Composite Structures 204 (2018) 778–790

Contents lists available at ScienceDirect

Composite Structures

journal homepage: www.elsevier.com/locate/compstruct

Integration of material and process modelling in a business decision support system: Case of COMPOSELECTOR H2020 project

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ARTICLE INFO

Keywords:
Business decision
Material model
Model selection
KPIs
Material selection
MODA
Interoperability
BDSS
BPMN
DMN
Data
Metadata

ABSTRACT

This paper shares and contributes to a ground-breaking vision developed and being implemented which consists in the integration of materials modelling methodologies and knowledge-based systems with business process for decision making. The proposed concept moves towards a new paradigm of material and process selection and design by developing and implementing an integrated multi-disciplinary, multi-model and multi-field approach together with its software tool implementation for an accurate, reliable, efficient and cost effective prediction, design, fabrication, Life Cycle Engineering (LCE), cost analysis and decision making. This new paradigm of integrated material design is indeed endowed with a great potential by providing further insights that will promote further innovations on a broad scale.

1. Introduction

It has become increasingly evident that the selection and design of composite materials and manufacturing processes are only possible by taking into account multiple influences at different physical scales and complex business processes [1]. To be reliable, this process must be built upon a physical and engineering framework and based upon methods that are systemic, effective and efficient in modelling complex, hierarchical materials and process [2].

For composite material design and selection, understanding and quantifying the links between material structure at the nano/mesoscale/microscale and their macroscopic effects is, therefore, essential and requires the integration of several models that have overlapping scales (polymer chemistry, matrix-fibre interface, fibre properties and topologies, etc.) [3,4]. This implies the need for development and integration of models to describe the behaviour of composite materials at different scales as well as material-processing-property relationships [5]. In parallel, high performance requires not only comprehensive material properties modelling but also understanding of risks, costs, and business opportunities for a range of decisions, from material selection to designing functional structural components and systems. Last but not least, design and selection of materials and manufacturing processes must also accommodate societal requirements for health and sustainability [6,7].

Developments and improvements have been taking place in disparate communities considering different types of models and phenomena on several different length scales, with advancements in so-called "multiscale" approaches [8] and multi-disciplinary design optimisation [9–11]. Nevertheless, they are far from being sufficient for materials design and selection, and suffer from a lack of integration across different types of models and related communities (especially discrete/continuum, modelling/experimental, material/process, science/engineering/business). This is a truly challenging task and calls for the definition of workflows and model coupling/linking that

Composelector website BDSS.

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https://doi.org/10.1016/j.compstruct.2018.06.121
Received 27 April 2018; Accepted 29 June 2018
Available online 12 July 2018

account, at finer scales, for various kinds of heterogeneities and physics. Since material selection and design for a particular functionality is intimately associated with the manufacturing process, attention should be given to link composite material and manufacturing selection in a systematic integrated approach including process-structure and structure–property relations.

The complexity and the interdisciplinary of this topic that require a fully integrated framework consisting of materials models coupled to process models allowing the seamless integration of material and process modelling workflows, solvers, post-processors together with business models and interoperability modules. The interoperability implies by definition the use of standards based abstract workflow definitions which can be stored, mined and re-used [13], together with specific communication protocols and conversion tools [14].

COMPOSELECTOR H2020 project proposes to develop a Business Decision Support System (BDSS), which integrates materials modelling, business tools and databases into a single workflow to support the complex decision process involved in the selection and design of polymer-matrix composites (PMCs) by means of an open integration platform which enables interoperability and information management of materials models and data and connects a "rich" materials modelling layer with industry standard business process models. Material and process models, software integration and along with archiving of data and metadata are presented here in the context of "multiscale" models. The presented application case exhibits how advanced selection and design process could be handled using the proposed approach. The application case is translated into a workflow consisting of materials modelling and materials data components using the materials modelling data (MODA) template [13] extended to include process models. This defines on a high level the requirements regarding input data, materials models and their coupling and linking, and the post-processing of raw data in order to arrive at the key performances needed.

2. BDSS definition and requirements

The developed BDSS proposes to integrate material and process modelling, business tools and databases into a single workflow to support the complex decision process involved in the selection and design of polymer-matrix composites by means of an open integration platform which enables interoperability and information management of materials models and data and connects a "rich" materials modelling layer with industry standard business process models. The BDSS is built on three "pillar" technologies (Fig. 1):

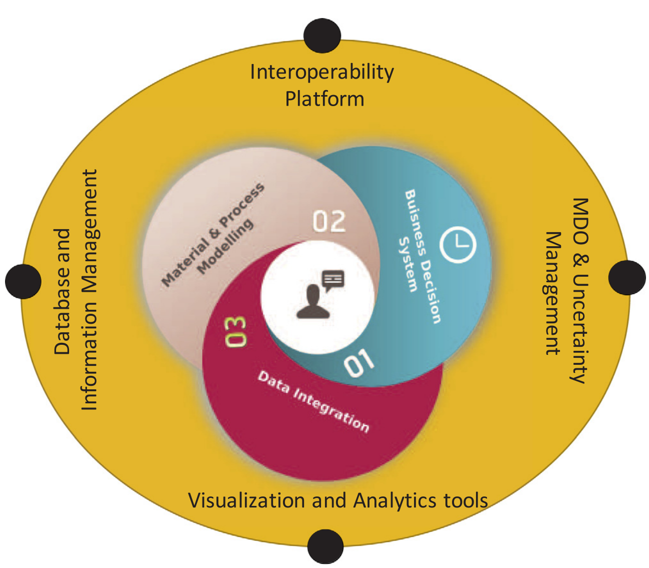

Fig. 1. BDSS core elements and pillars.

1. Materials and Process Modelling
2. Business Decision System
3. Data Integration

These pillars, represented by individual software tools, are interconnected and integrated into the BDSS platform. The interoperability layer will also seek compatibility with platforms from other BDSS projects, by contributing and adhering to the European Materials Modelling Ontology (EMMO) metadata and interoperability standard emerging via the collaboration within the context of the European Materials Modelling Council. The integration of different existing software solutions by means of an interoperability and metadata layer allows for carrying out multidisciplinary/multi-objective optimisation and analytics for material and process evaluation, uncertainty management and selection, spanning through "cradle-to-grave" lifetime of a product.

In line with the core elements shown in (Fig. 1), the functionalities integrated in the BDSS are presented in the following subsections.

2.1. Tailored Knowledge Apps to support decision makers

Typically, the tools are accessible via web based environment. The Knowledge Apps are integrated with business process systems based on the Business Process Model Notation (BPMN 2.0) standard [16]. This standard integration of defined business processes guarantees that the developed BDSS will be easily adaptable to any industrial sector. In particular, decision requirements and decision models will be integrated in the business process workflow and automated tasks as well as human interaction for business decision activities will be supported.

2.2. Actionable choices

Decision Makers require actionable choices that are the result of multi-criteria optimisation over all stages of product development, taking uncertainties, risks and opportunities into account. Choices should even extend to allow back engineering from the end-goal. In order to support this requirement, the BDSS as proposed in COMPOSELECTOR has a strong focus on the integration and innovative development of a Multi-Disciplinary Optimisation (MDO) framework, which will allow for time, resources and costs saving while increasing performance and functionality. One of the key enablers of the approach proposed is the ability to account for different class/aspects of uncertainty within models, experiments, design processes, cost of modelling, personnel and expertise. The material selection process involves distinct but coupled subsystems with large number of design parameters, constraints, and performance metrics and multidisciplinary formulation with multiple objectives and constraints. Surrogate model and a Bayesian Network Classifiers mapping approach are proposed for efficient search and uncertainty modelling and management, imprecise problem formulation will be incorporated. modeFRONTIER [15] is used in this context. Using modeFRONTIER, design teams can upload and organise models and data, create and reuse multiple optimisation strategies, execute huge numbers of jobs on a distributed execution network interfacing with HPC systems and cloud environments and perform data analysis using an array of post processing tools, safe in the knowledge that project integrity is safeguarded by reliable project versioning that aggregates design changes continuously under controlled conditions.

