the process (MD inventory stockout).	-5%	5
7	**Life cycle length of the MD** Lifetime of an MD from purchase to decommissioning.	TBD	4
8	**Daily human resources saturation** Average saturation level measured over a day.	[60%, 80%]	2,9

5.10 Decisions

This section describes the decisions of the use-case. These descriptions are grounded on the As-Is situation with respect to the To-Be goals.

1. Decide on the sterilization process operative management. The set of decisions includes: the selection of which kit of those in the queue to be processed at a given time depending on system state and surgery daily schedule, the management of WIP in each area (i.e., dirty, clean, sterile areas), automatic resource loading decisions, and the staff schedule. In addition, the set of decisions includes process controls as described in Section 5.8 (e.g. alternative cycles and process parameters). Particular attention should be devoted to the management of high-priority kits, to be delivered as soon as possible, and last-minute modifications of the surgery schedule. Indeed, the operating list and the number of surgeries performed is variable and affected by miscommunicated changes and emergencies.
    a. *Actor(s):* technical director
    b. *Challenge(s):* non-disclosure constraint for the kit (i.e., the kit, as composed by multiple MDs over multiple trays, should not be separated in different loads), eligibility and technological constraints for allocating MDs onto a certain machine, technological constraints to simultaneously load two MDs on a machine, maximum load capacity.
    c. *Time Horizon/Frequency:* Day / Daily
2. Decide on the repair of a worn MD. At the inspection process (IAP), each MD must pass a quality and conformance check resulting in: (i) fit for use and continue in the kit, (ii) in need of maintenance, or (iii) not fit for use or maintenance and should be removed and sent for recycling. Worn MDs and broken MDs must be substituted with a new/as-new one. The decision is whether to send the MD to repair or to recycle loops.
    a. *Actor(s):* technical director
    b. *Challenge(s):* hidden correlation between the decision and the risk of breakages
    c. *Time Horizon/Frequency:* at occurrence
3. Decide on the inventory management of new/as-new MDs. Decision on the quantity (number) of each type of MD in the spare MD-stock.
    a. *Actor(s):* technical director + CEO
    b. *Challenge(s):* service level to be assured (avoidance of kit stoppages and /or incompleteness)
    c. *Time Horizon/Frequency:* Month / Weekly
4. Decide on the number of kits of a certain type that populates the system (overall WIP). Given the set of kit variants, the number of kits of a certain variant might affect the performance of the sterilization center.
    a. *Actor(s):* technical director + CEO
    b. *Challenge(s):* given set of kit variants, maximum capacity of the system
    c. *Time Horizon/Frequency:* Year / Annual

5.11 KPIs

This section describes the key performance indicators for the use-case.

The following list focuses on KPIs related with external KPIs, mostly related to the service level, which is the major priority of the company:

- Fill rate. Meeting customer demand on time is very important for the company. This metric shows the fraction of customer demand that is met through immediate stock availability, without backorders or lost sales.
- Stockout. Lack of availability of a certain kit variant in the sterile inventory upon request
- TTS (Lateness). Time delay between the request of a certain sterile kit and the actual availability in the sterile inventory. This metric indicates indirectly the response-time of the sterilization centre at stockout occurrence.
- Number of incomplete sterile kits (*i.e.,* kits with not complete composition that are stored in the sterile inventory and might orbit in the hospital).

The following list focuses on internal KPIs:

- Area-based lead time. The metric indicates the time interval from the kit arrival to a certain area (i.e., dirty, clean, sterile) to its exit from the same area. A similar metric is the queue time, indicating the time interval from the kit arrival to a certain area (*i.e.,* dirty, clean, sterile) to the starting of its processing in that area. For example, the process lead times is computed from the kit arrival at the sterilization centre to the kit storage at the sterile inventory. Being related to the service level and the response capability of the system, the metric is of particular interest when considering the production lead time as the sum of area-based lead times. The goal is to reduce the time between the arrival of high priority kits and their dispatch.
- Work-In-Progress (WIP). The metric indicates the average number of kits waiting for process in a certain area (*i.e.,* dirty, clean, sterile). WIP is maintained in the dirty and clean areas overnight. The inventory of sterile kits is located in the sterile area of the center.
- Saturation of resources (*i.e.,* automatic and manual stations) and workload balance. The current state of usage denotes low saturation on the average and high saturation peaks, resulting in an unbalanced profile. The metric indicates both the average saturation and load peaks as, for example, the difference between max and average values of the machine saturation.
- Sterilization cost (energy and consumables). The metric includes the cost for sterilization (including materials and energy cost).
- MD reintegration and replacement. The metric includes the costs related to MD management: the cost for MD repair and replacement (wear and breakages), and the MDs' reintegration cost (lost MDs). The latter factor is of specific interest since it is related to the occurrence of uncontrollable external events, *i.e.,* MD losses in operating *theatres*.
- Product lifetime. Product lifetime (or life cycle length) is correlated to the number of sterilization cycles and the product usage in operating *theatres*. The metric of interest is the average number of sterilization cycles before replacement on a selected set of medical devices.
- Actual kit usage. Once the kit is sterile, it might spend a long time before usage which might indicate inefficiencies in the management of the centre. The metric used is the "time in orbit" as the time interval between the exit from the sterilization centre and the actual usage of the kit. The metric is affected by differences in scheduled/actual surgeries for kits and

scheduled/actual appointments in departments, and by the stochastic arrival of patients at emergency.

- Number of kits blocked in the system. The metric indicates how many kits, at the inspection process, need a reintegration/replacement of MDs while the MD is not available in the inventory (stockout).

5.12 Notes on as-is process

This section provides notes about the current As-Is state of the use-case.

The described decisional processes are currently solved with best practices and experience-based rules by the technical director of the sterilization centre. Best practices are applied to manage the production (*e.g.,* kit priorities, machine loading rules, and general process control). Mainly, the planned surgery schedule and estimated demands from departments and emergency are used to define the kit priority in the dirty area; then, an FCFS (First Come First Serve) production management rule is followed in clean and sterile areas. Experience-based management may be grounded implicitly on constraints of the problem such as eligibility constraint or prioritization needs.

Strategic decisions are selected by the CEO in coordination with the technical director of the centre.

Investment decisions on the number and type of resources and on the number and skills of operators are not included in this project. Herewith they are considered as problem constraints.

Set optimization (*i.e.,* to define the composition of each kit variant) and other contractual decisions are periodically revised jointly with the Hospital and are not included in this project.

6 Gr3n use case

6.1 Nomenclature and glossary

Polyethylene terephthalate (PET)	Polyethylene terephthalate (PET) is a type of plastic that is widely used in packaging applications, especially for food and beverage containers, mostly (around 70% of the market) in the fashion industry for textile, with its most well-known name of polyester fibre.
Virgin PET	Virgin PET, also known as virgin grade PET, refers to PET that has not been previously used or recycled. It is made from new, raw materials. It is regarded as an excellent material for many applications and is widely used for making liquid containers (bottles). Its origin is currently from ethylene and paraxylene, two oil-derived raw materials. [3]
Recycled PET	Recycled PET, also known as rPET, is produced from post-consumer PET waste that has been pre-processed. [3]
Feedstock	In the PET recycling process, feedstock refers to the raw material that is used as input into the recycling process to produce recycled PET. The feedstock for PET recycling is typically post-consumer PET waste, such as bottles or packaging material that has been used and discarded.
Mono-ethylene glycol	Mono-ethylene glycol (MEG) is a colourless, odourless, and slightly viscous liquid organic compound with the chemical formula (CH2OH)2. It is also known as ethylene glycol monomer or simply ethylene glycol.
Purified Terephthalic Acid	Purified Terephthalic Acid (PTA) is a white powder that is used as a feedstock in the manufacture of polyester fibre and PET.
Contamination	Contamination refers to the presence of any unwanted or harmful materials in the recycled PET material that can negatively impact its quality and usability in new products.
Pre-processing	Pre-processing refers to the process of cleaning and refining post-consumer PET waste or textile waste into a usable form that can be easily used for recycling.
Recycling	In the context of PET, recycling refers to the process of collecting, sorting, cleaning, and processing post-consumer PET waste into new products, such as rPET, which can be used as a raw material in the production of new PET products, such as bottles or packaging material. While in the context of textile, recycling refers to the process of collecting, sorting, and processing used or discarded textile products, such as clothing or fabric scraps, into new textile products, such as yarn.
Polymerization	Polymerization is a chemical process that is used in PET manufacturing to transform monomers, such as PTA and MEG, into long chains of repeating units known as PET polymer. If MEG and PTA satisfied the appropriate quality requirements, polymerization is equally appliable to virgin or recycled monomers.
Depolymerization	Depolymerization is a chemical process that is used in PET recycling to break down PET polymer into its constituent monomers, such as PTA and MEG.

Separation	Separation is a process used in PET recycling to isolate materials or components from a mixed stream of PET waste. During the separation process, the mixed stream of PET waste is subjected to physical or chemical treatments, such as sieving, magnetic separation, or density separation, to separate different types of PET waste.
Crystallization	Crystallization is a process used in PET recycling to purify and solidify rPET resin, which can then be used as a raw material in the production of new PET products. During crystallization, the rPET resin is heated and melted to a specific temperature, and then cooled slowly to allow the PET polymer to form crystals, which helps to remove impurities and improve the clarity and strength of the material.
Purification	Purification is a process used in PET recycling to remove impurities and contaminants from recycled rPET resin, making it suitable for use in the production of new PET products. During the purification process, the rPET resin is subjected to a series of treatments, including filtration, washing, and chemical treatments, to remove any residual contaminants that may be present, such as dirt, oils, dyes, or other materials.
Distillation	Distillation is a process used in PET recycling to separate and purify the monomers, such as PTA and MEG, from the depolymerized PET waste. During the distillation process, the depolymerized PET waste is heated and subjected to a series of treatments, including fractional distillation, to separate the PTA and MEG monomers.
Reactor	A reactor is a vessel or container used in chemical processes to carry out chemical reactions under controlled conditions of temperature, pressure, and other variables. In the context of PET recycling, reactors are used in several steps of the process, such as depolymerization and polymerization.
Mother liquor	Mother liquor is a term used in chemical processes to refer to the residual liquid that remains after a solid has been separated or isolated from a solution. In the context of PET recycling, mother liquor may refer to the residual liquid that remains after the monomers, such as PTA and MEG, have been separated and purified from the depolymerized PET waste.

