Platform release for testing via demo cases

Authors

Lead: Ansys
Collaborators: RISE, VTT, FhG-ISC, WALKI, Gnanomat, CIDETEC, Skeleton, Polymaris, CEA, FhG-ICT, IWNiRZ, IPC, AITIIP, Arjowiggins

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Technical References

Project Acronym	INN-PRESSME
Project Title	open INNovation ecosystem for sustainable Plant-based nano-enabled biomateRials deploymEnt for packaging, tranSport and conSuMEr goods
Project Coordinator	Ulla Forsström VTT Technical Research Centre of Finland Ltd
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[1] PU = Public
PP = Restricted to other programme participants (including the Commission Services)
RE = Restricted to a group specified by the consortium (including the Commission Services)
CO = Confidential, only for members of the consortium (including the Commission Services)

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Document history

V	Date	Beneficiary	Author
V0.1	2021-11-05: WP2/3 Update of Materials & Process Attributes – review meeting with TC's, 1,3,4,5,6,8 to expand harmonization of attributes across all TC's; presentation of process parameter optimisation opportunity using machine learning and Ansys Granta platform	Ansys	Donna Dykeman
V0.2	2021-12-02: WP2/3 Materials Information Management – Progress Update – review of progress with same stakeholders at 2021-11-05 meeting	Ansys	Donna Dykeman
V0.3	2022-01 to 2021-05: Various meetings with TC leads to harmonize attributes, understand TC progress, and development/delivery of Excel record structure to individual Pilot Lines, and to focus on implementation of management system with 3 forerunner TCs (1, 5, 9) as recommended by the coordinator and partners	Ansys	Donna Dykeman
V0.4	2022-05 to 2022-06: Refinement of schema and implementation in Granta MI	Ansys	Donna Dykeman
V1.0	2022-06-06: Deliverable draft shared with consortium members for review	Ansys	Donna Dykeman
V1.1	2022-07-01: Reviewed the final corrections approved	VTT	Ulla Forsström

Summary

This delivery outlines the purpose of implementing a materials information management system in the INNPRESSME project for the purpose of curating a Product+ reference database and ensuring quality assurance for results from partners to SEP clients. The deliverable presents a high-level strategy and timeline for implementation and will require the support of Pilot Line partners to achieve. A solution diagram is proposed, Personas, Use Cases and User Stories, which will continue to be consolidated throughout the project.

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1 Introduction

One of the challenges the INNPRESSME project aims to overcome is that nano-enabled, bio-based material selection in the design processes of manufacturing organizations is not well established, as indicative of the lack of commercialized products. As such, employing materials and processing information management best practices as established by Ansys (formerly Granta Design Ltd.) can support the upscaling of the Pilot Line products towards their commercialisation goals by digitalization of their structure, processes, properties and performance (SPPP).

The remainder of this section outlines the progress against Task 2.2, Subtask 2.2.2 for implementation of the materials and process information management system, Granta MI, with the collaboration of project partners.

Granta MI is an enterprise level materials and information management adopted by industry for in-house management needs and connection to design and simulation environments, and also readily used to support collaborative projects to promote FAIR data principles and business models after the project.

1.1 Task Description

The aim of this deliverable is to outline the implementation strategy for the materials and process information management needed to support the activities of the INNPRESSME project and future SEP, and to direct partners on materials information management best practices.

The main objectives were as follows:

- Define the products of the project for which materials and process records can be curated for selection.
- Understand how nano-enabled, bio-based materials and processes can be presented digitally for selection in early-to-detailed design phases.
- Capture partner requirements for records curation for the remainder of the project to support partner exploitation as a SEP business.

The outcomes are listed here, and it is noted whether or not they are publicly disclosed at this time. Since this project is an Innovation Action and the SEP intends to exploit project results, not all industrial R&D will be disclosed publicly in this deliverable:

- List of project products as defined by the Test Cases and Pilot Lines (shared publicly)
- Records for products agreed with partners to inform selection (not shared publicly)
- Detailed schema designed and implemented to capture materials, processes, characterisation pedigree and results with data/information samples provided by partners (not shared publicly)
- Configuration of a web-based interface for OITB use cases for selection and partner collaboration on data/information curation, including Access Rights, importers, etc. (some details shared publicly)

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1.2 Task Scope

For implementation of the materials and process information management system, Granta MI, the following objectives were met:

