User Requirements

Polymer / Composite

Pilot	Main requirement	DiMAT toolkit	Sub-requirement	Status M12	Status M24 [confirmed, tentative, rejected]
Polymer	During polymer compound manufacturing process, the toolkit shall indicate the percentage or amount of each polymer and additive to make the mixture and obtain the desired properties	DiCMDB DiKAF DiMEC-LCA DiMDF DiMM DiMMS	CMDB shall be queried for data used in previous processes - this can serve as a reference or a starting point with the support of APIs and data export capabilities	confirmed	confirmed
			Before initiating the process KAF shall be used in order to get suggestions on the amounts of materials - KAF can be queried based on material properties and retrieve materials that satisfy these properties and if this information is available, as well as propose polymers/additives to construct the material	tentative	confirmed
			The toolkit shall present LCA data about the polymers and additives used	tentative	confirmed
			Properties and associated datasets shall be made available via the built-in search functionality - the "materials relation app" will allow the discovery of parameters, materials and models, and the "correlation app" will provide means to investigate the best parameters choice based on existing data. Updated: The "search app" allows for searching properties and associated datasets; the "materials relation app" will allow the discovery of material models; the "correlation app" will provide means to investigate the best parameters choice based on existing data	tentative	tentative
			Given specific mechanical properties (and enough data) of the target final polymer, the MM toolkit shall provide the most suitable formulation/mixture of the starting material	confirmed	confirmed
			Molecular Dynamics models link the formulation with the mechanical properties - given the final mechanical properties, the toolkit shall determine the optimum formulation	confirmed	confirmed
	During compound formulation, the toolkit shall indicate the mechanical performance that could be achieved depending on the material and additives mix	DiCMDB DiMDF DiMM DiMMS	Similar to PC1r1.CMDB	confirmed	confirmed
			MDF shall be queried for tools containing relevant information given the material or additives - the "correlation app" will provide insights concerning the mechanical performance. Updated: the "search app" shall be queried for data containing relevant information given the material or additives; the "correlation app" will provide insights concerning the mechanical performance from data	tentative	tentative
			Given a specific formulation/mixture of the starting material (and enough data), the MM toolkit shall provide the mechanical properties of the final material	confirmed	confirmed
			Molecular Dynamics models link the formulation with the mechanical properties - given the composition, the toolkit shall determine the mechanical properties	confirmed	confirmed
	During compound production, the toolkit shall indicate the rheological performance that could be achieved depending on the composition of the compound	DiCMDB DiMDF DiMM DiMMS	Similar to PC1r1.CMDB	confirmed	confirmed
			The "correlation app" shall provide insights concerning the rheological performance. Updated: The "correlation app" shall provide insights concerning the rheological performance from data	tentative	confirmed
			Given a specific formulation/mixture of the starting material (and enough data), the MM toolkit shall provide the rheological properties of the final material	confirmed	confirmed
			Molecular Dynamics models link the formulation with the mechanical properties including rheological properties - based on the given composition, the toolkit shall determine the rheological properties	confirmed	confirmed
	During the compound production, the toolkit shall indicate in which feeder each material should be introduced	DiCMDB	Similar to PC1r1.CMDB	confirmed	confirmed
	During the compound production, the toolkit shall indicate the parameters and working conditions in the extruder (pressure, time, temperature, speed, etc)	DiCMDB DiMDF DiMMS DiMPS	Similar to PC1r1.CMDB	confirmed	confirmed
			The "Materials Relation" app shall provide information about the parameters. Update: The "correlation app" shall provide information about the parameters from data	confirmed	confirmed