6.2 Value chain analysis

GRN is a Swiss company that has invented the first economically viable and environmentally sustainable process for breaking down any type of PET and polyester into its two core components (i.e. monomers), which can be then re-assembled to obtain virgin-like plastics enabling endless recycling loops. The company is currently working on industrializing this process. The key objective is to commercialize a packaged system, called “Reactive Unit” (acronym RU), that implements in practice the patented technology for chemical recycling. GR3N intends to sell Reactive Units to Engineering, Procurement and Construction (EPC) contractors, to license the process to be used, and to provide all the after-sale services of maintenance. The long-term company’s goal is to become the world leading supplier of recycled PET and polyester. Figure 5 shows the value chain of GR3N pilot plant which will be the reference use case for Auto twin project, so in this case the plant is owned by GR3N itself.

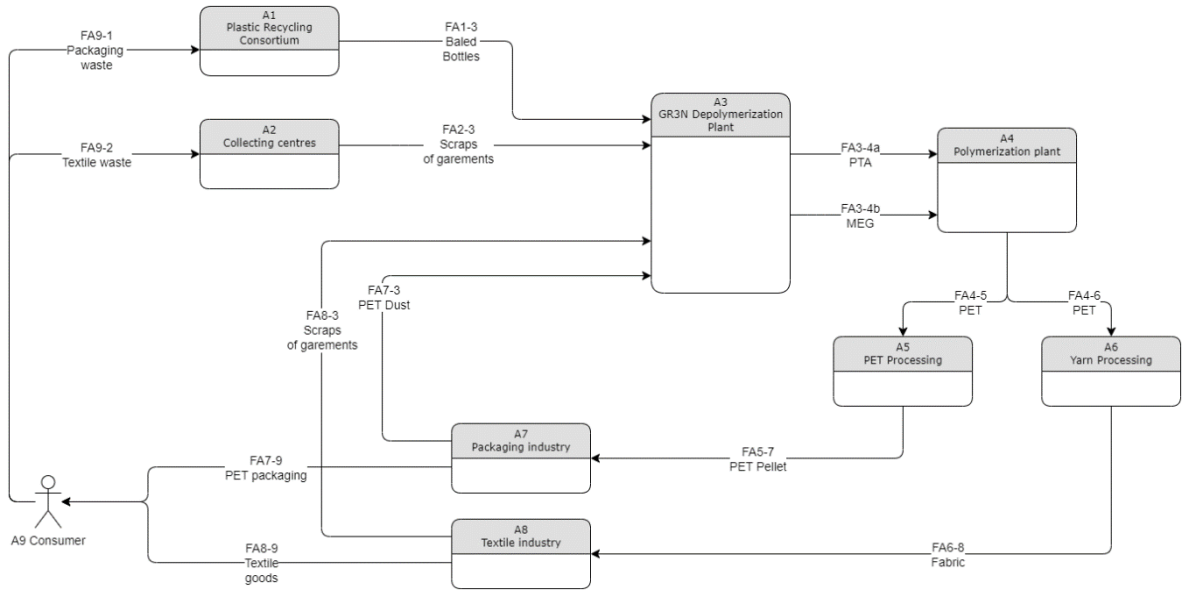

Figure 5 GR3N Value Chain Overview

The GR3N depolymerization plant, indicated as actor A3 inFigure 5, receives PET in the form of production off-cuts and scraps from the industry and collected wastes from consumer market, while the output of the recovery process are MEG and PTA, which are the core components for the polymerization process of PET. The polymerization plant is indicated as a separate actor A4 in the value chain diagram because in some cases polymerization could be performed by 3rd parties which buy the components from the owner of the depolymerization plant, but in other cases it could be integrated into the same facility.

ID	Actor Name	Description
A1	Plastic Recycling Consortium	National consortium for the plastic materials recycling (CO.RE.PLA in Italy)
A2	Collecting centres	Garbage collection centres directly controlled by the local municipalities
A3	GR3N depolymerization plant	It is the core of gr3n patented process and where PET waste is transformed back, via alkaline hydrolysis, to its composing monomers, MEG and PTA, to a quality undistinguishable from virgin-grade ones.

A4	PET polymerization plant	Repolymerization of PET starting from MEG and PTA obtained via depolymerization and purified thanks to gr3n proprietary process.
A5	PET Processing	Block representing the PET semifinished processing plants
A6	Yarn Processing	Block representing the production of the yarns starting from the virgin PET
A7	Packaging industry	Using recycled PET for packaging
A8	Textile industry	Using recycled PET for textile
A9	Consumer	Consumer market for PET products

6.3 Value chain flows

ID	Flow Name	Description	Entity	Trace
FA1-3	Baled bottles	PET collected by the recycling consortium is packed into batches of packaging pressed materials. The consortium characterizes each batch with structured attributes	Feedstock	Yes
FA2-3	Scraps of garments	Textile scrap collected by the local municipalities collection centres or directly by fashion brands.	Feedstock	Yes
FA7-3	PET Dust	Batches of PET dust. Packaging industry generates PET waste as scrap of production process of the finished consumer goods. Typically, this waste has the form of PET dust. The characterization of the flow material depends on the supplier	Feedstock	Yes
FA2-3	Scraps of garments	Batches of textile scrap Textile waste generated by the production of the final consumer goods. Typically, this kind of flow comes directly from the brand (H&M, Decathlon, etc.) production factories. The characterization of the flow material depends on the supplier	Feedstock	Yes
FA3-4a	PTA	Purified Terephthalic Acid obtained from depolymerized PET	Batch	Yes
FA3-4b	MEG	Mono-ethylene glycol obtained from depolymerized PET	Batch	Yes
FA4-5	PET	New virgin PET gained from polymerization	Batch	Yes
FA4-6	PET	New virgin PET gained from polymerization	Batch	Yes

FA5-7	PET Pellet	PET pellet used in the packaging industry	Batch	No
FA6-8	Fabric	Synthetic fabric produced with PET	Batch	No
FA7-9	PET packaging	Consumer goods produced wit PET	Batch	No
FA8-9	Textile consumer goods	Textile goods made with fabric	Batch	No
FA9-1	Packaging waste	Packaging waste from consumer goods	Batch	No
FA9-2	Textile waste	Textile waste from consumer goods	Batch	No

6.4 Value chain entity data

Each paragraph of this chapter reports the data related to a certain entity flowing in the value chain (mandatory for entities marked with trace=Yes in the flows table). The objective is capturing the information that could be useful for:

1. Tracking of the entity in the value chain and automated process-aware discovery towards autonomous digital twin generation
2. Association of the digital passport to the entity

6.4.1 FA1-3/Baled Bottles

Data name	Description/Availability/Format
ID	Identifier of the stock /Database/String
Weight	Weight of the stock /Database/Double
Receiving date	Data of reception/Database/Date
Source	Source of the stock/Database/String
Cost	Cost of the stock/Database/Double

6.4.2 FA2-3/ Scraps of garments

Data name	Description/Availability/Format
ID	Identifier of the stock /Database/String
Weight	Weight of the stock /Database/Double
Receiving date	Data of reception/Database/Date
Source	Source of the stock/Database/String
Cost	Cost of the stock/Database/Double

6.4.3 FA7-3/PET Dust

Pet dust/small fragments from industry, residual from moulding processes

Data name	Description/Availability/Format
ID	Identifier of the stock /Database/String
Weight	Weight of the stock /Database/Double
Receiving date	Data of reception/Database/Date
Source	Source of the stock/Database/String
Cost	Cost of the stock/Database/Double

6.4.4 F5/ Scraps of garments

Data name	Description/Availability/Format
ID	Identifier of the stock /Database/String
Weight	Weight of the stock /Database/Double
Receiving date	Data of reception/Database/Date
Source	Source of the stock/Database/String
Cost	Cost of the stock/Database/Double

6.4.5 F6/ PTA

Data name	Description/Availability/Format
ID	Identifier of the batch/Database/String
Weight	Weight of the batch/Database/Double
Production date and time	Date and time of production/Database/DateTime
Quality KPIs	Standardized metrics to measure the quality of the PTA produced by depolymerization/TBD/TBD
Isophthalic Acid Content	Content of Isophtalic acid/Database/Double

6.4.6 F7/ MEG

Data name	Description/Availability/Format
ID	Identifier of the batch/Database/String
Weight	Weight of the batch/Database/Double
Production date	Date and time of production/Database/DateTime
Quality KPIs	Standardized metrics to measure the quality of the MEG produced by depolymerization/TBD/TBD

6.4.7 F8/PET

Data name	Description/Availability/Format
ID	Identifier of the batch/Database/String

Weight	Weight of the batch/Database/Double
Production date	Date and time of production/Database/DateTime
Intrinsic Viscosity (IV)	It is the most important metrics to assess the mechanical properties of the PET and, consequently, its usage later on in the value chain/Database/Double