2.3. Integrated materials and process modelling

Innovative methodologies to connect models are being developed by enriching materials and manufacturing process-modelling framework with metadata schema and semantic interoperability. This is achieved by implementing approaches for Key Performance Indicators (KPI)-driven property calculations (See application case for more details) and by proposing advanced methods for model selection and model adaptivity. The developed modelling and simulation framework provides a unified environment and supports interoperability for modelling linked and coupled physical phenomena making the integration of new workflows much faster and less error prone. It is worth to mention that the platform supports multi-model coupling/linking to transfer information between models for an integrated workflow covering all scales and process stages of the application case. Therefore, removing the need to artificially isolate individual processes in the quest for a tractable problem.

2.4. Interoperability and metadata

Interoperability involves the development of an effective approach for materials information management across modelling and experiment, materials modelling integration and communication including reference standards and standardised methods for the representation, storage and communication of models. It also supports knowledge management of models and workflows, a key feature for business systems and value chain interactions [18]. Proper definition of interfaces, data structures, schemas and associated metadata is a prerequisite to guarantee interoperability among different materials modelling components as well as to support knowledge management across materials modelling data, business data, or LCE models. The BDSS platform overcomes the incompatibility in existing components by i) developing and implementing a “unified data and model representation architecture” using abstract classes defining common generic interfaces, and ii) using metadata schemas to facilitate semantic interoperability. This effort includes i) designing and implementing metadata schemas and Application Programming Interfaces (API) for materials and processes models and ii) designing and developing case study specific templates for materials modelling workflow chains, allowing to replace individual commercial/open-source codes in materials modelling. The metadata schemas for materials and processes models are being developed in order to describe also materials and related business and LCE data. This will lead to a rigorous quantification of all levels of materials structure in a large number of distinct material configurations, a repository for materials data and source of input data for materials modelling.

3. BDSS platform architecture

The BDSS integrates materials modelling, business tools and databases by following a well-defined ISO standard business process format (Fig. 2), Fig. 3). The business layer will be based on two well-defined standards: BPMN 2.0, the last version of the Business Process Model Notation standard defined by the Object Management Group (OMG), ISO standard ISO/IEC 19510:2013 [16], and the DMN [17], the Decision Making Notation standard, also defined by the OMG. The use of a standard representation (ISO standard ISO/IEC 19510:2013) and the Decision Model and Notations (DMN) [17] for business processes will make available the decision-making strategy across the different sectors and users. The BDSS could be connected with any third party platform. The developed workflows in MuPIF [20] are software components defining documented interface enabling to set input parameters, execute workflows and query outputs, thus allowing integration into other integration platforms such as Pipeline Pilot, Knime (Fig. 2).

BPMN includes graphic representations for business process workflows, and an associated XML-based executable representation, which can be used in business related engineering applications (Fig. 4). The DMN standard, which has been designed to work alongside BPMN, provides a mechanism for modelling the decision-making represented in a BPMN task within a business process model. By using DMN, it will be possible to specify sequence of actions to be followed after a decision has been taken, including those that are required to meet a certain directive, decide who or what participant should perform an activity or create specific values to be consumed later in the process. DMN supports the identification of the most important decisions, describing their impact on the global business objectives. User interaction is an essential element required for business decision activities. The single workflow will account for the complete production chain involving all the major processes and, at the same time, all possible parameters affecting the costs and other important factors under consideration. In this way, the BDSS decision layer will be able to control, manage and automate the repeatable decisions central to its business by effectively applying business rules, analytics and optimisation technologies.

MuPIF interoperability platform [20] provides high-level support for simulation tool data exchange and steering and servers as the simulation platform, where the distributed simulation workflows are defined and executed [21]. In MuPIF, the generic abstract classes are introduced for models (simulation tools) and generic data types, such as

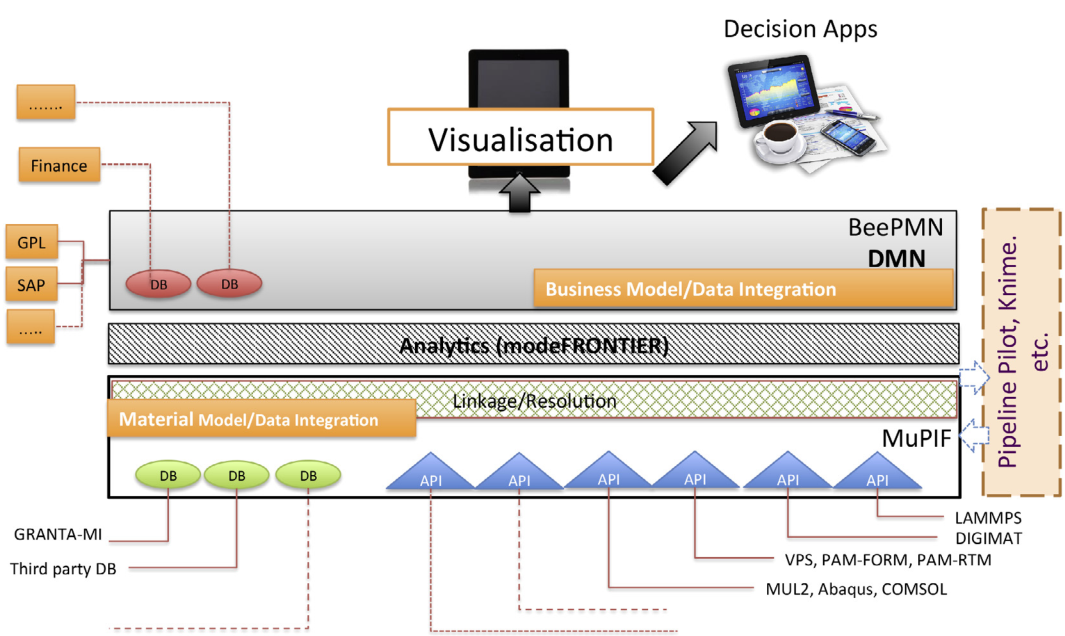

Fig. 2. High-level implementation view of BDSS. The BDSS gathers information from all points in the platform in view of end user informed decisions.

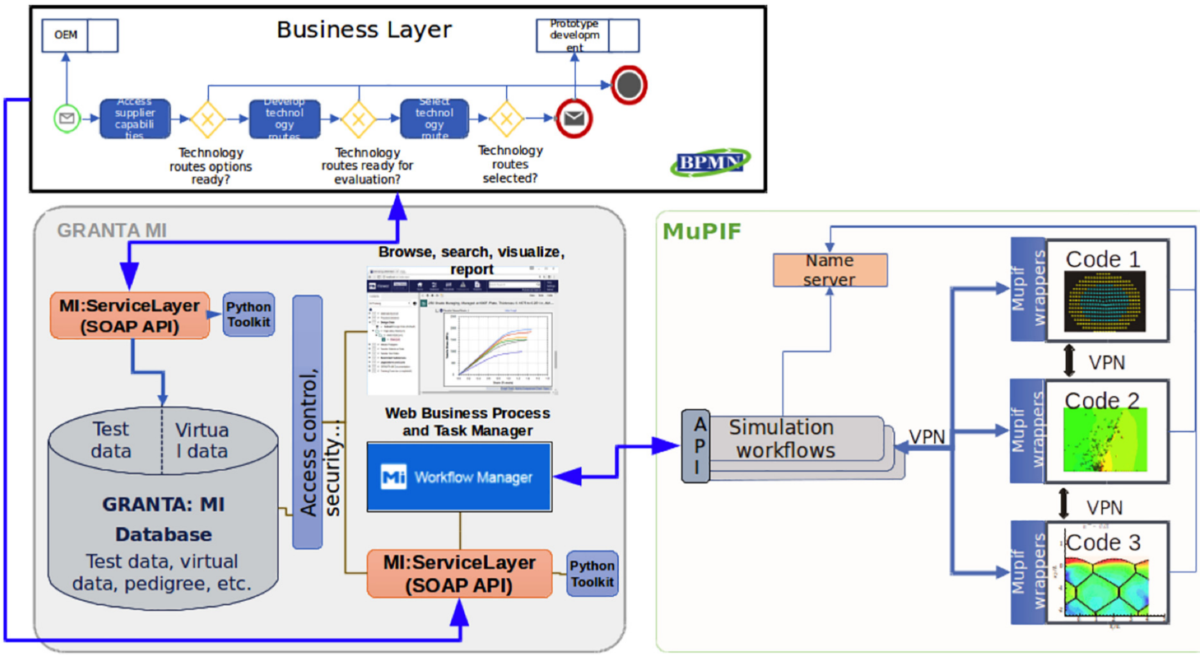

Fig. 3. High level Architecture between Business layer, Database and Simulation platform.