1. **Configuration** of Granta MI and adaptation of technology to support specific domain knowledge for nano-enabled, bio-based materials:
    - Schema for standard records for materials/process/characterization pedigree and results
    - Data exchange formats and workflows
    - Analysis workflows
    - Data quality assurance
    - User Access Rights
2. **Interoperability** with evolving initiatives (EMMC/EMCC NBMP project infrastructure):
    - EMMC ontology, notably for characterisation of the lower length scales
    - CHADA if there are novel characterisation methods identified which can benefit from this approach
3. **Searchability** for reference data for use cases for the use of M&P data/information in design and decision-making for products
    - Compatibility with FAIR data management principles fulfilled by metadata where appropriate of characterisation methods, batch information

1.3 Project Scope

To address both the Task Scope and the INNPRESSME Project Scope, we began by assessing the Test Cases and their viable M&P products which can fit into the concept of searchable records for selection in design processes. Table 1 reports the potential material products of the INNPRESSME project, each line representing a unique product. There are roughly 30 products identified to-date, applied in ~60 Pilot Line stages across the 9 Test Cases (i.e. some are used as intermediary constitutions in the construction of a composite or final part such as an electrode).

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Table 1: Material products across all Test Cases

TC	PL	Partner	Material - Form (Descriptors)	Generic Form
3, 5, 8	16	AITIIP	3D Printed Products	3D Print, Bulk Material
3, 4, 9	3	Polymaris	Polyhydroxyalcanoates (PHA) - Resin (Base Matrix)	Bulk Material
5	Commercial	CEA	Bio-based Polyamide (PA) - Resin (Base Matrix)	Bulk Material
2	7	VTT	Poly Lactic Acid (PLA)-X or PLAX - Resin (Base Matrix), bio-plastic dispersion (nano-enabled)	Bulk Material
8	Commercial	AITIIP	Bio-based Polyurethane (B-PU) - Resin (Base Matrix)	Bulk Material
8	Commercial	AITIIP	Bio-based Polypropylene (B-PP) - Resin (Base Matrix)	Bulk Material
8	Commercial	AITIIP	Bio-based Ethylene-vinyl acetate (B-EVA) - Resin (Base Matrix)	Bulk Material
3, 5, 6, 8, 9	4	IWNiRZ	Bio-based Silane - coating (3 modifications + original)	Coating
1	5	CIDETEC	Cellulose electrolyte (containing CNC) - Ink	Coating
1	5	CIDETEC	Cellulose electrolyte (containing CNF) - Ink	Coating
7	5	CIDETEC	Bio-based slurries for ultracap electrode manufacturing - Ink	Coating
7	6	Gnanomat	Carbon nanomaterials as active electrode material – Powder	Coating
8, 9	10	FHG-ISC	Material bioORMOCER® - Coatings (functional for antibacterial, antifungal performance)	Coating
2, 4, 5, 6, 8, 9	10	FHG-ISC	Material bioORMOCER® - Coating (bio-based lacquer)	Coating
7	12	CIDETEC	Roll-to-Roll electrodes for ultracapacitors – Coated substrate	Coating
1, 2	14	VTT (Sutco)	Poly Lactic Acid (PLA)-X or PLAX dispersions on substrates - Coating	Coating
1, 2	14	VTT (Sutco)	Material Lacquer via existing dispersion coating methods on the PLAX Coated substrates - Composite	Composite
1, 2	14	VTT (Sutco)	Material Barrier Products (nanoenabled) - Coating	Coating
3, 5, 6, 9	8	CEA	Bio-plastic compounds (nano-enabled) PA10,10 and PA11 + fibres + treatments – Composite	Composite
6	9	IPC	Bio-plastic compounds with micro fibres - Composite	Composite
8	16	AITIIP	Material bio-plastic compounds (nano-enabled) - Composite	Composite