6.4.8 F9/PET

Data name	Description/Availability/Format
ID	Identifier of the batch/Database/String
Weight	Weight of the batch/Database/Double
Production date	Date and time of production/Database/DateTime
Intrinsic Viscosity (IV)	It is the most important metrics to assess the mechanical properties of the PET and, consequently, its usage later on in the value chain/Database/Double

6.4.9 F10/PET Pellet

Data name	Description/Availability/Format
ID	Identifier of the batch/Database/String
Weight	Weight of the batch/Database/Double
Production date	Date and time of production/Database/DateTime

6.4.10 F11/Fabric

Data name	Description/Availability/Format
ID of source stock	Identifier of the batch/Database/String

6.5 Process analysis

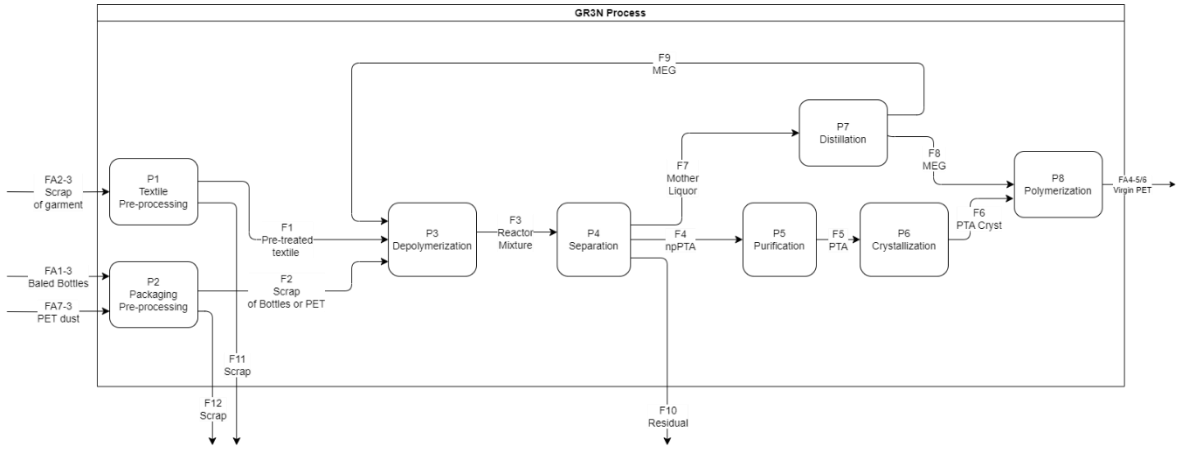

Figure 6 GR3N Process overview

6.6 Process flows

The table below reports the short description of the main entity flows of the process.

ID	Flow Name	Description	Entity	Trace
FA2-3	Scrap of garment	Recycled garment	Feedstock	YES
FA1-3	Baled bottles	Recycled bottles	Feedstock	YES
FA7-3	PET dust	Recycled PET	Feedstock	YES
F1	Pre-treated textile	Grinded textile scraps	Feedstock	YES
F2	Scrap of bottles or PET	Processed bottles or PET dust	Feedstock	YES
F3	Reactor mixture	Mixture of PTA, MEG and contaminants	Batch	YES
F4	npPTA	Not pur PTA	Batch	YES
F5	PTA	Purified Terephthalic Acid	Batch	YES
F6	PTA Cryst.	Crystals of PTA	Batch	YES
F7	Mother Liquor	Mixture of MEG, water and other soluble contaminants originally present inside the waste	Batch	YES
F8	MEG	Distilled pure Mono-Ethylene Glycol	Batch	YES
F9	MEG	Distilled pure Mono-Ethylene Glycol	Batch	YES

F10	Residual	Residual compounds, mainly unreacted fibres	Batch	YES
F11	Scrap	Residual scraps	Batch	YES
F12	Scrap	Residual compounds	Batch	YES
FA4-5 **FA4-6**	Virgin PET	Virgin PET	Batch	YES

6.7 Entity data

Each paragraph of this chapter reports the data related to a certain entity flowing in the value chain (mandatory for entities marked with trace=Yes in the flows table). The objective is capturing the information that could be useful for:

3. Tracking of the entity in the value chain and automatic derivation of continuous simulation model
4. Association of the digital passport to the entity

6.7.1 FA2-3/Scrap of garment

Data name	Description/Availability/Format
ID	Identifier of the stock/Database/String
Weight	Weight of the stock/Database/Double
Receiving date	Data of reception/Database/Date
Source	Source of the stock/Database/String
Composition	%PET,%PU,%Inseparable reactants,%Other/Database/Other

6.7.2 FA1-3/Baled bottles

Data name	Description/Availability/Format
ID	Identifier of the stock/Database/String
Weight	Weight of the stock/Database/Double
Receiving date	Date of reception/Database/Date
Source	Source of the stock/Database/String
Cost	Cost of the stock/Database/String

6.7.3 FA7-3/PET dust

Data name	Description/Availability/Format
ID	Identifier of the stock/Database/String
Weight	Weight of the stock/Database/Double

6.7.4 F1/ Pre-treated Textile

Data name	Description/Availability/Format
ID	Identifier of the stock/Database/String
Weight	Weight of the stock/Database/Double
Receiving date	Data of reception/Database/Date
Source	Source of the stock/Database/String

6.7.5 F2/ Scrap of bottles or PET

Data name	Description/Availability/Format
ID	Identifier of the stock/Database/String
Weight	Weight of the stock/Database/Double
Receiving date	Data of reception/Database/Date
Source	Source of the stock/Database/String
Cost	Cost of the stock, could be negative if is a paid feedstock

6.7.6 F3/ Reactor mixture

Data name	Description/Availability/Format
ID	Identifier of the batch/Database/String
Weight	Weight of the stock/Database/Double
Batch process start time	Start time of batch process/Database/Timestamp
Batch process end time	End time of batch process/Database/Timestamp

6.7.7 F4/ npPTA

Data name	Description/Availability/Format
ID	Identifier of the batch/Database/String
Weight	Weight of the stock/Database/Double
Batch process start time	Start time of batch process/Database/Timestamp
Batch process end time	End time of batch process/Database/Timestamp

6.7.8 F5/ PTA

Data name	Description/Availability/Format
ID	Identifier of the batch/Database/String
Weight	Weight of the stock/Database/Double
Batch process start time	Start time of batch process/Database/Timestamp

Batch process end time	End time of batch process/Database/Timestamp

6.7.9 F6/ PTA Crystals

Data name	Description/Availability/Format
ID	Identifier of the batch/Database/String
Weight	Weight of the stock/Database/Double
Batch process start time	Start time of batch process/Database/Timestamp
Batch process end time	End time of batch process/Database/Timestamp

6.7.10 F7/ Mother Liquor

Data name	Description/Availability/Format
ID	Identifier of the batch/Database/String
Weight	Weight of the batch/Database/Double
Batch process start time	Start time of batch process/Database/Timestamp
Batch process end time	End time of batch process/Database/Timestamp

6.7.11 F8/ MEG

Data name	Description/Availability/Format
ID	Identifier of the batch/Database/String
Weight	Weight of the batch/Database/Double

6.7.12 F9/ MEG

Data name	Description/Availability/Format
ID	Identifier of the batch/Database/String
Weight	Weight of the batch/Database/Double

6.7.13 F10/ Residual

Data name	Description/Availability/Format
ID	Identifier of the batch/Database/String
Weight	Weight of residual/Database/Double

6.7.14 F11/ Scrap

Data name	Description/Availability/Format
ID	Identifier of input batch/Database/String
Weight	Weight of scrap/Database/Double

6.7.15 F12/ Scrap

Data name	Description/Availability/Format
ID	Identifier of input batch/Database/String
Weight	Weight of scrap/Database/Double

6.7.16 FA4-5-FA4-6/Virgin PET

Data name	Description/Availability/Format
ID	Identifier of the batch/Database/String
Weight	Weight of the batch/Database/Double

6.8 Process steps

6.8.1 P1 Textile pre-processing

Textile scrap is treated to remove buttons, metal elements, and other non-textile components. At the end of the pre-processing, stocks are characterized.

6.8.1.1 Involved resources

ID	Resource	Capacity	Task/Use
M00	Operator	TBD	Opens the bags in which waste is contained Characterizes the incoming batch checking its correspondence with the expected lot. Feed the machines that will shred and prepare the waste for depolymerization
M10	Testing lab	TBD	Used during batch characterization

6.8.1.2 Main process control parameters

The table below reports the control parameters that affect the execution of the process tasks.

ID	Parameter	Impact on process
C00	Productivity	It must satisfy the nominal productivity of the depolymerization reactors.

6.8.1.3 Process monitoring

The table below reports the process data which is currently monitored and made available.

Data name	Description/Availability/Format
Batch ID	Id of the incoming feedstock/Database/String
Amount of scraps produced	Scraps produced/Database/Double

6.8.2 P2 Packaging pre-processing

Baled bottles are ground and reduced in shreds. At the end of the pre-processing, batches are characterized.

6.8.2.1 Involved resources

ID	Resource	Capacity	Task/Use
M00	Operator	1	Grinds the incoming batch, characterizes the incoming batch
M10	Testing lab	1	Used during batch characterization

6.8.2.2 Main process control parameters

ID	Parameter	Impact on process
C00	Grinding grain	Grinding grain influences process time

6.8.2.3 Process monitoring

The table below reports the process data which is currently monitored and made available.