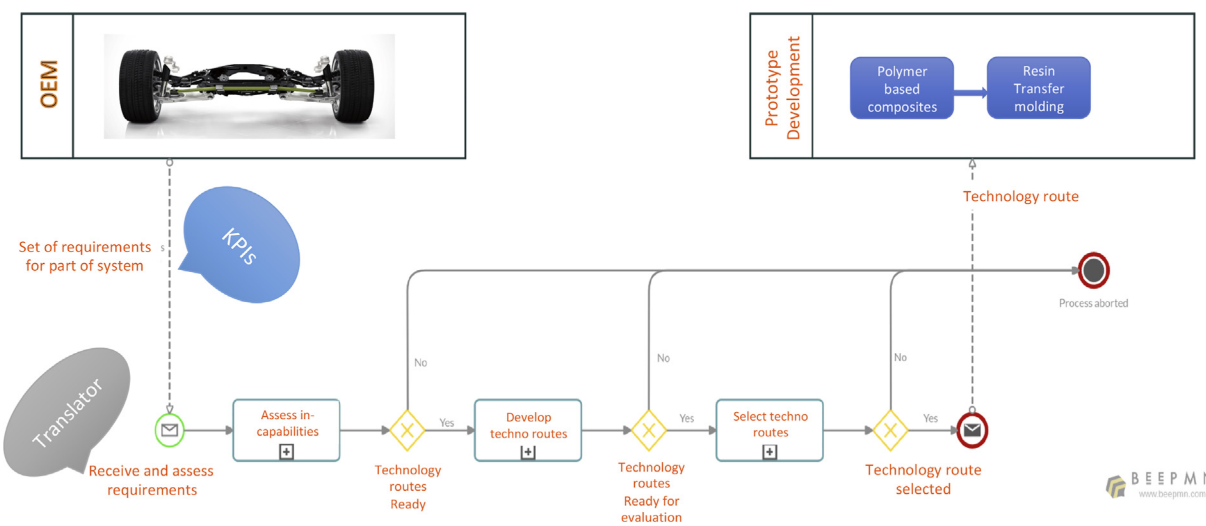

Fig. 4. Business Process Implementation in BPMN: The use of a standard representation for business processes will improve the decision-making strategy across the different sectors of the company.

properties, spatial fields, time steps, etc. The definition of abstract interfaces for models as well as for high level data types is one of the unique features of the MuPIF. It allows to achieve true plug&play architecture, where individual application as well as data representations can be plugged into existing workflows and be manipulated using the same generic interface. All classes are derived from top level abstract class, MuPIF-Object, declaring a generic interface common to all components. It defines the services allowing to attach the additional information about the individual object, so called metadata. The metadata plays an important role, as they allow to track the origin of the data, information about data units, etc. Some metadata have to be defined by user or simulation tool, some can be automatically collected by the platform. The interoperability in MuPIF is achieved by standardisation of application and data component interfaces, it is not relying on standardised data structures or protocols. Any existing data format can be plugged in and transparently used, provided the corresponding data interface is implemented.

From the software point of view, the BDSS is composed of three main modules: 1) the business layer, 2) the database and workflow manager and 3) the interoperability platform as shown in Fig. 3. All modules are connected with a well-defined Application Programming Interface (API), providing a loosely coupled modular and scalable solution. The business layer provides support for the creation and execution of material modelling business process, which are defined in terms of a standard representation of business process logic (the procedural flow of tasks) and business rules (declarative conditions leading to the conclusions of business decisions). This support is provided by a BPMN standard web-based graphical editor that support business workflow creation (the BeePMN editor), a business workflow engine that provides standard BPMN workflow execution support and a standard DMN engine for standard DMN rules execution. The BPMN engine provides support for fully automated tasks (like a request for model simulation to be delivered to the interoperability layer) and also for the so-called human tasks, where user intervention is required in order to complete a task or take a business decision.

The main user interaction entry point of the BDSS is web-based, allowing users to access core services through a standard web browser, providing an easy to use system, where users can connect from any location, at any time, from computers and also from mobile devices. The access to the BDSS is granted by using a single-sign-on approach, which provides user authentication and authorisation services in terms of the most up-to-date security standards. In this way, a clear separation of user roles can be provided, with strict control on simulation execution services and appropriate sharing of information supporting user interaction and collaboration.

The database and workflow manager layer (see Fig. 3) has two main tasks. On the one side, this layer provides the required database storage support for all data required and generated by the BDSS and on the other side, interacts with the interoperability layer to request simulation workflow executions. Requests for simulation workflow execution are usually received from the business layer, which after been completed with the required data, are passed to the interoperability layer for execution. This process can be fully automatic, when all information about required data is already defined, or can include user interaction if required. Also, this layer takes care of storing all data produced by simulation workflows, providing support for browse, search, visualisation and report operations.

The workflow presented in Fig. 4 and in Fig. 5 is an example of a business process, which represents a decision manager process for ”eligibility/approval” of a customer order, which requires simulation analysis and market information to determine its current business opportunity. A set of business rules has been defined by using DMN, which guides his decision process. This information can include the results of the simulation and results obtained from queries to databases and/or price information coming directly from real-time market sites. Based on that information, the decision maker takes a guided decision (implemented in terms of DMN) in order to determine the processing of the customer order. The decision-making node implements a decision process in DMN. Decisions are represented in terms of business rules, which automates the most common decisions and promote consistent results when used many times. The decision table (Fig. 5) are intended to produce an overall evaluation and decision. Based on this decision model, the decision maker is provided with all the information that is required to take a decision in this particular case, no more and no less. Of course, other business process workflows, which involve decision activities for risk evaluation, opportunity analysis, maximising impact or profit, can be represented in terms of business process workflows (BPMN 2.0) and decision-making rules (DMN). On Fig. 6 is depicted an example of DMN decision table for atomistic and mesoscopic models.

4. Model evaluation and selection

Selecting the appropriate model is of key importance for a reliable decision process. Specifically, the following features are analysed: i) effect of model resolution (uncertainty) on business decisions; ii) matching modelling strategies with business decision needs; iii) translation of process modelling value (cost/benefits), cost and triggers (part complexity/size/materials/process) and iv) evaluation of optimisation strategies for trade-offs in decisions. Furthermore, some selected case studies will permit to assess a judicious level of modelling complexity and recommend efficient simulation procedures, which should be as transparent and lean as possible for the end-users. Mechanisms for model selection are being developed and implemented within the BDSS. Typically, at each scale there can be a choice of several models with diverse quality, robustness and complexity (see Fig. 7). Notice that we use a “modelling strategy selection” instead of “model selection”. The reason is that individual models may have different dependencies, while strategies can have more or less defined dependencies. Based on the sensitivity measures, the model robustness, model utility and model complexity (see Fig. 7), we provide with an approach for the model evaluation and selection. The utility of a model is defined considering the problem on hand i.e. the user case and the attributes to be