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3, 5, 6, 8, 9	*4*	*IWNiRZ*	*Flax micro fibers - micro fibers*	*Fiber (micro)*
3, 5, 6, 8, 9	*4*	*IWNiRZ*	*Hemp micro fibers - micro fibers*	*Fiber (micro)*
1	*1*	*VTT*	*CNF, Cellulose nanofibril – Modified nano fibrils (wet form as hydrogels)*	*Fibril (nano)*
3, 9	*1*	*VTT*	*MFC, Micro Fibrillated Cellulose, Modified - Micro fibrils (High-consistency enzymatic fibrillation)*	*Fibril (micro)*
7	*1*	*VTT*	*CNF, Cellulose nanofibril, Unmodified - nano fibrils*	*Fibril (nano)*
3, 5, 8	*9*	*IPC*	*Filaments for 3D printing*	*Filament, Bulk Material*
4	*15*	*IPC*	*PHA - Multi-nano-layer Film*	*Film (nano)*
3, 9	*11*	*FhG-ICT*	*Material Expandable/Expanded Bio-polymer/MFC foam beads - Foam, Composite*	*Foam, Composite*
3, 9	*11*	*FhG-ICT*	*Material Expandable/Expanded Bio-polymer/NF foam beads - Foam Composite*	*Foam, Composite*
1, 2	*2*	*RISE*	*CNC, Cellulose nanocrystal - nano particulate (water dispersed)*	*Particulate (nano)*

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2 Solution Implementation Strategy

The main outcomes of implementation will be curated i) Datasets for selection and benchmarking based on the harmonized metadata, ii) Schema for data handling, iii) Protocols for data transformation (where appropriate and not infringing on partner IP), configuration of Granta MI for SEP use cases.

2.1 Harmonized Metadata Record Curation

Granta MI enables digital curation of datasets for materials and processes for their availability in professional, interactive engineering software tools to perform the following actions by end-users:

- Benchmarking against commercial grades in the property space
- Selection of records for design
- Assignment of records for design in CAD, CAE, PLM software environments
- Selection of records for modelling and simulation to predict properties and performance (SPPP relationships)
- World-wide reach through the SEP business, and Ansys channels

The metadata harmonization process was accomplished for all 16 Pilots Lines and their relevant Test Cases. Across all Test Cases there were ~8785 line-items to be harmonized for SPPP relationships. The metadata harmonization process resulted in a list and description of roughly:

- 30 Materials, or unique material products, categorized into 10 forms (e.g. bulk material, coating, composite, fiber, filament, foam, etc.), as shared in Table 1
- 40 Processes used in the production of the material and/or product
- 450 Attributes for SPPP relationships for materials, processes or products

Metadata harmonization was complimented by the leadership of Test Case leads, and participation of all Pilot Lines to complete survey for Test Cases they are providing capabilities to.

The next step of the record curation strategy was for Ansys to review its requirements for M&P curation and to relay anticipated attributes to the partners, gain their feedback on what is possible to deliver by end of the project, and propose methods to backfill the properties which will not be available. Ansys has the background capability to estimate material properties across a range of material families, and has already curate some bio-based materials (e.g. PLA, PHA and related composites, flax and hemp micro-fibres, etc.). There is a minimum set of properties for compatibility with Ansys owned MaterialUniverse™, which includes but is not limited to:

- ***General** – what's the material, composition, commercially available etc?*
- ***Mechanical** – e.g. linear properties such as Young's Modulus, Flexural Modulus, stress/strain behaviour, temperature dependence for polymers, fatigue data, shear data, impact strength.*
- ***Thermal** – e.g. CTE value or curve, diffusivity value or curve (or other application dependent property) as well as reference temperatures for service*
- ***Electrical** – e.g. Conductivity (resistivity) value or curve, temperature dependence*

