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Bringing together materials and business ontologies for protective coatings

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Abstract

This work discusses how to connect business decision support systems, implemented in terms of the BPMN and DMN standards, with materials modelling workflows. The suggested approach facilitates interoperability of materials modelling software tools covering the main phenomena involved in advanced corrosion protection and active protective coatings' behaviour. The proposed system integrates materials modelling methodologies with decision support in business processes using a knowledge-based architecture. Thus, this contribution showcases the missing link between business processes, materials science, and computational engineering workflows for industrially relevant use cases; here, specifically, corrosion and protective-coating modelling. At the implementation level, we report on novel features of the process modelling suite ProMo for ontology and process-topology based materials modelling workflow construction and documentation. ProMo is extended to address challenges specific to the H2020 project VIPCOAT which works toward establishing an open innovation platform for active protective coatings and accelerated corrosion tests, including assessments of their in-service durability. Connections between quantitatively reliable materials modelling tools, their integration into simulation workflows, and ontology-based knowledge representation are considered, addressing the use case from VIPCOAT.

Keywords

applied ontology, decision support system, multiphysics modelling and simulation, open innovation platform, process topology notation, protective coating ontology, workflow management system

1. Introduction

Digitalization efforts in the engineering and materials development domains are today introducing new methods for digital collaboration and open innovation, like the one proposed in VIPCOAT project. Development projects implementing digitalization approaches can offer multi-sided platforms, pursuing the goal of creating a collaborative environment to connect


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modellers (software owners, academia), translators [1], manufacturers, governmental bodies, and society to initiate and implement innovation projects. In parallel, an enormous amount of materials, manufacturing and processing data are currently generated by high throughput experiments and computations, possessing a significant challenge in terms of data integration, sharing and interoperability. A common ontology lays the foundation for solving these issues, enabling semantic interoperability of models, experiments, software and data, which is vital for using rational development design principles and testing and manufacturing of materials in general. The basic idea is to merge business decision support systems implemented in terms of the BPMN and DMN standards, with materials modelling workflows by using ontologies as a glue. The general approach used in the work is showcased by demonstrating interoperability for modelling phenomena involved in advanced corrosion protection. To this end, suitable business process models are constructed utilizing the BPMN and DMN standards and integrated with the materials modelling workflow constructions in the VIPCOAT open innovation platform (OIP) based on the ProMo (process modelling) ontological model for materials models and ontologizations of BPMN/DMN.

2. ProMo for modelling workflows

The process modelling tool ProMo is an ontology-driven computational engineering suite. It first builds an application-focused ontology that defines the fundamental entities and declares the variable classes. The ontology then provides the rules for defining the mathematical representation of each fundamental entity with a set of equations. Each equation is compiled into several target languages, including LaTeX for documentation and OWL for the uptake by knowledge-graph based semantic-web infrastructures [2]. The outcome can be used in a semantic network to generate APIs for the ProMo-generated simulation task and its interaction with databases, and the variable/expression set extends the ProMo ontology toward an application-specific ontology. This automated annotation mechanism avoids that simulation outcomes decay into dark data that have an unknown epistemic status and therefore cannot be reused [3]. ProMo uses a graphical representation of the model. The visual design language is currently subject to a CEN workshop agreement. In the suite, each fundamental entity is assigned to a graphical object, allowing for a pictorial composition of process models. Physical behaviour is represented as a network of extensive-quantity-communicating capacities. Each capacity stands for a part of the space. These volume elements are often referred to as control volumes, as one balances what goes in and out through the surface and is not consumed with the accumulation inside.

The ontology provides the basic building blocks, the fundamental entities. Then, those are combined to construct the overall model. The mereological information is encoded into the model's hierarchical tree. The internal nodes in the tree, we term composite entities. Replacing parts of the topology (usually, composite entities) by surrogates generates the skeleton of the modelling workflow. The model structure, thus its mereology, the block's nature and the interactions are described in OWL DL, thereby providing the data ontologies for the block interactions. The ProMo/semantic network enables auto-generation of APIs that provide mechanisms for multiple applications to communicate within a shared local data space. At

workflow run time, the tasks exchange data; specifically, simulation blocks receive data from other blocks upon request, and blocks can push information to other blocks within the same sequence. This exchange process is event-driven and can be represented as a discrete event system, e.g., by a Petri-net-like formalism. Thereby, the occurrence of an event (e.g., execution of a workflow step) is enabled once all the required data are available.