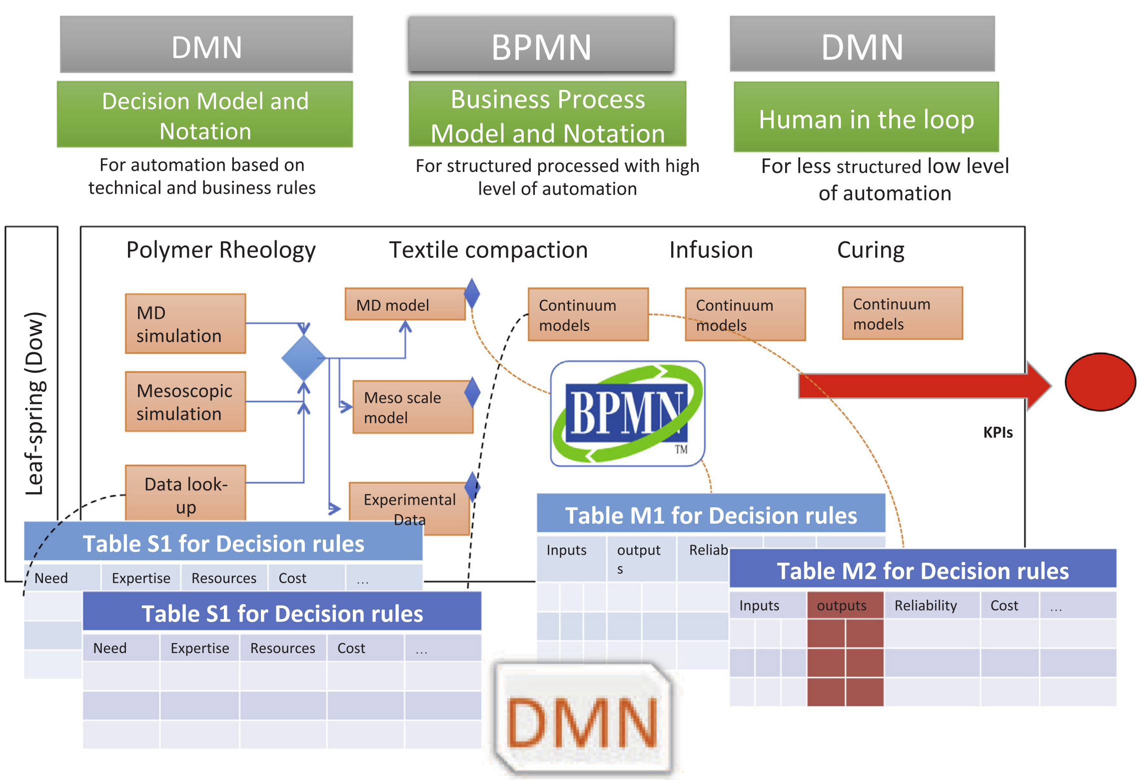

Fig. 5. The single graphical workflow as proposed in the BDSS includes standard BPMN task nodes, plus an activity node specifically designed to interact with the MuPIF simulation layer [17], task nodes to perform queries to databases and human interaction task nodes specifically design to interact with the BDSS.

Selection table for atomistic and mesoscopic model

	Input +				Output +			
	expertise	Cost (€)	time (hours)	reliability	atomistic	mesoscopic	feasible	Annotation
	boolean	integer	integer	integer	boolean	boolean	boolean	
1	No	-	-	-	-	-	No	-
2	-	<= 100	-	-	-	-	No	-
3	-	-	<= 6	-	-	-	No	-
4	-	-	-	<= 1	-	-	No	-
5	Yes	]100..1000[	> 6	>= 5	Yes	No	Yes	-
6	Yes	]100..1000[	> 6	]1..5[	-	-	No	-
7	Yes	>= 1000	]6..24[	>= 5	Yes	No	Yes	-
8	Yes	>= 1000	]6..24[	]1..5[	-	-	No	-
9	Yes	>= 1000	>= 24	]1..5[	No	Yes	Yes	-
10	Yes	>= 1000	>= 24	>= 5	Yes	No	Yes	-

Fig. 6. The single graphical workflow as proposed in the BDSS includes standard BPMN task nodes, plus an activity node specifically designed to interact with the MuPIF simulation layer [17], task nodes to perform queries to databases and human interaction task nodes specifically design to interact with the BDSS.

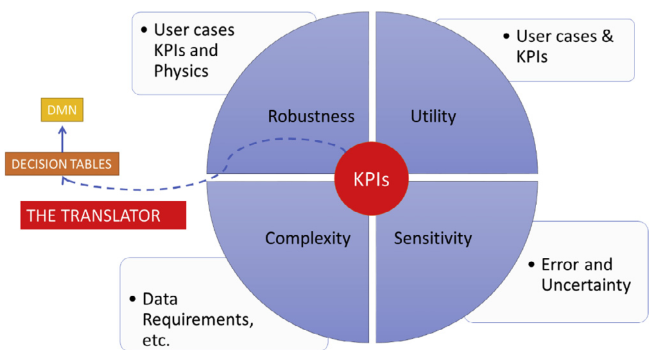

Fig. 7. Model Selection based on the model quality (i.e. reliability, sensitivity), robustness, model complexity and KPIs.

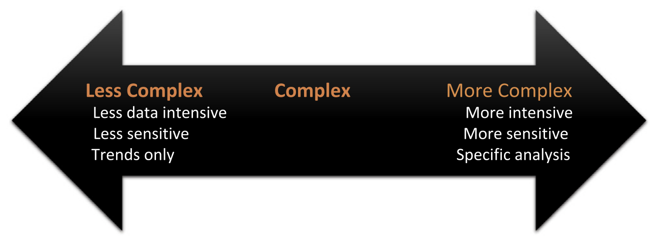

Fig. 8. Model complexity based model selection.

estimated. The utility of a model is determined according to the information we have reflecting the specific objective at hand. The decision might include theoretical and computational considerations. The robustness is defined as the degree that model is physics based. This represents the capability of the model to predict the physical properties and represent the physical reality. The complexity of model combines both model and software implementation complexities. The sensitivity analysis (estimation of sensitivity indices) permits to determine the most important uncertain input-parameters, their correlation and to quantify their impact on the predicted output.

Decision tables are constructed based on robustness, sensitivity and complexity. A weight ($0 < W < 1$) is assigned based on the quality (i.e. robustness, sensitivity, complexity) of the individual partial models. The need to separate this decision logic for model selection from the model selection and the user-case has motivated the use of DMN for model selection.

4.1. Model complexity

The decision on the complexity level for each model depends on the purpose of the modelling effort (Fig. 8) and data availability and accessibility. The factors that are used to estimate model complexity are:

1. Structure and the level of detail in the processes that make up the model.
2. The number of parameters and state variables
3. The sophistication of the mathematical relationships that describe each process
4. Number of processes in the model
5. The resources required to solve the model

4.2. Model robustness

Model output needs verification, interpretation and validation and should not be necessarily always believed to be the truth. Model robustness is therefore necessary and it is defined as the capability of the model to predict the physical properties even when some "perturbations" are present/introduced. In other words we should answer the following questions/requirements:

– Did the model represent the physical reality?
– Is there any documented verification and experimental validations of the model?
– What is the number of modelling assumptions that can be relaxed without overturning the conclusions (outputs)?

4.3. Model sensitivity

Sensitivity Analysis (SA) investigates how the variation in the output of a model can be attributed to variations of its input factors. The goal is to verify the consistency of the model behaviour and to assess the robustness of the model to uncertain inputs or model assumptions (Fig. 9). When used for model evaluation, SA is used to indicate whether there are "unnecessarily" represented processes in the model workflow and thus identify potential for model simplification. With this regard, the sensitivity analysis provides additional information beyond what is typically considered a part of an uncertainty quantification analysis. Based on the sensitivity indices, it is possible to determine the most important uncertain input-parameters, their correlation and to quantify their impact on the predicted output. For global sensitivity analysis, different types of sensitivity indices can be used, ranging from correlation measures between inputs and output to statistical properties of the output distribution.

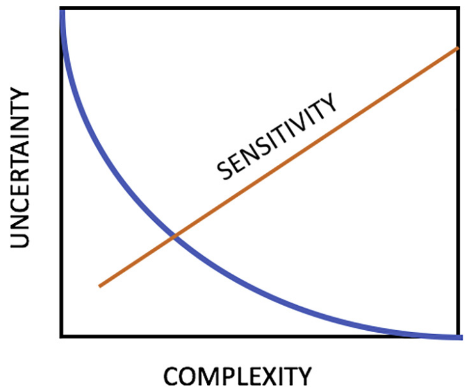

Fig. 9. Complexity-Sensitivity-Uncertainty: Model sensitivity increases with increasing model complexity and model uncertainty decreases with Model Complexity.