			The toolkit shall link the formulation with the mechanical properties	confirmed	confirmed
			The toolkit shall indicate the parameters and working conditions during the compounding process	tentative	tentative
	The toolkit shall visualise and store material properties to choose the right mixture for the compound manufacturing (CMBD) and analyse correlation between materials (KAF)	DiCMDB DiKAF DiMEC-LCA	The toolkit shall make relevant datasets and previous processes available based on the user query	confirmed	confirmed
			Similar to PC1r1.KAF	tentative	confirmed
			The toolkit shall present LCA data based on the materials used for the compounding process	confirmed	confirmed
	The toolkit shall provide the working conditions and machine parameters in the extruder in order to facilitate the melt spinning process (temperature, speed flow diameter, coiling temperature, godet speed, draw rate, etc)	DiCMDB DiMDF DiMMS DiMPS	Similar to PC1r1.CMDB	confirmed	confirmed
			The "Materials Relation" app shall provide information about the parameters. Update: The "correlation app" shall provide information about the parameters from data	confirmed	confirmed
			The toolkit shall link the formulation with the mechanical properties	confirmed	confirmed
			The system shall provide the working conditions and machine parameters	confirmed	confirmed
	The toolkit shall visualise and store yarn properties to choose the right mixture of compound vs. additives in the melt spinning process (CMBD) and analyse correlation between materials (KAF)	DiCMDB DiKAF DiMEC-LCA DiMMS	Similar to PC1r6.CMDB	confirmed	confirmed
			Similar to PC1r1.KAF, materials shall be queried based on the required properties	tentative	confirmed
			The toolkit shall present LCA data based on the materials used for the melt spinning process	confirmed	confirmed
	The toolkit shall provide the number of yarns and strands to build the twine, braids per meter, size of knots	DiCMDB DiMDF DiMMS DiMPS	Given the Multiscale FEM model of the yarn and strand, the toolkit shall determine the mechanical properties of a set of yarns	confirmed	Confirmed
			Similar to PC1r1.CMDB	confirmed	confirmed
			The "search app" shall allow searching for datasets that used similar input data	confirmed	confirmed
			Multiscale FEM model of the yarn and strand to determine the mechanical properties of a set of yarns - given the final mechanical properties, the toolkit shall determine the optimum configuration	confirmed	confirmed
			The system shall provide the number of yarns and strands to build the twine, braids per meter, size of knots	tentative	tentative
	The toolkit shall provide the number of meshes depth and the size of the mesh	DiCMDB DiMDF DiMMS DiMPS	Similar to PC1r1.CMDB	confirmed	confirmed
			The "search app" shall allow searching for datasets that used similar input data	confirmed	confirmed
			Multiscale FEM model of the mesh to determine its mechanical properties – given the properties of the mesh, the toolkit shall determine the optimum configuration	confirmed	confirmed
			The system shall provide the number of meshes depth and the size of the mesh	tentative	tentative
	The toolkit shall provide the parameters of the autoclave to dimensionally stabilise the net	DiCMDB DiMDF DiMMS DiMPS	Similar to PC1r1.CMDB	confirmed	confirmed
			The "search app" shall allow searching for datasets that used similar input data - the "materials relation app" will provide information about the parameters. Update: The "search app" shall allow searching for datasets that used similar input data; the "correlation app" will provide information about the parameters	confirmed	tentative
			Given the Multiscale FEM model of the mesh, the toolkit shall determine its mechanical properties	confirmed	Confirmed
			The system shall provide the parameters of the autoclave to dimensionally stabilise the net	tentative	tentative
	The toolkit shall provide the material properties of the yarns in order to produce the correct net and store the net properties	DiCMDB DiKAF DiMEC-LCA DiMDF DiMMS DiMPS	Similar to PC1r1.CMDB	confirmed	confirmed
			The toolkit shall query material properties of the yarn	tentative	confirmed
			The toolkit shall provide LCA data about the relevant net materials used in the net knitting process	tentative	confirmed