Data name	Description/Availability/Format
Batch ID	Id of the incoming feedstock/Database/String
Batch characterization	Structured attributes stored on PTurn platform/Database/TBD
Batch process start time	Start time of feedstock process/Database/Timestamp
Batch process end time	End time of feedstock process/Database/Timestamp

6.8.3 P3 – Depolymerization

Depolymerization is achieved through a microwave-assisted alkaline hydrolysis. It can be then repeated an unlimited number of times, without any degradation or side effects: "erasing" the history of that polymer and of its physical and chemical properties.

6.8.3.1 Involved resources

ID	Resource	Capacity	Task/Use
M00	Main reactor	60 Kg/h	Depolymerization of input batch
M10	Operator	1	Setup recipe parameters Control execution

6.8.3.2 Main process control parameters

ID	Parameter	Impact on process
C00	Temperature	Increases the amount of used energy and reduces the duration of the process
C10	Pressure	Control of reaction processes and efficiency of energy use
C20	Flow rate	Control of the speed of material in and out

6.8.3.3 Process monitoring

The table below reports the process data which is currently monitored and made available.

Data name	Description/Availability/Format
Temperature	Temperature of the reaction/Database/Double
Start time	Start of operation/Database/DateTime
Duration	Duration of the operation/Database/Double
Pressure	Pressure of reactor/Database/Double

6.8.4 P4 – Liquid solid Separation

Separation of Na2TA from the liquid part called Mother Liquor.

6.8.4.1 Involved resources

ID	Resource	Capacity	Task/Use
M00	Decanter	100 kg/h	The decanting unit adopts the centrifugal effect to separate solid components of the reacted mixture from the liquid ones (i.e., Mother Liqueur)
M10	Operator	1	Monitor the correct operation of the machine and intervene in case of malfunctioning.

6.8.4.2 Main process control parameters

ID	Parameter	Impact on process
C00	Temperature	Temperature is optimized compromising between productivity and residual humidity after separation

6.8.4.3 Process monitoring

The table below reports the process data which is currently monitored and made available

Data name	Description/Availability/Format
Batch ID	Identifier of the batch/Database/String
Batch process start time	Start time of batch process/Database/DateTime
Batch process end time	End time of batch process/Database/ DateTime

6.8.5 P5 – Purification

The reaction output is a mixture of building blocks derivatives, which are then isolated and purified.

Involved resources

ID	Resource	Capacity	Task/Use
M00	Na2TA Purification section	65 kg/h	The Na2TA salt produced at depolymerization is progressively purified, leading to a crude TA ready for the lasts step of crystallization.
M10	Operator	1	Monitor the correct operation of the machine and intervene in case of malfunctioning.

6.8.5.1 Main process control parameters

ID	Parameter	Impact on process
C00	Temperature and duration of the thermal treatment	It determines how much the organic contaminants are decomposed by means of thermal decomposition. It must be adapted to the type of feedstock used at depolymerization.
C10	Time passed inside the Activated Carbon	It influences the final quality of the crude TA but is based on a trade-off on productivity and on life expectancy for the AC filters.

6.8.5.2 Process monitoring

The table below reports the process data which is currently monitored and made available.

Data name	Description/Availability/Format
Batch ID	Id of the batch/Database/String
Batch process start time	Start time of batch process/Database/DateTime
Batch process end time	End time of batch process/Database/DateTime

6.8.6 P6 – Crystallization

Crude TA is crystallized in water to achieve the quality required to be defined PTA (Purified Terephthalic Acid)

6.8.6.1 Involved resources

ID	Resource	Capacity	Task/Use
M00	Crystallization reactors	48 kg/h	By a means of a process where the TA is first heated up at very high temperature and pressure, the monomer dissolves in water, releasing into it its residual contaminants. After that, the solution is progressively cooled by means of “flashing” steps, where the PTA crystal are recreated.
M10	Operator	1	Monitor the correct operation of the machine and intervene in case of malfunctioning.

6.8.6.2 Main process control parameters

ID	Parameter	Impact on process
C00	Temperature of the dissolution water	It determines the maximum solubility of the crude TA and, consequently, the maximum productivity of the system.
C10	Concentration of crude TA in water	It influences directly the productivity of the system.

6.8.6.3 Process monitoring

The table below reports the process data which is currently monitored and made available.

Data name	Description/Availability/Format
Batch ID	Identifier of the batch/Database/String
Batch process start time	Start time of batch process/Database/DateTime
Batch process end time	End time of batch process/Database/DateTime

6.8.7 P7 – Distillation

Mother liquor is distilled to separate MEG from water, contaminants and other chemicals.

6.8.7.1 Involved resources

ID	Resource	Capacity	Task/Use
M00	Thin Film Evaporator	20 kg/h	The distillation section of the plant is actually composed of two equipment, the first one being a so-called Thin Film Evaporator, a machine where the ML is boiled, leaving behind salts and non-volatile contaminants. This process happens under vacuum.
M10	Distillation column	20 kg/h	It's the core of the distillation process, under vacuum, where water, MEG and other chemicals are recovered.

6.8.7.2 Main process control parameters

ID	Parameter	Impact on process
C00	Temperature of the distillation column	It impacts the quality of the MEG produced

6.8.7.3 Process monitoring

The table below reports the process data which is currently monitored and made available.

Data name	Description/Availability/Format
Batch ID	Identifier of the batch/Database/String
Batch process start time	Start time of batch process/Database/Timestamp
Batch process end time	End time of batch process/Database/Timestamp

6.9 Objectives and impacts

The following table maps business objectives and technical objectives of the use case, assigning to each objective a priority level ranging from 1 (highest level of priority) to 3 (lowest).

Table 5 Technical objectives

ID	Business Objective	Technical Objective	Priority Level	Description
1	Predictive and prescriptive capabilities	Depolymerization reaction time prediction	2	Currently Gr3n has a rough mathematical model based on theoretical data to predict the reaction time. The objective is to use a more reliable model based on real data, possibly automatically inferred, capable to predict this time.
2		MEG (l/h) and PTA (kg/h) productivity prediction after the depolymerization reaction	2	Gr3n would like to predict how much MEG and PTA can be extracted from the depolymerization of a certain mix of input feedstocks. The uncertainty up to now is related to the fact that not all the feedstocks are characterized in terms of PET content and the amount of contaminants affecting the efficiency of reaction is not completely determined.
3		Polymerization reaction time prediction	3	Currently Gr3n has a rough mathematical model based on theoretical data to predict the reaction time. The objective is to create a more reliable model based on real data, possibly automatically inferred, capable to predict this time.
4		PET (kg/h) productivity prediction after polymerization reaction	1	The objective is being able to predict how much PET can be extracted from the depolymerization of a specific input feedstock mix.
5		Total process yield prediction	1	The objective is being able to predict the percentage of PET that can be actually extracted in relation to the original PET content of the input feedstock. (Assuming input feedstock PET content has been assessed to be 75%, how much PET gets out at the end? The whole 75% or less?)
6	Enable production planning	Feedstock PET content and price threshold definition	2	The objective is being able to decide if according to the current and future cost trends of facilities like energy, it is economically and environmentally sustainable to accept feedstocks with a

				certain percentage of PET content and with a certain price.
7		Optimize temporal sequence of feedstock mix	1	The objective is being able to select the best sequence over time (i.e., schedule) of a given list of feedstocks to minimize specific cost functions and environmental impact. Total cost and CO2 equivalent LCA indicators are function of process parameters and input feedstock mix. Each feedstock is characterized by quantity, price, composition (PET content, type) and possible customer constraints. The requirements are finding the best scheduling of production on a weekly basis, and identifying for each shift the feedstocks that should be used to feed the process and their sequence.
8		Learning and adaptation of DT to represent always the whole physical system	2	The objective is exploiting the huge amount of data collected from the field to learn or adapt automatically generated models of the processes whose precision and reliability are higher than the existing ones.
9	Reduce production costs and environmental impact	Reduce the electric energy needed in the depolymerization process of PET	3	The objective is reducing the amount of energy required in the depolymerization phase of the PET. *Note: The energy cost of depolymerization is very much intrinsic to the process, hence not many degrees of freedom to minimize it*
10		Optimize cooling water (CW) consumption	3	The objective is optimizing the consumption of cooling water. Note: Even if the objective is related to the overall KPIs optimization. Again, not many degrees of freedom to minimize it.
11		Reduce the thermal energy	3	The objective is reducing the amount of thermal energy used for the process. Note: Even if the objective is related to the overall KPIs optimization. Again, not many degrees of freedom to minimize it.
12	Improve human-twin relation	Create tools which can be used by different roles in the company without a	1	The developed modules should be used by plant managers without a deep knowledge on the process but no expertise in the usage of digital twins. The objective is to

		deep knowledge of all the processes		adapt the complexity of the underlying technologies to different types of users (CTO, CEO, CFO, COO, etc.), increasing the level of acceptance of the tools by the final end user.
13	Data exchange	Create the environmental product passport	1	The objective is to create a Product passport capable to trace and certify the environmental impact of produced PET batches relating to the used facilities (energy, etc.) and input feedstock. It is important to provide evidence of the provenance of the input material and of the amount of used facilities to certify that the product is recycled PET extracted from waste and additionally, if required, that the origin material comes from a specific supply chain.
14		Publish product passport through an IDS connector into PET Recycling Data Space	2	The objective is to make the product passport available through standard IDS data connectors that can be leveraged by actors of the textile and packaging value chains.

The following table defines a set of potential developments to reach the technical objectives abovementioned and maps each solution to corresponding Exploitable Results (ER) and project Objectives (OBJ) declared in the proposal and reported in Figure 2.

Table 6 Potential Developments.