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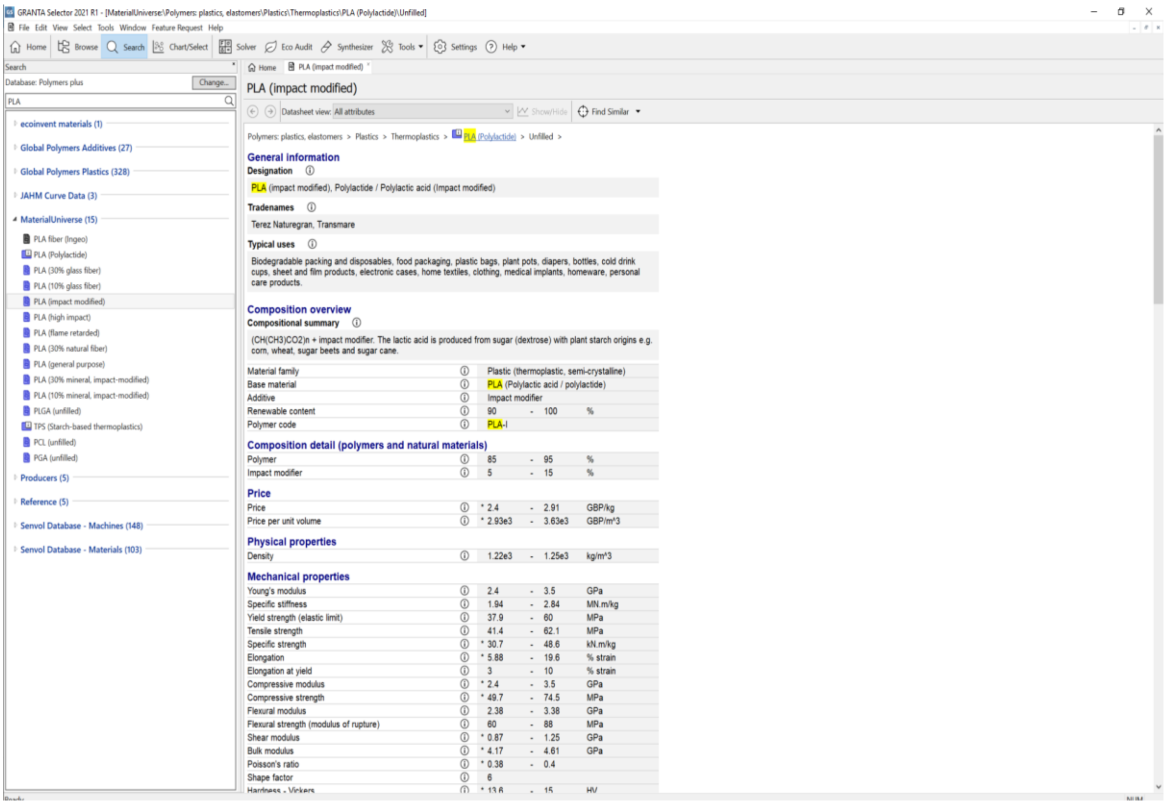
- ***Durability** – resistance to specific environments, e.g. fresh water, salt water, acids, solvents etc.*
- ***Eco** – CO2 footprint, Energy, Water, Restricted Substances*
- ***Manufacturing** – processes used, and additional information, supplier name and location. Other key manufacturing parameters like melt properties, viscosity, etc.*

For compatibility with Materials Data for Simulation™ (MDS), the material in question must be a material in MaterialUniverse™ (MatUni) and may optionally include additional curve data not provided in MaterialUniverse directly useful for solvers – mechanical, electrical, thermal, magnetic etc.

Figure 1 illustrates the two record types for the two Ansys products. These illustrations do not include all of the variations of data formats and representations of M&P records which can be accommodated by Ansys software but aim to give an impression of the differences between the two datasets.



(a)

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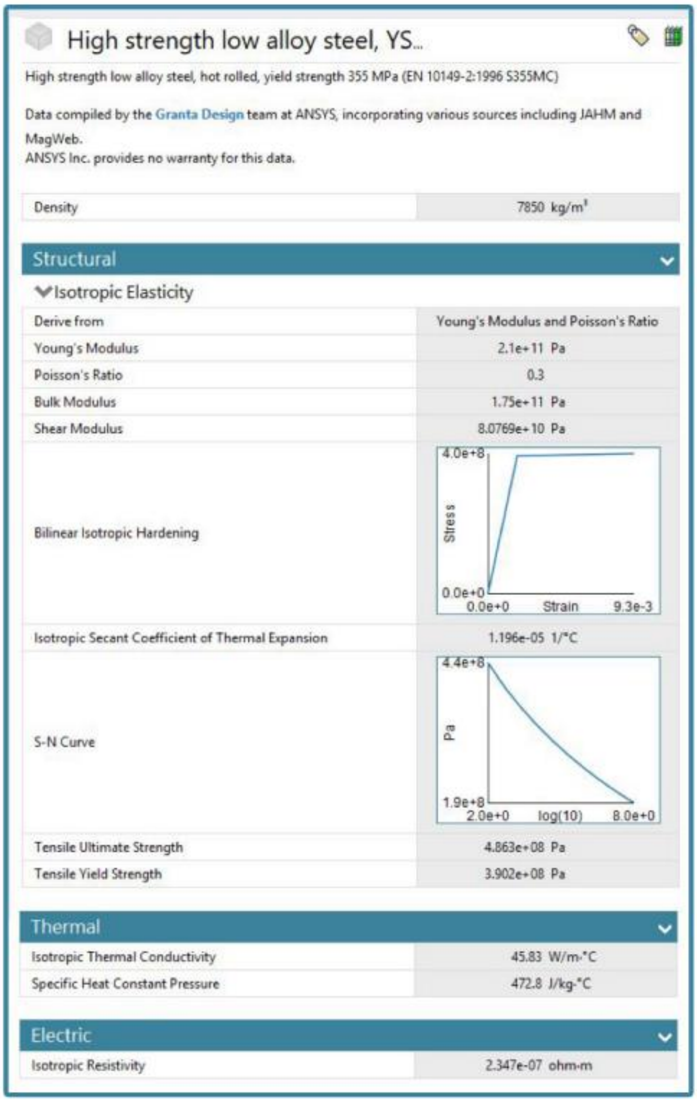