Hit	Characteristics							
Model	Class	Time	Uncertainty	Fidelity	Cost	Expertise	needs	weight
1	Molecular	Medium	High	Yes	High	Yes	Yes	0.2
2	Molecular	High	High	High	High	Yes	Yes	0.4
3	Continuum	low	Low	High	Low	Yes	Yes	0.9

Fig. 10. Sample decision table with its constitutive elements for model selection. The model selection and also the selection of the partial models should to be done/assessed by a framework for model assessment base on Model Robustness, Model Sensitivity, Model Complexity.

4.4. Modelling strategy

Figs. 10 and 11 illustrate the material modelling strategy. At the top level, the properties acting as key performance indicators can be modelled using various solvers technologies (for example finite elements, boundary elements, finite difference method, etc.) or models with varying physical complexity. Thus, a choice has to be made among the several models enabling the determination of one or more KPIs. The material input parameters required for this top modelling layer will either be provided by modelling at a lower scale, or by databases fed by literature or experiments. At this scale, databases or several modelling techniques and models with varying levels of complexity may be used for obtaining one or more material parameters required by the modelling level above. For example, some material properties may be obtained by a simple micro-mechanical model of the composite structure or by more complex modelling of the production process like, for instance, thermoforming or resin transfer moulding. The material parameters required for modelling at this scale may then be obtained by more or less complex models, for example molecular dynamics, coarse-grained models, etc., or by database lookup. The number of modelling layers may be increased by including layers with more refined methods, like atomistic models or others. It should be noted that the last scale of modelling will entirely depend on material or structure properties obtained from database lookup. Notice that for some strategies, not all scales (levels) have to considered/included, as can be replaced by including assumptions/heuristics. As illustrated in Fig. 11, at each level, various models exist for obtaining the required input for the next levels, or the KPI at the top level, respectively. This choice has to be made by considerations of availability, computing time and cost, as well as the precision required in the application case assembled in a DMN table Fig. 10. Considering that data, at a given scale, are only known to a certain degree (uncertainties), we can afford to choose less accurate models that are faster to evaluate, provided that the resulting error is of the order of the global uncertainties. In order to formalise this idea, key quantities will be considered uncertain at the finest scale, where the material is described, and at the coarsest scale, where the engineering problem is described. The chain of models will be allowed to transport these uncertainties through the scales, using robust uncertainty quantification or probabilistic analysis by sampling methods. In addition, the following statements and remarks should be added:Fig. 12.

– The business decision will influence how the modelling should be done based on cost, time, fidelity, etc.
– The global simulations workflows will be decomposed into individual tasks (determination of single KPI, process simulation, etc.). These tasks together with their input/output requirements will be identified for each case study.
– Alternative implementation of individual tasks (represented by so called task workflows) with different performance indicators (time requirements, cost, fidelity of results, etc.) will be implemented. The availability of alternative task workflows (yielding the specific action) would allow the BDSS to explore different modelling options based on different business and/or technical requirements (performance indicators).

This single workflow will allow accounting for the complete production chain involving all the major processes and, at the same time, all possible parameters affecting the costs and other important factors under consideration. Each workflow should define its performance indicators (as workflow metadata). The task workflows should have some general common inputs-outputs. The individual workflows will depend on additional parameters-properties, which can be obtained by simulation or from database, however this logic must be implemented into specific workflow. This way the BDSS is able to freely combine different alternatives without being concerned by i/o dependencies. In parallel, a business decision mechanism based on a balance between investment (complexity and number of inputs) and return will be implemented to decide on the type of models (in a chain) namely electronic, atomistic, mesoscopic and/or continuum Fig. 11.

The lines in Fig. 11 indicate that different models at relevant scales can be used to drive a variety of “actions”. Here, “action” refers to the estimation of specific technical or business KPI. Notice that each application case is translated into a workflow consisting of materials modelling and materials data components using the MODA (Modelling Data) materials modelling data templates as a starting point [13].

5. User-case application

The objective of introducing composites (carbon and glass reinforced polymer composites) into the body structure of a vehicle is to reduce weight and to improve energy efficiency. Reduction of mass potential is considerable when using composites, consequently the greatest hurdle lies not in merely achieving a significant mass reduction, it lies in the new technical and business (financial) challenges that will arise when composite structures are introduced into the high volume automotive sector. The technical novelty in this application is the use of carbon reinforced polymers (CRFP) in parallel with glass-reinforced polymers (GFRP).

The suspension leaf spring is one of the potential items for higher strength in automobiles. Composite leaf springs serve as the elastic elements and guiding mechanism of the suspension in automotive design (Fig. 13). The technical novelty in this application is the use of carbon reinforced polymers (CRFP) in parallel with glass-reinforced polymers (GFRP), which is the standard work piece material for this type of application. The proposed application case is towards the application of the BDSS for material selection and manufacturing process for composite leaf spring (Fig. 14). For the behaviour of the leaf spring, the mechanical strength and stiffness are major characteristics.

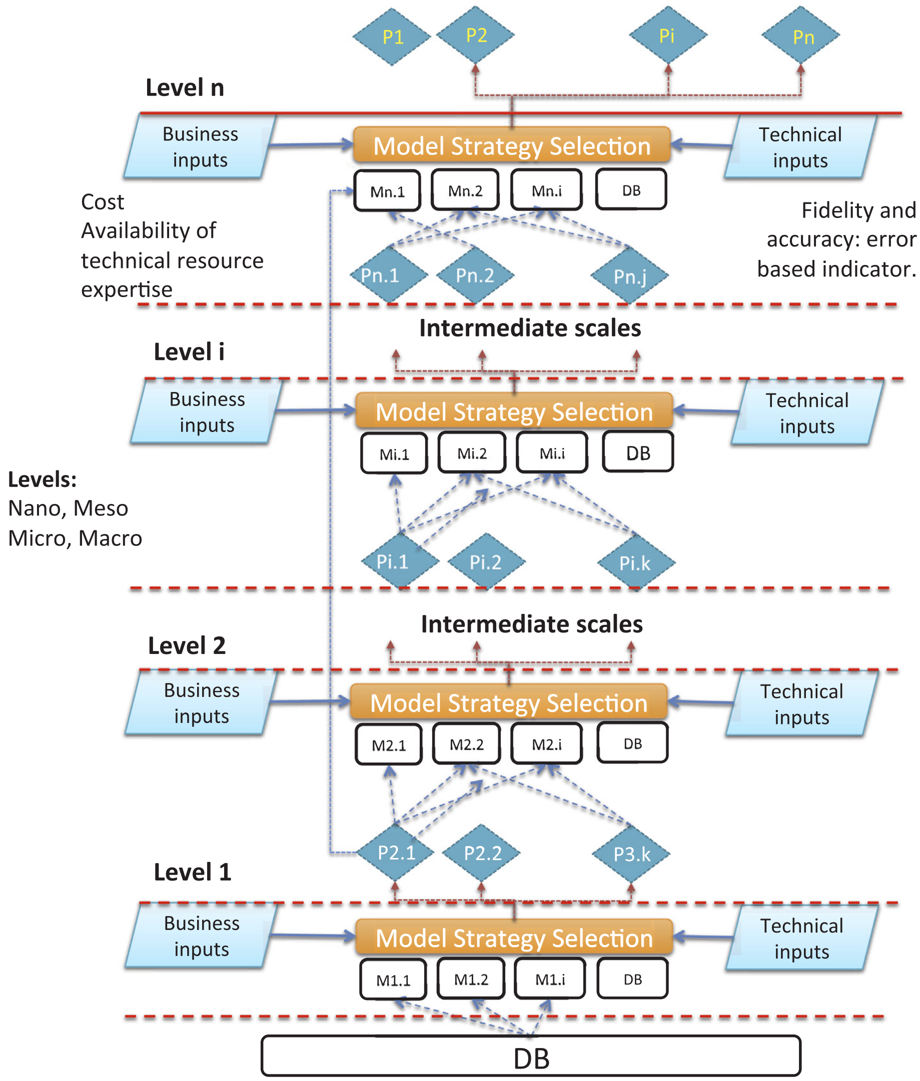

Fig. 11. Model Strategy Selection Strategy.