			The "materials relation app" shall provide information about the parameters - the "correlation app" will be used to optimise the parameters. Update: The "correlation app" shall provide information about the parameters	confirmed	confirmed
			Given the Multiscale FEM model of the yarn and strand, the toolkit shall determine the mechanical properties of a set of yarns	confirmed	confirmed
			The system shall provide the material properties of the yarns to produce the correct net and store the net properties	tentative	tentative
Composite	The toolkit shall indicate the optimised resin curing cycle (temperature ramp and hold time at curing temperature)	DiMPS	The toolkit shall indicate the optimised resin curing cycle	confirmed	confirmed
	The toolkit shall calculate the mechanical and physical properties requested for the defined material & assistance in requirements definitions	DiCMDB DiMEC-LCA DiMDF DiMD	CMDB shall host data that can be used for calculations as well as the calculation results for future reference - APIs and data export capabilities will be supported	confirmed	confirmed
			The toolkit shall provide LCA data about the materials used during the UAV component design process	tentative	confirmed
			The "correlation app" shall be used for the calculation of the mechanical and physical properties - the "materials relation app" will help to find related materials and properties. Update: The "correlation app" shall be used for analysing of the mechanical and physical properties from data; the "materials relation app" will help to find related material models	confirmed	confirmed
			The toolkit shall calculate the mechanical properties of the composite material	confirmed	confirmed
	During the manufacturing process, the toolkit shall detect deviations from the nominal cycle and suggest/command the appropriate corrective action	DiDTPC	Suitable IoT devices sensors shall be deployed (NTUAr15, NTUAr19) - data from the equipment are fed to virtual functions assuming these are open-source available or will be custom developed with aid from the pilot	confirmed	confirmed
	The toolkit shall provide LCC and LCA analysis after the process to ensure minimal impact and monitor the outcomes	DiMEC-LCA	The toolkit shall provide LCA/LCC data regarding the impact of the components used	tentative	confirmed

Glass / Graphite

Pilot	Main requirement	DiMAT toolkit	Sub-requirement	Status M12	Status M24 [confirmed, tentative, rejected]
Glass	DiMAT toolkits shall react on the order data of the customer to take the right features into account for the calculation of the bended product measurements, weight of the end-product and number of packages, as well as give the software feedback of those calculations in order to have the information (a) to update the order in the ERP and 3D model, (b) for the production and bending furnace	DiCMDB DiKAF DiMPS	CMDB shall be used to store (and later query) product data - APIs and data export capabilities will be supported, as well as pre-processing of data on upload	tentative	confirmed
			KAF shall be used to query materials based on properties to decide on manufacturing related details - it can predict the future product's state if relevant data have been stored in KAF from the pilot	confirmed	confirmed
			The toolkit shall allow for the calculation of the bended product measurements	tentative	confirmed
	DiMAT toolkits shall react on the order data of the customer and bended product measurements from DiMAT to take the right features into account for the calculation of the bending mold, as well as give the software feedback of those calculations in order to have the information (a) to update the order in the ERP and a 3D model, (b) for the production and bending furnace	DiCMDB DiKAF DiMPS	Similar to PC3r1.CMDB	tentative	confirmed
			Same as PC3r1.KAF	confirmed	confirmed
			The toolkit shall allow for the calculation of the bended product measurements	confirmed	confirmed
	DiMAT toolkits shall react on the order data of the customer and the bended product measurements to take the right features into account for the calculation of the flat glass measurements, as well as give the software feedback of this calculation in order to have the information (a) to update the order in the ERP and a 3D model, (b) secondly for the production and bending furnace	DiCMDB DiKAF DiMPS	Similar to PC3r1.CMDB	tentative	confirmed