ID	Name	Potential Development	AUTO-TWIN	
			OBJ	ER (WP)
D1	Depolymerization reaction time prediction model	Create a model, inferred from real data acquired from the plant to predict the time needed for depolymerization reaction when the reactor is fed with a specific feedstock mix. The model should keep into consideration the characterization of the input feedstocks.	OBJ1	ER1 (WP3)
D2	MEG (l/h) and PTA (kg/h) productivity prediction model	Create a model, inferred from real data acquired from the plant capable to predict the quantities of MEG and PTA that is possible to extract from a specific feedstock.	OBJ1	ER1 (WP3)
D3	Polymerization reaction time prediction model	Create a model, inferred from real data acquired from the plant to predict the time needed for polymerization reaction when the reactor is fed with a specific feedstock mix. The model should keep into consideration the characterization of the input feedstocks.	OBJ1	ER1 (WP3)
D4	PET (kg/h) productivity prediction model	Create a model, inferred from real data acquired from the plant to predict the quantity of PET that can be recovered from a specific feedstock in relation with the initial percentage of PET content.	OBJ1	ER1 (WP3), ER7 (WP4)
D5	Full plant digital twin	Create a digital twin of the plant that is capable to forecast the facilities utilization when the plant is loaded with a specified temporal sequence of feedstock. The model must keep into consideration the characterization of the feedstocks and the historical data to provide a result which is as much as possible near to the real behaviour of the plant. NOTE: the digital twin is not supposed to close the loop automatically on automation, but it is meant to be used by the scheduling optimization module to provide feedback to the plant	OBJ1, OBJ2	ER1 (WP3), ER3 (WP2)

		manager (decision maker) to support its decision making process.		
D6	Scheduling optimization module	Create a module targeted to the plant manager, capable to suggest the best weekly scheduling that minimizes specific cost functions related to facilities usage and environmental indicators. The model must keep into consideration the availability of feedstocks in the inbound warehouse and the forecasting of feedstock arrivals. The module must rely on the digital twin of the plant (R5) to generate its results and must be easily usable by the plant manager.	OBJ2, OBJ3	ER2 (WP2), ER3 (WP2), ER5 (WP3), ER6 (WP3),
D7	Price decision support module	Create a decision support module that enables the plant manager to decide if a feedstock with a certain PET content and price is eligible for recycling. The module should consider the current facilities costs, their trends and the forecasting of the plant behaviour, if a specific feedstock mix is loaded, to provide performance indicators in support of end user decision (both economic and environmental).	OBJ2, OBJ3, OBJ4	ER2 (WP2), ER3 (WP2), ER5 (WP3), ER6 (WP3), ER7 (WP4)
D8	PET batch digital passport	Create a digital passport of the PET batch that provides in a reliable way evidence of the material provenance and its environmental impact. The passport must be fed with data acquired from production and the initial characterization of the feedstock, linking to the information stored on the PTurn platform of Gr3n.	OBJ2	ER2/ER3/ER4 (WP2)
D9	Data Connector	Create or adapt an IDS compliant data connector that is capable to publish information related to PET batches and in particular to their digital passports (R7)	OBJ2	ER2, ER3, ER4 (WP2)

The following table maps the potential developments on the use case technical objectives, providing a view on the level of coverage of the initial requirements.

Table 7 Objectives - Developments map

	Objective	Result								
		D1	D2	D3	D4	D5	D6	D7	D8	D9
1	Depolymerization reaction time prediction	■								
2	MEG (l/h) and PTA (kg/h) productivity prediction after the depolymerization reaction		■							
3	Polymerization reaction time prediction			■						
4	PET (kg/h) productivity prediction after polymerization reaction				■					
5	Total process yield prediction				■	■				
6	Feedstock PET content and price threshold definition	■	■	■	■		■			
7	Optimize temporal sequence of feedstock mix	■	■	■	■	■		■		
8	Learning and adaptation of DT to represent always the whole physical system	■	■	■	■					
9	Reduce the electric energy needed in the depolymerization process of PET	■				■				
10	Optimize cooling water (CW) consumption		■			■				
11	Reduce the thermal energy		■	■		■				
12	Create tools which can be used by different roles in the company without a deep knowledge of all the processes						■	■		
13	Environmental product passport								■	
14	Publish product passport through an IDS connector into PET Recycling Data Space									■

The following table reports a set of measures that have been identified as possible indicators of the impact of applying the AUTO-TWIN results to the use case. This list has been defined with the current knowledge of the objectives and potential developments of the following research activities. Therefore, they will be adjusted during the validation phase. As stated in DoA, the baseline values for the impact measures will be defined in D1.2.

Table 8 Target impact measures

ID	Impact measures	Expected target value	Related user objective
1	**Software development time** Time needed to complete the commissioning of the automation software for a new part of the plant or for a new plant as a whole	Reduce	
2	**Depolymerization time model accuracy** The accuracy of the depolymerization time prediction model generated by the automatic digital twin generation compared to the value generated by the simple material/energy balance model.	+/- 5%	1,7,8
3	**MEG and PTA prediction model accuracy** Accuracy of the prediction model compared to the value generated by the simple material/energy balance model.	+/- 5%	2,7,8
4	**Polymerization time model accuracy** Accuracy of the prediction model compared to the value generated by the simple material/energy balance model.	+/- 5%	3,7,8
5	**PET productivity prediction model accuracy** Accuracy of the prediction model compared to the to the value generated by the simple material/energy balance model.	+/- 5%	4,7,8
6	**CO2 equivalent indicator** Value of CO2 equivalent indicator for a Kg of PET produced for a reference feedstock mix.	-20%	7,13,14
7	**Overall productivity** Productivity of the plant fed with a specific reference set of input feedstocks respect to a reference hand optimized production plan.	+5%	5,6,7

8	**Production plant reconfiguration ease** This will be assessed in terms of how much time is required to develop a production recipe for a new feedstock incoming to the plant	-30%	7,8
9	**Electricity consumption forecasting model accuracy** Range of credibility of the forecasting is improved with respect to correct off-line modelling. Indicator is the reduction of the overall range	-50%	6,7,8,9
10	**Thermal energy forecasting model accuracy** Range of credibility of the forecasting is improved with respect to correct off-line modelling. Indicator is the reduction of the overall range	-50%	11

6.10 Decisions

This section describes the decisions of the use-case. The description applies both to packaging (*i.e.,* PET dust and baled bottles) and to feedstock (i.e. textile mix) plants. Packaging and feedstock are not mixed on the same plant and reconfiguration PET from/to feedstock is not considered.

1. Decide on the production process operative management. The set of decisions includes: the selection of which mix/product variant to be produced at a given time depending on system state (*e.g.,* inventory levels, current production), and the management of pre-processing activities and the intermediate storages/inventories feeding the depolymerization process. Particular attention should be devoted to reconfigurations (changes of mix/variant) to maintain the thermo-chemical process equilibrium point which might change varying the product mix/variant; thus, reconfigurations should assure a smooth transition. Advanced control of the flow rate and process parameters (temperature, etc) is also included.
    a. Actor(s): Production Department
    b. Challenge(s): -
    c. Time Horizon/Frequency: Week / Daily
2. Decide on the inventory management. The set of decisions includes the management of feedstock and packaging inventories between the pre-processing processes and the depolymerization process. Also, the decision includes that a certain product is allocated to a certain storage, and the replenishment rule. Stockout must be avoided to maintain the continuous process.
    a. Actor(s): Technical leader / Purchasing Department
    b. Constraint(s): space availability, limited number of storages (silos), quality levels should be not mixed (preferably), …
    c. Time Horizon/Frequency: Week / Daily
3. Decide on the management of utilities. The set of decisions includes utilities (e.g., electricity, steam, cooling water and N2) management to assure production with potential increases of efficiency / reduction of costs. The systems providing utilities are often highly consuming; therefore, energy efficient strategies are included in the set of decisions (e.g., flow rate management, off/on policies, parameters optimization, load balance).

a. Actor(s): Production department

b. Constraint(s): -

c. Time Horizon/Frequency: Day / Continuous

4. Decide on the energy storage (chemical energy storage). The set of decisions includes the management of the hydrolysis process according to the production schedule. The hydrolysis enables the reintegration of necessary chemicals for the reaction and, being exothermic, releases energy. Stockout of chemicals must be avoided to maintain the continuous process.

   a. Actor(s): Production manager

   b. Constraint(s): Space availability, availability of chemicals for the reaction must be guaranteed.

   c. Time Horizon/Frequency: continuously

6.11 KPIs

This section describes the key performance indicators that the company is interested in. The following list focuses on KPIs related with external KPIs:

- Efficiency indicators. Relative values with respect to the output kg of PET (for global system performances). Relative values respect to the output (locally), technical efficiency.
- Processing time. Time required to perform a certain process, *e.g.,* depolymerization

The following list focuses on internal KPIs:

- Deviation from equilibrium point / number of reconfigurations. Transition from-to a *thermo-chemical equilibrium point* may cause lack of efficiency and are hard to be managed. The aim is to *limit* as much as possible the reconfigurations.
- Utility consumption. The company manages its production (or gets under control the deviations from the production target level) by adjusting some process specifications such as temperature. Utility costs play an important role in increasing the company's efficiency in terms of profitability because this is the main expense for their production process. This metric represents the amount of electrical energy (or natural gas) that has been consumed over a specific time, in units of kWh (or MCM). It consists of electricity (average power kWh/h), thermal energy (MJ/h), N2 consumption (flow kg/h), and cooling water (average power of the auxiliary system and flows) consumption.
- Materials. Chemical processes are evaluated in terms of material consumption input/output. In details: as input are included the feedstock (quality: percentage of the PET and contaminations), MEG, NaOH (sodium hydroxide) constrained by a specific known receipt; as output are included the reactive mix and PET crystals.
- LCC indicators: including CO2-eq emissions of the process, utilities, efficiency etc.
- Accuracy. The accuracy of predicted value is an important KPI for the company. This metric *evaluates* the difference among any estimated value and the actual value obtained from the real system, e.g., system efficiency, utilities usage, efficiency indicators, etc.