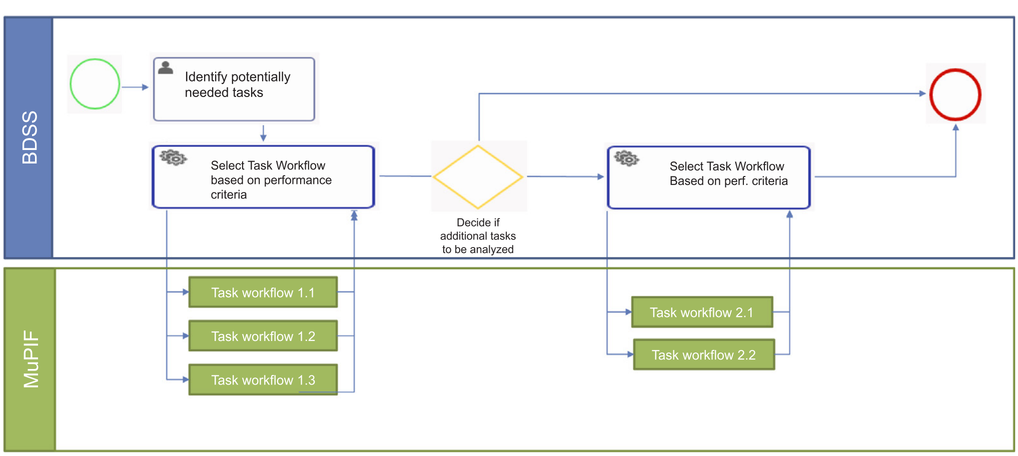

Fig. 12. Business decision should influence how the modelling should be done based on cost, time and fidelity, for example.

5.1. Key performance indicators

This application would illustrate the capability of BDSS for material and process selection for large production: (72000 parts/year +/−20%). In this specific application, the KPIs are: mechanical performances, weight, time cycle, processing, material usage, cost and life cycle engineering (see Table 1). The example of the leaf spring could be extended to all the application where the integration of the composite material in the car body structure is concerned. The individual models and associated modelling workflows are depicted on

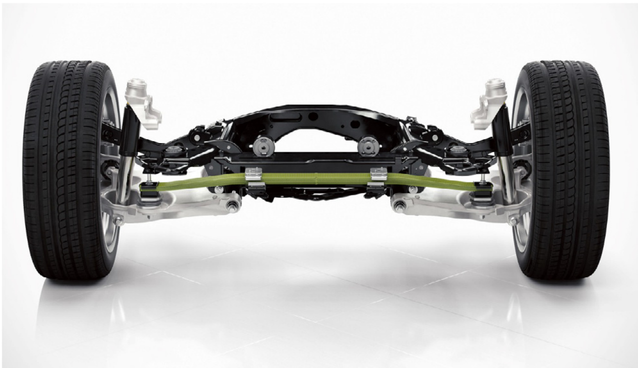

Fig. 13. Transverse Rear Leaf spring (1 per vehicle). The thickness: should come from optimisation e.g. 22 mm in the middle, 18 mm at the end. For the behaviour of the leaf spring, the stiffness and the mechanical strength and stiffness are major characteristics.

Fig. 15.

At design level, the challenge of balancing technical requirement (static and dynamic performances) with manufacturing aspects and weight reduction remains. The composite and part design (i.e. structural design) is the first important decision for material selection phase. The potential of structural design allows for the weight optimisation of the structure, not only by improving geometrical shape but also designing the final material for certain requirements i.e. structural design optimisation. The car body structure is accounting for 20–25% of the overall vehicle weight. It is also the main load-carrying structure, providing overall vehicle properties, governing handling and, more importantly, the passive safety of the vehicle. By reducing the weight of the body structure, consequent weight reductions of related systems such as engine, brakes etc. can follow which will further reduce the overall weight of the vehicle. The objective is to reduce the weight of leaf spring without any reduction on load carrying capacity and stiffness.

Table 1
Leafspring Technical and Business Key Performance Indicators.

KPI1	Minimum Stiffness: 300 N/mm
KPI2	Minimum Tensile Strength (MPa): 700
KPI3	Elongation to break 3.5%
KPI4	Production rate: 72000 parts/year +/−20%
KPI5	Flexibility: cope with a variety of sizes
KPI6	Weight reduction of 50% versus steel
KPI7	Value of weight saving: 5 Euro/kg

When focusing on high volume manufacturing such for the automotive industry, material cost is one of the main the greatest barrier for the use of composites. Consequently, despite great lightweight potential, the challenge is to achieve the weight reduction with a feasible business application. Such applications demand new approaches to composite design and manufacturing. Initial material and process selection influences many of these aspects, choices here can restrict later design and weight reduction potential by limiting structural design potential, influencing material utilisation and process efficiency.

The choice of composite material system, as well as manufacturing

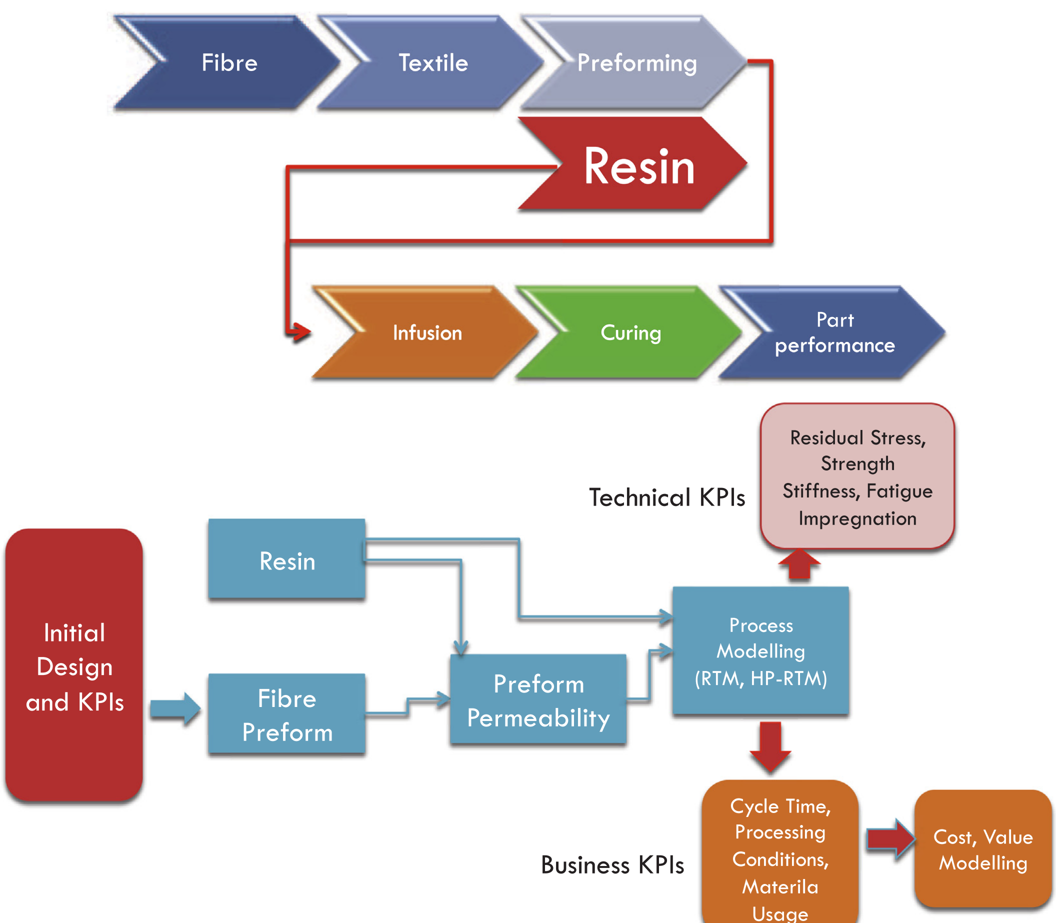

Fig. 14. Workflow describing the operational steps in the leaf-spring composite manufacturing process and related business KPI. The underlying approach for workflow selection is to connect the simulation workflow outputs and the business and technical KPIs that deliver relevant data to allow decision making.