			Same as PC3r1.KAF	confirmed	confirmed
			The toolkit shall allow for the calculation of the mold, depending on coated glass	tentative	confirmed
	DiMAT toolkits shall react on the order data of the customer and the bended product measurements to take the right features into account for the calculation of the processing, decision-making of processing moment and 3D model, as well as give the software feedback of this calculation in order to have the information (a) to update the order in the ERP and a 3D model, (b) for the production and bending furnace	DiCMDB DiKAF DiMPS	Similar to PC3r1.CMDB		
			Same as PC3r1.KAF	confirmed	confirmed
			The toolkit shall allow for the calculation of edge processing, drillings, cutouts to manage individual contours	tentative	tentative
	DiMAT toolkits shall react on the order data of the customer, flat glass product and the bended product to take the right features into account for the calculation of expected process time and energy consumption, as well as give the software feedback of this calculation in order to update the order in the ERP and a 3D model, (b) for the production and bending furnace	DiCMDB DiKAF DiMEC-LCA DiMPS	Similar to PC3r1.CMDB	tentative	confirmed
			Same as PC3r1.KAF	confirmed	confirmed
			For a given order, the toolkit shall provide data about the expected process impact and energy consumption given the environment of plant and furnace	tentative	confirmed
			The toolkit shall provide actual data of process time and energy consumption of previous calculations/ processes	tentative	confirmed
	DiMAT toolkits shall react on the order data of the customer, flat glass product and the bended product and bending mold (if necessary), as well as give the software feedback of this calculation in order to have the information (a) to update the order in the ERP and a 3D model, (b) for the production and bending furnace	DiCMDB	Similar to PC3r1.CMDB	tentative	confirmed
	The order data shall be translated into production data for DiMAT toolkits to calculate the needed temperature, which is firstly feedback for the production software with a 3D model, and secondly information for the bending furnace	DiCMDB DiMDF DiMMS DiMPS	Similar to PC3r1.CMDB	tentative	confirmed
			The "search app" shall find related secondary data for the "correlation app" to analyse	confirmed	confirmed
			The toolkit shall determine the viscoelastic properties of the glass by interpolating in a material database - model n layers of bent glass with adhesive to predict the homogenised strength of the component	confirmed	confirmed
			The toolkit shall allow for the calculation of temperature for bending depending on actual thickness, strain rate, etc	confirmed	confirmed
	The order data shall be translated into production data for DiMAT toolkits to calculate the needed position in the furnace as well as the quantity of sheets in the furnace, which is firstly feedback for the production software with a 3D model, and secondly information for the bending furnace	DiCMDB DiMPS	Similar to PC3r1.CMDB	tentative	confirmed
			The toolkit shall allow for calculation of position in furnace and quantity of sheets in furnace	tentative	tentative
	The toolkit shall allow for the prediction and process control	DiDTPC	Sensors/IoT devices shall be installed and transmit data (NTUAr15, NTUAr19) to feed to suitable virtual functions - the results are displayed to the operator to decide on appropriate actions	confirmed	confirmed
	The bending furnace shall give information firstly to the production software and ERP, and secondly to DiMAT for actual data analysing (improvements of expected data) and reporting	DiCMDB DiMEC-LCA DiMDF	Similar to PC3r1.CMDB	tentative	confirmed
			The toolkit shall provide data from the furnace regarding energy consumption etc. of the bending process	confirmed	confirmed
			The MDF "search app" shall allow searching for datasets that used similar input data	tentative	confirmed
	The toolkit shall provide an accurate FEM model which is critical for new geometry design in the bending process, execution of virtual experiments and generation of data for ML model training - the deviation from simulation results and real experiment should be minimised	DiCMDB DiKAF DiMMS DiMPS DiDTPC	Similar to PC3r1.CMDB	tentative	confirmed