3. Ontology and BPMN based platform for protective coatings

The business process model and notation (BPMN) 2.0 standard offers the possibility to graphically construct and automatically orchestrate business processes and any kind of computational workflows. BPMN offers a standardized bridge for the gap between business process (BP) design, process implementation, and materials modelling, cf. Fig 1. BPMN can also handle B2B BP concepts, such as they are used in the VIPCOAT framework for open innovation (OI), as well as advanced modelling concepts. Ontologies for BPMN 2.0 are in existence already [4]. Here we report on the development of a generic ontology that goes beyond this state of the art by enabling a fine-grained BP representation consistent with the quadruple-helix OI model. The quadruple-helix model has been enjoying an increasing uptake [5], and in the VIPCOAT H2020 project, it is applied to protective-coating related innovation. The knowledge dimension is one of the most relevant aspects of BP modelling. It considers knowledge used, mobilized, and produced during an activity (accounting for different types of knowledge), as well as the sources of knowledge, their localization, the flows between knowledge sources and activities, collaborations and interactions, etc. The core of the ontology is extracted from the BPMN 2.0 meta-model [6] and enhanced with taxonomies, concepts, relations and attributes in order to meet requirements from open innovation in materials modelling. Once populated with BP data, the ontology yields a knowledge base (KB) that can be exploited by virtual agents to support operators at a step-by-step BP execution. Decision nodes, supporting the DMN standard, are included in order to implement decision models in terms of business rules. Decisions are represented in terms of business rules [7], which automates the most common decisions and promotes consistent results when used many times. The results of the simulation and market prices or life cycle engineering (LCE) obtained from other tasks are also taken into account. Keeping decision logic separated from process logic provides better consistency across the whole enterprise, making also decision logic auditable and traceable.

4. Conclusions

The reliability of a decision-making process depends on the availability and quality of the information, but also on the flow of the information and the modelling and simulation processes and tools necessary to confidently describe and evaluate the critical key performance indicators (KPIs) of a given product development business, accounting for a business case (BC), an industrial case (IC), and a translation case (TC), following EMMC ASBL nomenclature [8]. BPMN and DMN together with the ProMo process-modelling software provide strong support to representing processes and the associated decision making. We demonstrate this in the context of protective coating, linking business processes, materials science, and computation engineering workflows.

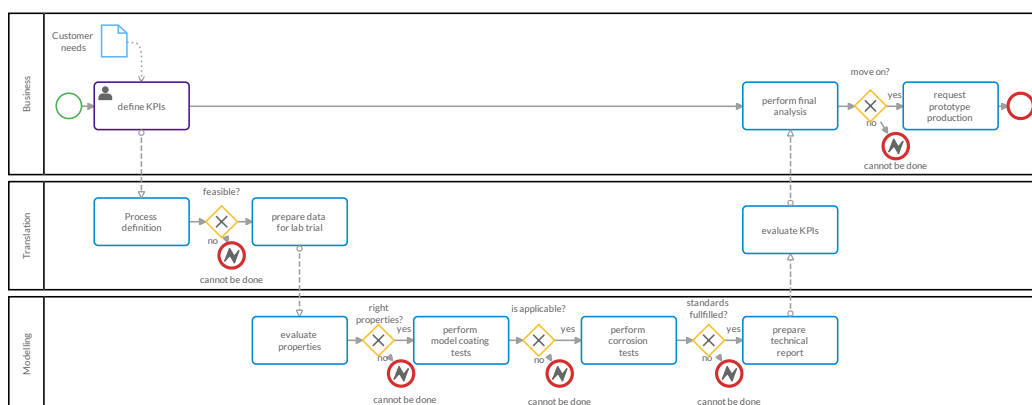


Figure 1: BPMN in an OI context: Bridging gaps between business, translation, and modelling activities.

BPMN and ProMo can be used at this stage to provide the missing link between business processes and materials science/engineering workflows. As a result of this methodology, we produce an interconnected database, multi-model, multidisciplinary optimization and data-analytics software tool for business decision support in a unifying framework.

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