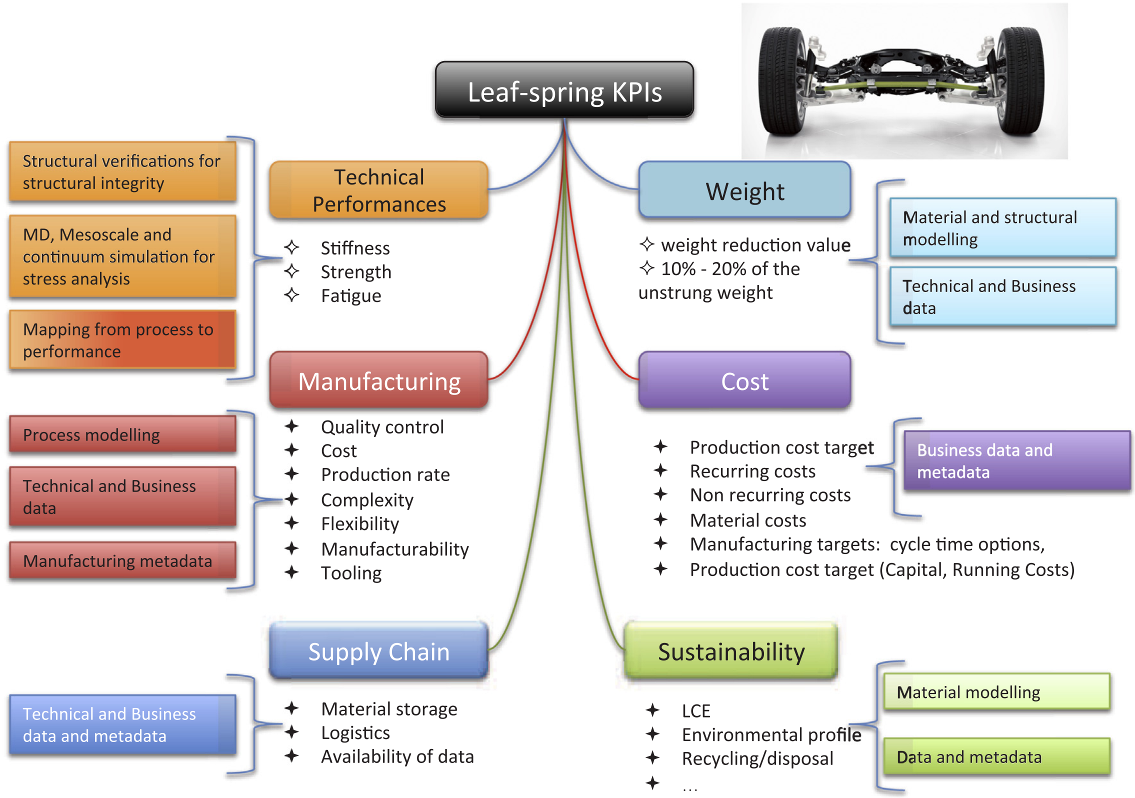

Fig. 15. Key Performance Indicators for material and process selections for the leaf-spring design and manufacturing.

Table 2
Chain of models.

MODEL 1	ATOMISTIC model (MD)
MODEL 2	MESOSCOPIC model (DPD)
MODEL 3	CONTINUUM model (properties of the tows)
MODEL 4	CONTINUUM model (modelling of the preforming)
MODEL 5	CONTINUUM model (fluid mechanics of impregnation)
MODEL 6	CONTINUUM model (curing)
MODEL 7	CONTINUUM model (final component)

process, greatly influences the final properties of the structure. For instance, liquid composite moulding processes are often more cost effective using virgin materials, fibre and resin, purchased at lower levels in the value chain. As a result, the manufacturing process becomes more complex and requires longer cycle times. Compression moulding processes on the contrary are rapid and require simpler tools and therefore less investment. These material systems, however, consequently become more expensive since the pre-impregnation of the fibres increases the value of the material system. In addition, manufacturing constraints will limit the weight reduction potential of the composite, although they will also increase the industrial relevance of the results and therefore are especially important for composites in conceptual design.

5.2. Material specifications

Epoxy Resins are used for this application. Epoxy resins are reasonably stable to chemical attacks and are excellent adherents having slow shrinkage during curing and no emission of volatile gases. Four (4) formulations with well-known ingredients (molecular structure) and well know properties will be used:

– **Epoxy I:** Longer Cure; Higher mechanical properties (Aromatic Amines); DER 330/331 epoxy + DETDA (Ethacure 100)

– **Epoxy II:** Medium Cure, Medium mechanical properties (Cycloaliphatic Amines); DER 330/331 epoxy + IPDA 30 min cure time

– **Epoxy III:** Faster Cure: 15 min cure time; Lower mechanical properties (Aliphatic Amines); DER 330/331 epoxy + TETA/DETA - typical 60 min + cure time

– **Hardener:** is mainly used to cure the epoxy resin, which causes a chemical reaction without changing its own composition. The curing time mainly depends on the hardener and epoxy mixing ratio.

– **Process Temperature:** Process temperature is another parameter to influence flowtime to cure: e.g. we could go to 15 mns cure time for the IPDA if you use higher processing times. By properly selecting the % of reinforcement and its orientation it is possible to achieve higher order stiffness and consequently higher natural frequency.

– **Formulations baseline:** 1:1 (resin–hardener ratio) with possibility to go up down 10% at both sides.

Both glass and carbon fibre option will be evaluated. Glass fibres, with a Young's modulus similar to aluminium (70 GPa), exist in different grades of strength and provides a good combination of low cost and high material properties. Carbon fibre comes in different grades: high strength (HS), intermediate modulus (IM) and high modulus (HM) are common. The most common fibre-reinforced composites are competitive engineering materials, carbon fibre composites in particular. Compared to other engineering materials, carbon fibre composites possess almost unsurpassed weight specific mechanical properties. Their greatest drawback, as described in the introduction, is their cost being very expensive at around 20 Euro/kg.