			KAF shall be used to retrieve information about materials	tentative	confirmed
			The toolkit shall determine the viscoelastic properties of the glass by interpolating in a material database - model n layers of bent glass with adhesive to predict the homogenised strength of the component	confirmed	confirmed
			The toolkit shall provide an optimised FEM model of laser glass bending process which is capable of calculating accurate final bending geometry according to various process parameters	tentative	confirmed
			Sensors/IoT devices shall be installed and transmit data to monitor the operation	confirmed	confirmed
	The toolkit shall provide comprehensive glass materials properties data for simulation and modelling	DiCMDB DiKAF DiMMS	Similar to PC3r1.CMDB	tentative	confirmed
			Glass related materials and properties shall be included to KAF	confirmed	confirmed
			The toolkit shall determine the viscoelastic properties of the glass by interpolating in a material database	confirmed	confirmed
	The toolkit shall train a ML-based surrogate model to embed the results from optimised FEM simulation to facilitate real-time prediction during the glass bending process	DiCMDB DiMMS DiMPS DiDTPC	Similar to PC3r1.CMDB	tentative	confirmed
			The toolkit shall determine the viscoelastic properties of the glass by interpolating in a material database	confirmed	confirmed
			Real-time prediction of the glass shape	tentative	tentative
			Sensors/IoT devices shall be installed and transmit data (NTUAr15, NTUAr19) that are then given as input to forecasting virtual functions	confirmed	confirmed
Graphite	The toolkit shall quickly obtain information on the performance of the battery built with different types of carbons by optimising the testing process both in terms of efficiency and time to quickly identify those with superior characteristics, and adjust the production process accordingly	DiCMDB DiKAF DiMM	CMDB shall be used to store experimental results, as well as query and export data to other toolkits	confirmed	confirmed
			KAF shall be used in order to acquire data about graphite or battery related materials, but such data must be made available to KAF in advance	confirmed	confirmed
			MM shall provide the correlations between the starting materials properties and target parameters (given enough data)	confirmed	confirmed
	Through LCA assessment, the toolkit shall find the best approach to minimise the environmental impact of the process	DiCMDB DiMEC-LCA	Similar to PC4r1.CMDB	confirmed	confirmed
			At the end of the testing process, the toolkit shall provide LCA data about the process	confirmed	confirmed
	Through correlation analysis of the data provided by the various tests, the toolkit shall identify the tests that do not bring useful information or that bring information already provided by other tests, to keep only those that contain fundamental information aimed at guaranteeing optimisation of the test phase	DiCMDB DiMM	Similar to PC4r1.CMDB	confirmed	confirmed
			MM shall provide the correlations between the starting materials properties and target parameters (given enough data)	confirmed	confirmed

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ID	Requirement definition	Requirement type	DiMAT toolkit	Status M24 [confirmed, tentative, rejected]
DRAXISr1	The toolkit's outputs shall be based on user input, rather than real-time data	Functional/Technical req	Di$^{MEC-LCA}$	confirmed
DRAXISr2	Data shall be collected from the pilots and maintained in order to provide the required outputs	Functional/Technical req	Di^{CMDB}	confirmed
			Di^{KAF}	confirmed
			Di$^{MEC-LCA}$	confirmed
			Di^{MMS}	confirmed
			Di^{MPS}	confirmed
			Di^{DTPC}	confirmed
DRAXISr3	The toolkits shall manage user access for every pilot partner	Security req	Di^{CMDB}	confirmed
			Di$^{MEC-LCA}$	confirmed
			Di^{MDF}	confirmed
			Di^{MD}	confirmed
			Di^{MMS}	confirmed
			Di^{MPS}	confirmed
NTUAr1	The toolkit shall be able to access real-time data from IoT devices at appropriate rates	Functional/Technical req	Di^{MDF}	rejected
			Di^{DTPC}	confirmed
NTUAr2	The toolkit shall be able to predict the behaviour of the modelled system	Functional/Technical req	Di^{DTPC}	confirmed
NTUAr3	The toolkit shall be able to connect with at least the 2 other toolkits of the corresponding DiMAT suite	Functional/Technical req, Interface req	Di^{KAF}	tentative