6.12 Notes on as-is process

This section provides notes about the current As-Is state of the use-case.

GR3N is currently in the installation phase of the demo-plant; therefore, the operative management of the plant is not yet implemented. GR3N will deal with the daily operation of the demo-plant in the future. Nevertheless, the every-day management of industrial plants will be left to GR3N's customers.

Currently, GR3N determines its sales price with a practical rule, i.e., the company determines its own sales price based on the reference price being appeared in the market. Using a dynamic pricing strategy, which depends on its inventory level and customer type, might help the company to manage its stocks more efficiently, increase its revenue, and cut down some stock-related costs. Additionally, the company uses a simple policy to decide whether to accept returning items. Specifically, the company accepts a returning item when the percentage of PET in the item is larger than the company's minimum target level. The reasoning behind this policy is that the plant performance is directly affected by the percentage of PET in returning items in terms of cost and time (transition time to a new equilibrium). The target value that the company uses has been set based on their past experience. However, it can be set according to multiple criteria and some multi-objective optimization techniques can be used to this end. Examples may include acceptance/rejection decisions related to prices/contracts with a specific customer, similarly work/discard decisions upon accepted materials.

GR3N is interested in providing services related to the operative management to the plant and to technical optimization of the processes.

All decisions are intended to be taken by the production manager and / or plant manager.

7 Libattion use case

7.1 Nomenclature and glossary

Cell	Single unit of device that converts chemical energy into electrical energy, in this use case we are considering Li-ion cells
Battery	Collection of cells connected to reach desired voltage and capacity
BMS	Battery management system, electronic equipment which keeps charge balanced between different cells that are wired in parallel
Bus bar	Metal strip or bar which connects all the strips in a battery and conveys power to the battery terminals

7.2 Value chain analysis

Libattion is a Swiss-based company that manufactures battery solutions for different sectors. It is focused on integrating innovative cutting-edge battery technologies into industrial vehicles, electro mobility and stationary systems. At the beginning of the AUTO-TWIN project, one of their most mature products has been chosen as a use case, the E-Brick. The E-Brick is a modular Li-ion rechargeable battery system used for light electrical vehicles or home appliances, built with up-cycled 18650 Li-ion battery cells, meaning that the battery is built using cells recovered from used batteries. During the execution of the project Libattion will analyze the integration of the AUTO-TWIN solutions for further products like the stationary energy storage system.

An IoT device which measures data about the life of the battery is installed in the E-Brick, and allows to download data which will be used to create a digital twin of the product. This digital twin will b store information about the lifecycle of the product and will support the management of the product.

The current production for the E-Brick is currently in a manual prototypal phase, so there isn't much information about process data, but an industrial grade production line is now under design and should be ready in M12 of the project, Figure 7 illustrates the value chain for the E-Brick production line that will be built.

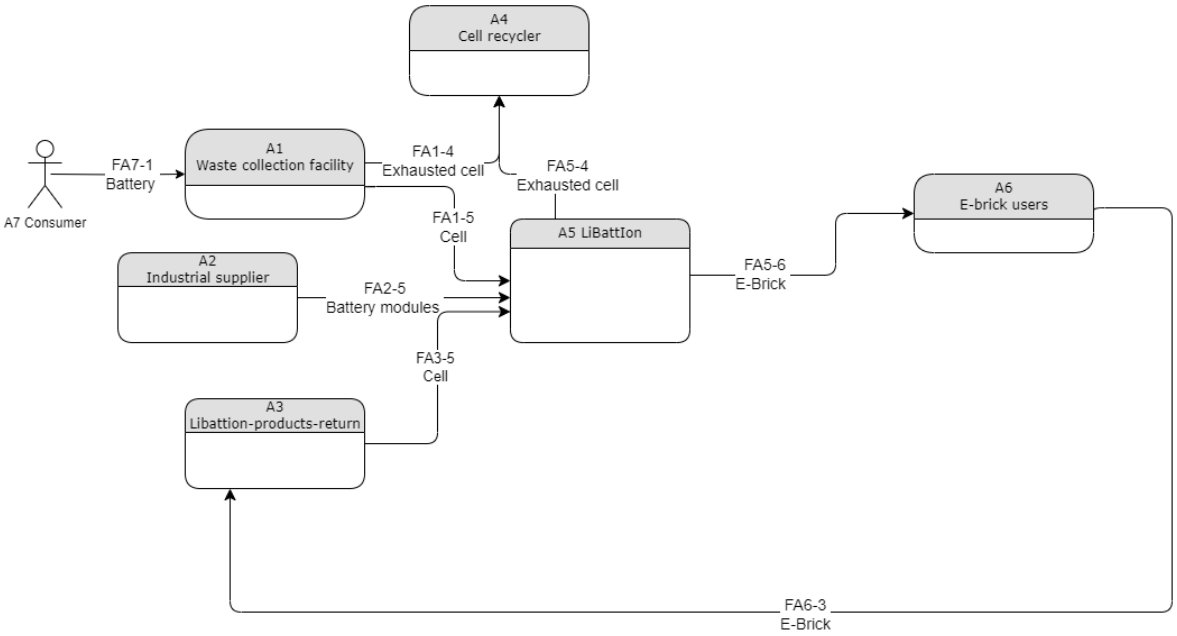

Figure 7 Libattion value chain schema

Libattion facility is indicated as actor A5 in the value chain, the inputs are cells coming from battery recovery facilities and from used batteries coming from industrial suppliers.

ID	Actor Name	Description
A1	Waste collection facility	Recycle waste collection facility
A2	Industrial supplier	Industrial supplier of used battery modules
A3	Libattion-products-return	Libattion E-Brick recollection point
A4	Cell recycler	Cell recycling facility where cells are disposed, and raw materials recovered
A5	Libattion	Libattion facility
A6	E-Brick users	Light electric vehicle (forklift, golf cart) manufacturers, portable energy storage manufacturers, etc.
A7	Consumer	Consumer market for batteries

7.3 Value chain flows

ID	Flow Name	Description	Entity	Trace
FA7-1	Batteries from consumer market	Batteries from consumer market are collected and disassembled in waste collection facility	Battery	NO
FA1-4	Exhausted cell	Faulty or damaged cells are sent to battery (or cell) recycler	Cell	NO
FA1-5	Cell	Not damaged cells are sent to Libattion	Cell	YES*
FA2-5	Battery modules	Batteries modules collected and tested by external suppliers	Battery module	NO
FA5-6	E-Brick	Small modular transportable storage module, available in different voltages	Battery	YES
F6-3	E-Brick	E-Bricks are collected from authorized recovery facilities	Battery	YES
FA3-5	Cell	Cells recovered from E-Brick	Cell	YES*
FA5-4	Exhausted cell	Exhausted cells in Libattion are sent to the battery (or cell) recycler	Cell	NO

7.4 Value chain entity data

Each paragraph of this chapter reports the data related to a certain entity flowing in the value chain (mandatory for entities marked with trace=Yes in the flows table). The objective is capturing the information that could be useful for:

1. Tracking of the entity in the value chain and automated process-aware discovery towards autonomous digital twin generation
2. Association of the digital passport to the entity

7.4.1 FA1-5/ Cell

** There are still doubts at which extent data about cells will be collected when outsourcing activities to third parties*

Data name	Description/Availability/Format
Cell producer	Producer of the cell/Test document/String
Cell capacity class	Capacity of the cell/ERP/ String Enumeration (Red, Yellow, Orange, Green)
Test date	Date of test execution/ERP/Date

7.4.2 FA5-6/ E-Brick

Data name	Description/Availability/Format
E-Brick ID	Identifier of the E-Brick/ERP/String
Lifecycle data	Charging cycles and cell balancing/IoT device/Table

7.4.3 FA6-3/ E-Brick

Description/Availability/Format	Description/Availability/Format
E-Brick ID	Identifier of the E-Brick/ERP/String

7.4.4 FA3-5/ Cell

** There are still doubts at which extent data about cells will be collected when outsourcing activities to third parties*

Data name	Description/Availability/Format
Cell producer	Producer of the cell/Test document/String
Cell capacity class	Capacity of the cell/ERP/ String Enumeration (Red, Yellow, Orange, Green)
Test date	Date of test execution/ERP/Date

7.5 Process analysis

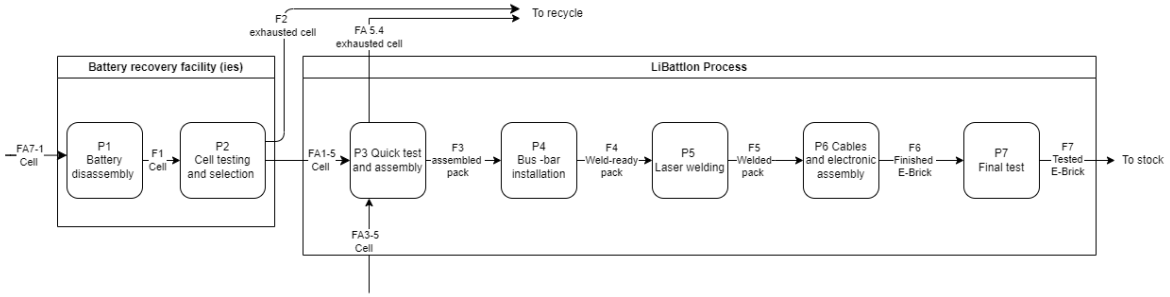

Figure 8 Libattion process overview

7.6 Process steps

ID	Process name	Description
P1	Battery disassembly	Batteries are disassembled and cells are removed
P2	Cell testing and selection	Cells are tested at the battery recovery facility and classified by producer and capacity; operation is included in the process diagram since the operation is performed by Libattion staff
P3	Quick test and assembly	Cells are picked up and tested by a robot, then inserted into battery holding rack
P4	Bus-bar placement	Place the bus bar with cells together
P5	Laser welding	Cells are welded to bus bar
P6	Cables and electronic assembly	Cables and electronic are added
P7	Final test	Charge and discharge tests