(b)

Figure 1: Two record types for materials selection in (a) MaterialUniverse™(MatUni) and (b) Materials Data for Simulation™ (MDS), respectively

At the time of this deliverable, Ansys is working with partners to refine a set of attributes which can be compiled for each product in Table 1.

2.2 Schema for FAIR Data Management

A first version of the schema was proposed in an earlier deliverable which is confidential to the project, along with metadata for batch characterisation to ensure all partners are transferring the same level of details when passing products between themselves.

2.3 Protocols for Data Handling

The Statistical Data and Design and Simulation Data are two database table concepts which are readily used in the Ansys Granta MI implementation strategy for manufacturing organizations and can use available protocols for data roll-up to average values, a standard

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deviation or other precision denotation, and other statistical calculations, or can be configured for specific data handling strategies such as data pooling for large design of experiments for qualification. As we continue to explore the dataflows of partners, these tables may be populated and supported by semi/fully automated data handling protocols. At this time, further investigation is needed.

2.4 Configuration of Granta MI

A high-level Solution Diagram was shown in D2.2, confidential to the project. The solution indicated a starting point in Granta MI™ to store data and information relevant for materials, process and product management for various end-points such as interfaces for search, selection, assignment for design, simulation, analysis, administration, etc. One type of end-point is the MI Explore™ interface which can be configured to apply filters, visualize the material process, or product by a representative illustration, and provide brief datasheets which link to more details data (Figure 2).

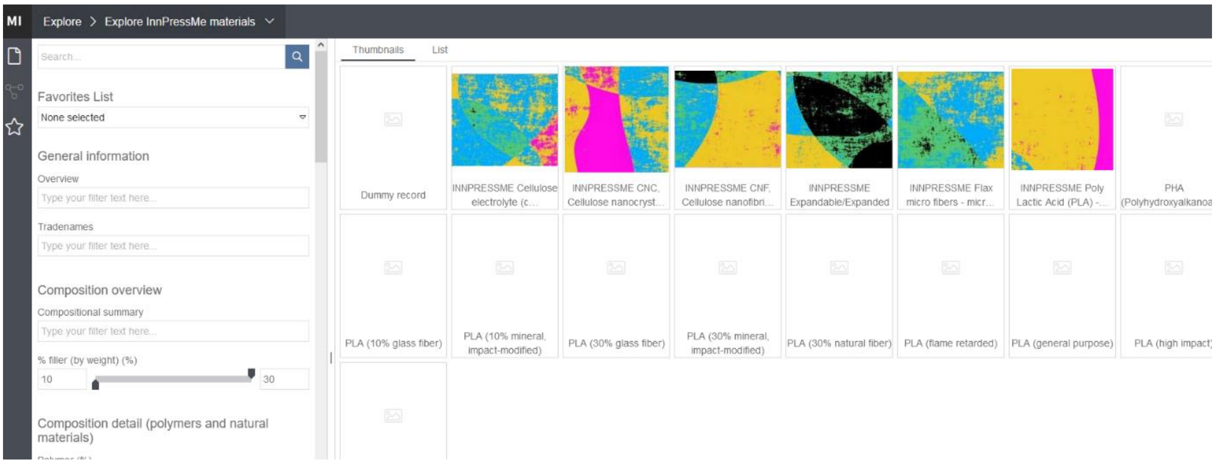

Figure 2: MI Explore™ for visual selection of INNPRESSME material products

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3 Conclusion

Our next deliverable is due at M48, *D2.7 Final Platform release for OITB Implementation through SEP*. To reach this goal, several broader targets are set with partners to ensure we achieve preparation of the platform and also the ambition to have a Product+ dataset at the end of the project for selection and benchmarking activities to support the upscaling of nano-enabled, bio-based products. Timelines for milestone delivery is dependent on the development timelines of Pilot Lines and Test Cases.

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