			Di^{MDF}	confirmed
			Di^{MMS}	confirmed
			Di^{MPS}	confirmed
			Di^{DTPC}	confirmed
NTUAr4	The toolkit shall offer an intuitive UI	Interface req	Di^{KAF}	confirmed
			Di$^{MEC-LCA}$	confirmed
			Di^{MD}	confirmed
			Di^{MMS}	confirmed
			Di^{MPS}	confirmed
			Di^{DTPC}	confirmed
NTUAr5	The toolkit shall be accessible only by authorised users	Security req	Di^{CMDB}	confirmed
			Di^{KAF}	confirmed
			Di$^{MEC-LCA}$	confirmed
			Di^{MDF}	confirmed
			Di^{MM}	confirmed
			Di^{MD}	confirmed
			Di^{MMS}	confirmed
			Di^{MPS}	confirmed
			Di^{DTPC}	confirmed
NTUAr6	The toolkit shall store long-term data to cloud databases	Functional/Technical req	Di^{DTPC}	tentative
NTUAr7	The toolkit shall provide sufficient documentation	Guidelines req	Di^{CMDB}	tentative
			Di^{KAF}	confirmed
			Di$^{MEC-LCA}$	confirmed
			Di^{MDF}	tentative
			Di^{MM}	confirmed
			Di^{MPS}	confirmed
			Di^{DTPC}	confirmed
NTUAr8	The data required or generated by the toolkits shall be transmitted over secured channels	Security req	Di^{CMDB}	confirmed
			Di^{KAF}	confirmed
			Di^{MDF}	confirmed
			Di^{MPS}	confirmed
			Di^{DTPC}	confirmed
NTUAr9	The toolkit shall offer communication over at least 3 different protocols (e.g., HTTP, MQTT, CoAP)	Functional/Technical req	Di^{KAF}	tentative
			Di^{DTPC}	confirmed

ID	Requirement definition	Requirement type	DiMAT toolkit	Status M24 [confirmed, tentative, rejected]
NTUAr10	The toolkit shall be able to suggest optimal parameters concerning material processes	Functional/Technical req	Di^{KAF}	tentative
			Di^{MM}	confirmed
			Di^{MPS}	confirmed
			Di^{DTPC}	tentative
NTUAr11	The toolkit shall support data visualisation through dashboards in the User Interface	Interface req	Di^{CMDB}	confirmed
			Di^{KAF}	confirmed
			Di$^{MEC-LCA}$	confirmed
			Di^{DTPC}	confirmed
NTUAr12	The toolkit shall support data formatted in at least 3 different formats (e.g., CSV, RDF, JSON)	Functional/Technical req	Di^{CMDB}	confirmed
			Di^{KAF}	confirmed
			Di^{MMS}	confirmed
			Di^{DTPC}	confirmed
NTUAr13	The toolkit shall be appropriately updated when necessary	Usability and Quality req	Di^{CMDB}	confirmed
			Di^{KAF}	confirmed
			Di$^{MEC-LCA}$	confirmed
			Di^{MDF}	confirmed
			Di^{DTPC}	confirmed
NTUAr14	The toolkit shall incorporate at least one (e.g., EMMO) of the most popular material ontologies	Functional/Technical req	Di^{KAF}	confirmed
			Di^{MDF}	confirmed
			Di^{MD}	tentative
			Di^{MMS}	confirmed
NTUAr15	The digital twin shall be able to communicate with the physical counterpart	Functional/Technical req, Interface req	Di^{MMS}	confirmed
			Di^{DTPC}	confirmed
NTUAr16	The DTPC toolkit shall prohibit users from causing undesirable effects to the physical equipment	Security req	Di^{DTPC}	confirmed
NTUAr17	The toolkit shall store and handle credible and semantically useful and correct data	Functional/Technical req	Di^{KAF}	confirmed
NTUAr18	The toolkit shall issue alerts when an error occurs	Security req	Di^{DTPC}	confirmed
NTUAr19	The DTPC toolkits shall communicate with the physical counterpart through IoT devices	Functional/Technical req, Interface req	Di^{DTPC}	confirmed
NTUAr20	Availability of services of the toolkits shall be checked and measured frequently	Usability and Quality req	Di^{CMDB}	confirmed
			Di^{KAF}	confirmed
			Di^{MDF}	confirmed
			Di^{DTPC}	confirmed
NTUAr21	Interfaces of the toolkits shall be aligned with publicly available definitions	Interface req	Di^{CMDB}	confirmed
			Di^{KAF}	confirmed
			Di^{DTPC}	confirmed
CERTHr1	The toolkit shall be able to leverage GPU acceleration for training and inference of machine learning models	Functional/Technical req	Di^{MM}	confirmed
CERTHr2	The toolkit shall be able to incorporate techniques to avoid overfitting under normal conditions (sufficient data quality and quantity)	Functional/Technical req	Di^{MM}	confirmed
AMSr1	The toolkit shall check the input data analysing the format and the range to avoid extrapolation of predictions	Functional/Technical req	Di^{CMDB}	confirmed
			Di^{MM}	confirmed
			Di^{MMS}	confirmed
			Di^{MPS}	confirmed
			Di^{DTPC}	confirmed
CETMAr1	The toolkit shall be able to communicate and exchange data with the calculation code, even if it installed on a different server	Interface req	Di^{MD}	confirmed
			Di^{MMS}	confirmed
			Di^{MPS}	confirmed

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