7.7 Process flows

ID	Flow Name	Description	Entity	Trace
FA7-1	Battery	Used battery from waste collection	Battery	NO
F1	Cell	Untested cell	Cell	NO
FA1-5	Cell	Tested and usable battery cell	Cell	YES*
FA3-5	Cell	Tested and usable battery cell from Libattion used products	Cell	YES*
F2	Exhausted cell	Exhausted Li-ion cells sent to recycling	Cell	NO
F3	Assembled pack	Pack of cells assembled with bus bar installed	Pack	YES

F4	Weld-ready pack	Pack closed, with bus bars in place and inserted into a jig ready to be welded	Pack	YES
F5	Welded pack	Pack with cells welded to contacts	Pack	YES
F6	Finished E-Brick	Libattion main product, a Li-ion battery	E-Brick	YES
F7	Tested E-Brick	Tested final product	E-Brick	YES
FA 5-4	Exhausted cell	Exhausted Li-ion cells discarded after internal test are sent to recycling	Cell	NO

7.8 Process steps

7.8.1 P1 – Cell disassembly

Batteries are disassembled to remove cells, this process is not managed by Libattion so there is no traceable information.

7.8.2 P2 – Cell testing and selection

Operator picks up a cell, inserts the cells into the testing machine and starts the test machine, the tests are conducted in batches. The results of the test are saved in a database. Then the operator puts the cell in different racks depending on the producer and capacity of the cell.

Currently the process in the pilot plant is conducted by Libattion staff, but in future plans it will probably be outsourced to battery recovery facilities. There are still doubts if and how traceability for single cells will be feasible in this new configuration.

Cells are classified according to their producer and then divided into 4 classes; *RED: 3150-3200 mAh, YELLOW: 3200-3250 mAh, ORANGE : 3250-3300 mAh, GREEN 3300-3450 mAh.*

Shipments of cells from disassembly point currently don't have a fixed frequency but are on average 4000 cells/week, the objective is to reach 40000 cells/week

7.8.2.1 Involved resources

ID	Resource	Capacity	Task/Use
M00	Operator	1 operator	Operator takes cell and puts the cell into the machine. When the machine is full, the operator runs the test.
M10	Testing machine	500 cells	Test equipment used to classify cells

7.8.2.2 Main process control parameters

The table below reports the control parameters that affect the execution of the process tasks.

ID	Parameter	Impact on process
C00	Process duration (7h)	Time required to test all the batteries

7.8.2.3 Process monitoring

The table below reports the process data which is currently monitored and made available.

Data name	Description/Availability/Format
Cell producer	Producer of the cell/Test document/String
Cell capacity class	Capacity of the cell/ERP/String enumeration (Red, Yellow, Orange, Green)
Test date	Date of test execution/ERP/Date

7.8.3 P3 – Quick test and assembly

The operator puts an empty battery holder in the robot working area, configures the robot for the appropriate topology and start the process. The topology of the battery specifies the quality of cell for each position in the schema, if a cell of the needed quality level is not available in the stock, a higher quality cell is chosen. The robot starts picking a battery for the first position in the rack, performs a quick voltage test and, if the test fails discards it, otherwise the cell is put into the position required by the battery design schema.

7.8.3.1 Involved resources

ID	Resource	Capacity	Task/Use
M00	Operator	1	Operator loads and unloads the robot
M10	Robot	1	Robot used to test and insert cells into the battery holder

7.8.3.2 Main process control parameters

ID	Parameter	Impact on process

7.8.3.3 Process monitoring

The table below reports the process data which is currently monitored and made available.

Data name	Description/Availability/Format
Battery test result	Result of test/ERP/Boolean
Battery quality	For each position in the matrix, quality of the placed cell/ERP/ String enumeration (Red, Yellow, Orange, Green)
Operation time	Time of operation/ERP/Double

7.8.4 P4 – Bus bar application

The operator moves the battery holder out of the robot working area, applies the upper cover of the rack, then inserts the rack into the welding jig and places the bus bars, the operator closes the welding jig.

The assembled module is moved to welding station by the operator.

7.8.4.1 Involved resources

ID	Resource	Capacity	Task/Use
M00	Operator	1	Operator performs the operation
M10	Welding jig	NA	Jig applied to the pack keeping all components in place for the next welding operation

7.8.4.2 Main process control parameters

ID	Parameter	Impact on process
C00	E-Brick voltage	Voltage of the produced E-Brick, it influences the bus bar topology and electronic placement

7.8.4.3 Process monitoring

The table below reports the process data which is currently monitored and made available.

Data name	Description/Availability/Format
Operator id	Id of the operator/ERP/String
Operation time	Time of operation/ERP/Double

7.8.5 P5 – Laser welding

Operator places the welding jig on to the welding machine, selects the welding program, then starts the welding process. The operator unloads the welding machine and moves the welded module to the next station.

7.8.5.1 Involved resources

Resource	Capacity	Task/Use
Operator	1	Operator loading and unloading the machine
Laser welding machine	1	Automatic laser welding machine

7.8.5.2 Main process control parameters

Parameter	Impact on process
Welding program	Welding programs depends on the E-Brick voltage (different series-parallel connections)

7.8.5.3 Process monitoring

The table below reports the process data which is currently monitored and made available.

Data name	Description/Availability/Format
Product ID	E-Brick ID/ERP/String
Quality check results	Quality check results for the welding operation/ERP/String enumeration (success, fail)
Operation time	Time of operation/ERP/Double

7.8.6 P6 – Cables and electronic assembly

Cables and electronics are installed by an operator, assembly is inserted into the external case and the case is closed.

7.8.6.1 Involved resources

Resource	Capacity	Task/Use
Operator	1	Operator assembles the final product

7.8.6.2 Main process control parameters

Parameter	Impact on process

7.8.6.3 Process monitoring

The table below reports the process data which is currently monitored and made available.

Data name	Description/Availability/Format
Product ID	Id of the E-Brick/ERP/String
Operation time	Time of operation/ERP/Double

7.8.7 P7 – Final test

The E-Brick is tested through a 7-hour charge-discharge test.

7.8.7.1 Involved resources

Resource	Capacity	Task/Use
Testing machine	12	Machine used to test the complete e-brick

7.8.7.2 Main process control parameters

Parameter	Impact on process

7.8.7.3 Process monitoring

The table below reports the process data which is currently monitored and made available.

Data name	Description/Availability/Format
Product ID	Id of the E-Brick/ERP/String
Voltage	Voltage of the E-Brick/BMS/Double
Cell balancing	Voltage balance between cells/BMS/List<Double>

7.8.8 P7 – E-Brick check

Returning E-Brick is checked, data are downloaded from the cloud portal.

7.8.8.1 Involved resources

Resource	Capacity	Task/Use
Operator	1	Operators tests the incoming e-brick

7.8.8.2 Main process control parameters

Parameter	Impact on process

7.8.8.3 Process monitoring

The table below reports the process data which is currently monitored and made available.

Data name	Description/Availability/Format
Product ID	Id of the E-Brick/ERP/String

7.9 Objectives and impacts

The following table maps business objectives and technical objectives of the use case, assigning to each objective a priority level ranging from 1 (highest level of priority) to 3 (lowest).

Table 9 Libattion technical objectives

ID	Business Objective	Technical Objective	Priority Level	Description
1	Predictive and prescriptive capabilities	Predict battery health status	2	Now, the prediction of the remaining life of a battery and the current health of a battery is done by a standard formula and Libattion currently has no access or control over this formula since it is provided by a 3rd party, that does not take in account the actual usage pattern and composition of the battery into account. The objective is improving the prediction model considering also the usage pattern, intensity and the composition of the pack to make a more accurate assessment of the health status and the remaining useful life of the battery.
2		Trace batteries and cells through their complete lifecycle	3	The objective is being able to trace the cells of a battery during operation, including the cells that return to Libattion because they are reused or should go to recycling. The feasibility of tracing single cells is still under investigation.
3		Predictive maintenance for battery warnings/errors and replacements	2	The objective is to detect forthcoming failures before they appear to apply proper remedy actions and inform the battery customer service.
4	Enable production planning	Trace Data from Production Into E-Brick and the Battery management platform	2	The objective is to introduce further tests during the last step of the production of the batteries and fully trace results to identify the actual performance of the battery when it leaves the factory.
5		Prediction of arrival rates of used batteries coming back to the plant and inventory levels	3	The objective is to receive data in advance from centres in which batteries are disassembled and cells tested. The feasibility of tracing single cells is still under investigation and this objective could be removed.
6	Reduce service costs and environmental impact	Avoid testing used batteries coming back to the plant	3	The objective is to collect all the usage information to avoid executing performance tests on the incoming batteries and to improve the decision

				making about the actual health status of the cells.
7	Improve human-twin relation	Visualize battery usage, battery status and create a graphical user interface for battery management	1	The objective is providing the end user with an automatically generated visual overview of the status of his batteries, their current capacity and additional information like warnings and maintenance cycles.
8		Implement a battery management and visualization tool to automatically analyse performance	2	The objective is providing the end user of the battery with suggestions on how he can optimize the use and settings of the battery according to his needs (max performance, max lifetime, etc.)
9	Data exchange	Record cells and battery pack data into the ERP	3	The objective is automatizing the procedure to associate the output of the machine which measures the capacity of the battery with the serial number of the cells. Currently, this is a time-consuming manual task.
10		Exchange data with the battery management platform (Brick tracker)	2	The objective is publishing the measurements made on the cells onto the battery management platform. In this way, the measure data should be uploaded through the cloud to the battery management software.