5.3. Modelling data (MODA)

The MODA defines a high level the requirements regarding input

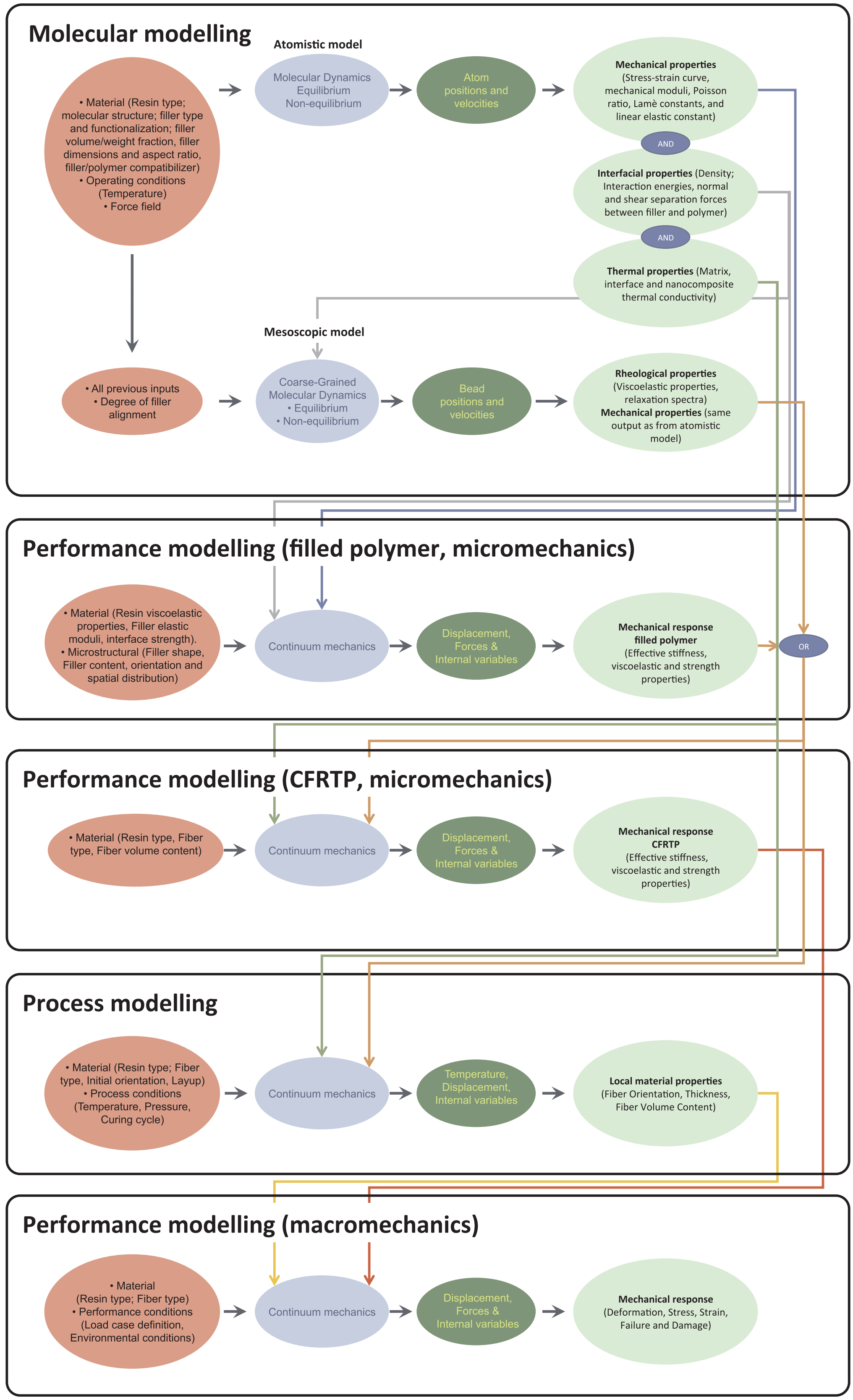

Fig. 16. Schematic representation of possible MODA workflow[13].

data, materials models (Table 2) and their coupling and linking, and the post-processing of raw data (Fig. 16) in order to arrive at the properties/technical KPIs needed for the validation of the application cases.

The atomistic model (**Model 1**) is used to calculate the system equilibrium density d at different temperatures, different degree of curing, and different chemistries. From the fitting of the two portions of the $d = f(T)$ curves in the rubbery and glassy regimes the glass transition temperature T_g can be estimated. The same model will be used to predict the elastic constant C_{11} and the bulk modulus K for the resin at different degree of curing and different temperatures. C_{11} and K are obtained by unidirectional compression/tension and hydrostatic compression/tension simulations, respectively. Finally, the Young modulus and Poisson's ratio are calculated from C_{11} and K via the fundamental relationships of linear elasticity. The temperature dependence of the Young modulus at a given degree of curing T_g can also be estimated by sigmoidal fitting of E vs T data as an alternative method. Model 1 is also employed to predict stress-strain curves for the resin at a given degree of curing and in the presence of a given amount of filler. From these data, Young modulus, tensile strength, and failure strain for the pure resin and the filler-loaded systems can be estimated. Model 1 is finally used to derive molecular quantities required to calculate the input parameters for Model 2 (Mesoscopic model), e.g., the polymer characteristic ratio, the monomer molecular volume and the solubility parameters of polymer and fillers.

Model 2 is adopted to predict the extension of the interface and the Young modulus at the interface between the resin and the filler at each given degree of curing, resin chemistry, filler loading, and filler aspect ratio. Model 2 is also employed to determine the rheological (i.e., viscoelastic properties) and thermal conductivity of the resin and the relevant filler-loaded composites as a function of the degree of curing and filler loading. Finally, Model 2 is adopted to estimate the structure and the time course of the curing reaction as a function of the chemistry.

The continuum model (**Model 3**) will be used to simulate the properties of the tows made of thousands of filaments. The aim is to estimate the mechanical properties of the tows and to produce a kinematic model of UD composite preforms that will be used in model 4.

The continuum model (**Model 4**) will be used to simulate the preform of the fibre bed. The shape and local flow characteristics of the deformed fibre bed (reinforcement) will be realistically defined for the impregnation (Model 5) and the curing processes (Model 6). The output of Model 4 will be used in for selecting the most suitable preform and preform configurations. Model 4 will predict the reinforcing fibre volume fraction and for a given set of preforming constraints and processing parameters.

Model 5 is adopted to simulate the impregnation process of the resin. Model 5 uses the outputs of Model 1 and Model 2: rheological properties of the resin, the resin kinetics and the viscosity over temperature, etc. As output, Model 5 provides volume fraction of resin, pressure field and resin velocity.

Model 6 is adopted to simulate the curing process of the thermoset requires a complete set of reliable material data. Model 6 requires a set of simulated inputs that are provided by Model 1 and Model 2. Model 6 will include solving energy and momentum equations in conjunction with pre- and post-curing, cure kinetics, thermoset shrinkage, thermal dilatation and appropriate Material Relation MR model ([13]) of the polymer to predict temperature and residual stress fields. Model 6 will be used to predict the material microstructure evolution due to curing.

Simulated deformation and stress results after curing (Model 6) will be used in **Model (7)** to estimate the leaf-spring structural properties.

6. Conclusion

In this paper, a new approach aiming at coupling material modelling with business data and models have been presented. The objective is develop a Business Decision Support System (BDSS), which integrates materials modelling, business tools and databases into a single workflow to support the complex decision process involved in the selection and design of polymer-matrix composites (PMCs) by means of an open integration platform which enables interoperability and information management of materials models and data and connects a "rich" materials modelling layer with industry standard business process models. The BDSS and the modelling capabilities as developed within COMPOSELECTOR will be used both optimal material use and control of material production. The results of such calculations will permit the fast qualification of existing products but also open new opportunities for optimal and advanced material selection thanks to the integration of materials modelling, business tools, and databases into a single workflow. The challenges implied by the massive use of composite materials e.g. in aerospace and transports fields, are tremendous. Diminishing cycle-time, automatised processes, and improving material selection are a key factor to lower the costs and increase the competitiveness. For transport applications, for instance, enhancing the performance and footprint by improving performances over mass (e.g. size and strength per mass) is among the most notable material selection and design challenges. In terms of polymer based composite material selection and design, this challenge can be won only via a tool that allows effective, rational and fast screening, assessing and cross-comparing of all the different and complex drivers that govern them. An indicator of the industrial impact of such a system is a series of three patents taken out by Boeing in recent years. Particularly, the integration of material modelling in business decision support system, as proposed in COMPOSELECTOR, will contribute to increase the fraction of critical decisions informed by modelling and simulation and anticipate the reengineering effects in a quantitative way. Furthermore, it is expected that an improved composite material selection made possible by the use of the developed business decision platform will allow substantial improvements in the design and process manufacturing as well. Indeed, the integration of materials in BDSS can transform the way engineers understand, and ultimately design and manufacture materials and will contribute to a better-informed decision-making process in the early development stages of products, particularly with regards to the analysis and selection of composite material and their manufacturing processes. The ability to integrate complex components (composite material behaviour, process design and LCE for instance) to study their interactions. Indeed, one of the main features of the BDSS as described in this paper is the possibility of flexible integration and connection to external third partly applications. Therefore, offering the possibility to balance among performances, manufacturing as well as economic and life cycle aspects.

Acknowledgement

The authors would like to acknowledge the support of EU H2020 COMPOSELECTOR project (GA no: 721105). The authors would like to express their appreciation to the EMMC community for many useful inputs, exchange and valuable comments. The views expressed on this paper reflect the views of the authors. The European Commission is not liable for its content and the use that may be made of the information contained herein.

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Further reading

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