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Chemical enterprise model and decision-making framework for sustainable chemical product design

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ABSTRACT

The chemical product substitution process is undertaken by chemical industries for complying with regulations, like REACH in Europe. Initially devoted to chemists, chemicals substitution is nowadays a complex process involving corporate, business and engineering stakeholders across the chemical enterprise for orienting the search toward a sustainable solution. We formalize a decision making process framework dedicated to the sustainable chemical product design activity in an industrial context. The framework aims at improving the sharing of information and knowledge and at enabling a collaborative work across the chemical enterprise stakeholders at the strategic, tactical and operational levels. It is supported by information and communication technologies (ICT) and integrates a computer aided molecular design tool. During the initial intelligence phase, a systemic analysis of the needs and usages enables to define the product requirements. In the design phase, they are compiled with the help of a facilitator to generate the input file of a computer aided product design tool. This multiobjective tool is designed to find mixtures with molecular fragments issued from renewable raw materials, and is able to handle environment-health and safety related properties along with process physicochemical properties. The final choice phase discusses the solution relevancy and provides feedback, before launching the product manufacturing. The framework is illustrated by the search of a bio-sourced water–solvent mixture formulation for lithographic blanket wash used in printing industry. The sustainability of the solution is assessed by using the sustainability shades method.

1. Introduction

The chemical manufacturing industry is on the frontline of sustainable development as its product and process activities often strongly impact the environment and people's health and safety. Indeed chemical industries are reconsidering the products that they use and produce, under the pressure of regulations like REACH [1] and VOC directives [2] or of consumers wanting eco-labeled products. They do so from a "doubly green chemistry" perspective: one green for the use of renewable raw materials and one green for the reduction of their impacts [3]. The management of sustainability during the product development cycle is becoming the new paradigm of chemical manufacturing industries [4–6]. It is inducing a shift from a cost-driven development to a sustainability-driven development [7]. Within the sustainability context and driven by the 12 principles of green chemistry and the 12 principles of green engineering [8,9], specific issues must be looked at: the use of renewable materials, the minimization of energy and material resources consumption, the evaluation of impacts on environment, the consideration of health and safety, the selection of appropriate criteria to assess sustainability [10] and the selection of consistent life cycle methods covering economics, environmental and social issues [11]. However these issues are a concern for hard science engineers that are not the only people to be involved when designing a new product. Indeed, the chemical product development process involves many stakeholders across the chemical enterprise. The market department will get involved for cost analysis, market trends and user needs assessment. R&D chemists, chemical engineers and process operation engineers bring knowledge and expertise in product properties, in process constraints and in product and process design. The quality

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Nomenclature

BPMN	business process modeling notation
CAMD	computer aided molecular design
CAPD	computer aided product design
DSM	Design Structure Matrix
EHS	Environmental, Health, Safety
ICT	Information Communication Technology
LCA	Life Cycle Analysis
LISI	levels of information system interoperability
LCIM	level of conceptual interoperability model
MDE	model driven engineering
MMI	Man Machine Interface
OCL	Object Constraint Language
OIM	organizational interoperability maturity
PSE	process system engineering
QFD	Quality Function Deployment
QSAR	Quantitative Structure Activity Relationship
QSPR	Quantitative Structure Property Relationship
RED	property name expressing the ratio of Hansen Solubility Radius versus the HSP sphere radius for a given product
RM-ODP	Reference Model of Open Distributed Processing
SBVR	Semantics of Business Vocabulary and Rules
SME	Small Medium Enterprise
UML	Unified Modeling Language
VOC	Volatile Organic Component
XML	Extensible Markup Language

management department is responsible for ensuring the product quality through norms and means to achieve it. The business process experts will be managing production and chemical supply chain; corporate managers.... Hung et al. [12] wrote: '*Effective product development depends on the integration of a variety of specialized capabilities, strong functional groups with interdisciplinary teams and multiple progressive pressures. New product development [...] involves cross-function integration, a complicated interdisciplinary activity that requires many knowledge inputs to generate a suitable product solution as well as an appropriate project plan in the time-competitive environment*'. This stresses the importance of information and knowledge management between people that are coming from different cultures and the importance of bringing them to consider all the sustainability issues together.

In this context, we develop an ICT based decision-making frame to improve the collaborative participation between all stakeholders in the development of sustainable chemical products. To our knowledge it is the first time that such a framework is coupled with a computer aided molecular design for finding chemical product, and that this coupling is specially aimed at sustainable chemical product development. Section 2 surveys a background on chemical product development activity issues and on enterprise-wide product engineering. Section 3 reviews limitations of existing approaches and tools. It identifies five challenges and suggests solutions. Section 4 describes our ICT solution and computer-aided chemical product development. It is split into a description of the chemical enterprise perspective and of the different phases of the decision process. It incorporates a distributed computing solution aiming at finding chemical products satisfying predefined requirements within a sustainable context. Section 5 describes a detailed industrial based case study aiming at finding a novel ink wash-blanket solvent in a printing manufacture.

2. State of the art

2.1. Chemical product development

Hill [5] stated that chemical product development covers "(1) chemical product design and development, and (2) product-oriented process design and development", also called chemical product engineering [4]. We restrict ourselves to the first issue in this paper.

2.1.1. Product classification

Refs. [13,14] classified products in basic, structured and configured-consumer products. Basic/functional chemicals encompass commodity, intermediate and specialty chemicals that are designed for achieving one function (solvent, reactant) and for matching only a few key physicochemical properties (solvent power, boiling point, etc.). Structured products and configured-consumer products combine many properties and functions in a single product, which is often a mixture. Structured products (cream, films, etc.) or industrial chemicals are assemblies of basic chemicals [4,15]. Some of their properties can be set by the product manufacturing process itself [5,16], which induces a simultaneous design of the product and process. Configured-consumer products (drug delivery patches, post-it note, drug pill...) target the end-user markets and are assemblies of several industrial products with a focus on their physical construction [15]. For all product classes, the set of requirements is complex. It can include qualitative sensory factors, environment, health, safety (EHS) impact-related properties, stability and flowing considerations along with more traditional physicochemical properties. Costa et al. [4] focused on product perceived quality factors and identified three property classes: product properties, process-related properties and usage-related properties to encompass all the product technological requirements.

2.1.2. Product design solutions

For designing a new chemical product, the traditional trial and error bottom-up approach is intrinsically inefficient. It proceeds as follow: given a raw material, perform chemical, physical or biochemical transformations to make a molecule; then check properties and see a posteriori if the expected requirements are matched. Instead, top-down reverse engineering approaches focus in needs first: they define a priori a set of target property values and search for complying molecules, either into databases or by building them from a pool of small chemical elements. Reverse engineering is nicely implemented within computer-aided molecular design (CAMD) tools [17–19]. Those tools rely upon a multi-objective optimization technique to build candidate molecules and upon property estimation models to evaluate the candidate performance vs. the set of a priori target property values. The use of accurate property prediction methods is recommended to legitimate the CAMD predictive process. Nevertheless, experimental synthesis and validation completes the CAMD process. Within the CAMD tools, the objective function can aggregate any types of property for which exists an estimation model based on the molecular and product structure. We identify group contribution methods [20–23], QSAR/QSPR methods [24], similarity models for toxicity models [25] and arbitrary scaling methods for sensorial properties [26].

For mixture products, each mixture component can be designed and property models with linear or non-linear dependency on the mixture composition must be considered. Most computer aided product design (CAPD) tools perform a sequential search of each product components individually for example by using CAMD, before checking mixture properties and mixture stability [27–30] or decompose the overall problem into a subset of subproblems [31]. This prompted us to develop in parallel to the present paper