The following table defines a set of potential developments to reach the technical objectives abovementioned and maps each solution to corresponding Exploitable Results (ER) and project Objectives (OBJ) declared in the proposal and reported in Figure 2.

Table 10 Potential Developments.

ID	Name	Potential Development	AUTO-TWIN	
			OBJ	ER (WP)
D1	Battery health status prediction module	Create a module that implements a battery health status prediction algorithm based on the acquired usage data. The algorithm should be able to predict the trend of the battery performance and possible forthcoming failures and should be integrated into the existing Libattion platform.	OBJ1, OBJ3, OBJ4	ER1 (WP3), ER5 (WP4), ER7(WP4)
D2	E-Brick monitoring module	Install an improved IoT device on each E-Brick to collect all the operation parameters of the battery cells and to store them on a dedicated cloud system, making them available to the battery digital twin.	OBJ1	ER1 (WP3)

D3	Data Connector	Create or adapt IDS compliant data connector that allows the connection to external measuring systems located in other actors of the value chain to share (cell?) battery pack data acquired outside Libattion facilities	OBJ2	ER2, ER3, ER4 (WP2)
D4	Final station enhancement	Modify the final station of the process to automate the acquisition of data from testing procedure of the whole battery and assess its initial status updating the battery digital twin.	OBJ1	ER1 (WP3)
D5	Battery digital twin	Implement a digital twin of the battery that stores historical status data (like measures, feedback, etc.) and manages the execution of prediction algorithms. The digital twin, integrated into Libattion platform, must provide feedback to the end user through a dedicated GUI (about status, warnings, etc..) and to the the onboard battery management software.	OBJ1, OBJ2, OBJ3	ER1 (WP3), ER2/ER3/ER4 (WP2), ER5 (WP4)
D6	Battery optimal operation module	Create a module that, based on the acquired historical data of the specific E-Brick applies algorithms that suggest optimized usage procedures (and maybe explains why the usage made by the end user caused problems)	OBJ2, OBJ4	ER4 (WP2), ER7 (WP4)
D7	Capacity test automation	Create a software connection module (possibly using also dedicated hardware) capable to collect the capacity measures from the machine and upload them on the ERP, associating the read values to the cell serial numbers.	OBJ4	ER7 (WP4)

The following table maps the potential developments on the use case technical objectives, providing a view on the level of coverage of the initial requirements.

Table 11 Objectives - Developments map

	Objective	Result						
		D1	D2	D3	D4	D5	D6	D7
1	Predict battery status	■				■		
2	Trace Batteries and cells trough their complete live cycle		■					■
3	Predictive maintenance for battery warnings/errors and replacements					■	■	
4	Trace Data from Production Into E-Brick and the Battery management platform		■		■			■
5	Prediction of arrival rates of used batteries coming back to the plant and inventory levels	■				■		
6	Avoid testing used batteries coming back to the plant					■		
7	Visualize battery usage, battery status and create a graphical user Interface for battery management					■		
8	Implement a battery management and visualization tool to automatically analyse performance					■		
9	Record cells data into the ERP		■		■			■
10	Exchange Data with the Battery management platform (Brick tracker)			■				■

The following table reports a set of measures that have been identified as possible indicators of the impact of applying the AUTO-TWIN results to the use case. This list has been defined with the current knowledge of the objectives and expected results of the following research activities. Therefore, they will be adjusted during the validation phase. As stated in DoA, the baseline values for the impact measures will be defined in D1.2.

Table 11 Target impact measures

ID	Impact measures	Expected target value	Related user objective
1	**Battery life duration** Life duration due to determination of real state-of-health value	+10%	3,7
2	**Service costs saving** Saving on additional costs for testing	100 EUR/Battery	3
3	**Battery replacement cost** Cost related to unexpected battery replacement	-10%	
4	**Planning flexibility** Planning flexibility	Increase (+25%)	5
5	**Quality control system availability** Data availability provides access to a quality control system	Existing	

7.10 Decisions

This section describes the decisions indicators that are most common in literature and that can be of possible interest for the use-case.

1. Decide on the production process operative management. The set of decisions includes: the selection of which product of those in the queue to be processed at a given time depending on system state, the disassembly/assembly decision related to a certain product, and the decision of assembly different quality cells in the same product so that the quality of finished product is affected.
    a. *Actor(s):* technical director
    b. *Challenge(s):* uncertain estimation of state of health (SOH) and remaining useful life (RUL)
    c. *Time Horizon/Frequency:* Day / Daily
2. Decide on whether to refurbish or recycle incoming products. Collected cells and e-Bricks are tested and each must pass a quality check resulting in an estimation of SOH and RUL. As a consequence, the decision whether to recycle or to process the products is made. Also, an e-brick might be completely remanufactured or refurbished in one of its parts.
    a. *Actor(s):* technical director

b. *Challenge(s):* hidden correlation between the decision and product quality

c. *Time Horizon/Frequency:* at occurrence

3. Decide on sales prices of refurbished and brand-new batteries based on the on-hand stocks. This is also known as dynamic pricing. It is typically based on the changes in real-time product supply and demand, and one of its main advantages is to enable levering demand and managing on-hand stocks efficiently.

    a. *Actor(s): technical director*

    b. *Challenge(s): The frequency of price changes is an important criterion to be considered. When implementing a dynamic pricing policy, possible intangible negative impacts (e.g. burden costs of making frequent price changes, lack of experience in its implementation), and possible adverse customer reactions should be taken into consideration.*

    c. *Time Horizon/Frequency: Instantaneous.*

4. Decide on the collection and management of a certain product according to quality level, i.e., SOH (state of health). The decision is related to the on-line tracking of product quality (digital twin of the product) so that collection and maintenance services might be offered.

    a. *Actor(s): technical director*

    b. *Challenge(s): It might be costly to establish such an online tracking system. It may require a feasibility analysis.*

    c. *Time Horizon/Frequency: Daily/Weekly*

7.11 KPIs

This section describes the key performance indicators that are most common in literature and that can be related to the use-case.

The following list focuses on KPIs related with external KPIs, mostly related to the service level:

- Satisfaction rate of customers purchasing refurbished batteries
- Fill rate. Meeting customer demand on time. This metric shows the fraction of customer demand that is met through immediate stock availability, without backorders or lost sales.
- Stockout. Lack of availability of a certain product variant in the inventory upon request.
- Return rate of used batteries. The return rate of a certain product variant might be related to the state of health of products and to their aging behavior.

The following list focuses on internal KPIs as related to plant performance:

- Accuracy of estimations related to remaining lifetime of batteries
- Inventory-based KPIs such as Turnover Rate, Average Inventory, and so on. The inventory turnover rate is the number of times a company sells and replaces its stock in a period, usually one year. Average inventory is the amount of inventory a company has on hand during a particular time period. Average inventory is the amount of inventory a company has on hand during a particular time period. It can be calculated and kept track for returned stocks, work-in-process, and finished goods.
- Operational expenditures (Transferring, Handling & Collecting, Quality Check, etc.)

Production amount of brand-new batteries

8 Summary of use-case features

The following table summarize key features representing the flows and the processes of the three use-cases and it is aimed to be used for a simple and immediate description of use-case system complexity from a modelling point-of-view.

Table 12 Use-case features summary table (Note: * LIB is in the startup phase of activities)

Provider	**Croma (CRO)**		**GR3N (GRN)**	**Libattion (LIB) ***	
System Category	Discrete		Continuous	Discrete	
Flows of auxiliary materials and utilities	Not significant		Multiple flows of chemicals and auxiliary materials	Not significant	
Number of Variants	10 - 100		around 10	2 families, variants to be defined	
How many variants are simultaneously in the system?	Multiple at stages		Single at stages Multiple in system	Multiple at stages	
Priority Rules at Processes	Best practices, Priorities due-date dependent and variant dependent		Schedule	FCFS	
Stages	7		[5 - 8]	[5-7]	
Stage Buffers	Yes		Not applicable	Yes	
Parallel resources at a single stage	Yes		No	No	
Area-based WIP Limit	No		Not applicable	No	
Processing Mode	Automatic	Manual	Automatic	Automatic	Manual
Processing Time	Deterministic	Stochastic	Deterministic	Deterministic	Stochastic
	Independent	Variant-dependent	Independent	Variant-dependent	Variant-dependent
In-Out Patterns	One-to-One	One-to-One	One-to-One, One-to-Many, Many-to-One, Many to Many	One-to-One	One-to-One, One-to-Many, Many-to-One

Substructures	Serial + Parallel	Serial + Parallel (possibly cyclic after quality check)	Industrial plant: serial Demo plant: serial + cycle for purification Chemicals: cycling	Serial	Serial + Parallel (possibly cyclic after quality check)
Load/Unload + machine setup mode	Manual		Automatic	Manual	
Changeover (change of product variant)	Not significant		Significant	Not significant	
Transfer Time	Deterministic		Deterministic	Deterministic	
Handling mode	Manual		Not applicable	Manual	

9 References

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