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Co-constructive development of a green chemistry-based model for the assessment of nanoparticles synthesis

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ABSTRACT

Nanomaterials (materials at the nanoscale, 10^{-9} meters) are extensively used in several industry sectors due to the improved properties they empower commercial products with. There is a pressing need to produce these materials more sustainably. This paper proposes a Multiple Criteria Decision Aiding (MCDA) approach to assess the implementation of green chemistry principles as applied to the protocols for nanoparticles synthesis. In the presence of multiple green and environmentally oriented criteria, decision aiding is performed with a synergy of ordinal regression methods; preference information in the form of desired assignment for a subset of reference protocols is accepted. The classification models, indirectly derived from such information, are composed of an additive value function and a vector of thresholds separating the pre-defined and ordered classes. The method delivers a single representative model that is used to assess the relative importance of the criteria, identify the possible gains with improvement of the protocol's evaluations and classify the non-reference protocols. Such precise recommendation is validated against the outcomes of robustness analysis exploiting the sets of all classification models compatible with all maximal subsets of consistent assignment examples. The introduced approach is used with real-world data concerning silver nanoparticles. It is proven to effectively resolve inconsistency in the assignment examples, tolerate ordinal and cardinal measurement scales, differentiate between inter- and intra-criteria attractiveness and deliver easily interpretable scores and class assignments. This work thoroughly discusses the learning insights that MCDA provided during the co-constructive development of the classification model.

1. Introduction

Nanotechnology is the manipulation of matter at the nanoscale (one billionth of a meter, 10^{-9} meters) to produce materials (i.e., nanomaterials) with enhanced performances. During the last decade it has experienced a sizeable development (Iavicoli, Leso, Ricciardi, Hodson, & Hoover, 2014; Shapira & Youtie, 2012; 2015). Plethora of nanotechnology applications are emerging in several industrial sectors (e.g., biomedical, cosmetics, electronic, energy, engineering, textile, packaging, food and drinks) and due to its pervasive nature there is a pressing need for assessing the implications of this fast-pace development on the environment, economy and society (Iavicoli et al., 2014; Karn & Wong, 2013; Shapira & Youtie, 2015). Achieving this objective involves the use of multiple assessment criteria, which represents a complex decision problem with conflicting viewpoints. This paper contributes to this area by proposing a Multiple Criteria Decision Aiding (MCDA) approach to support environmentally sustainable synthesis of nanomaterials.

The synthesis stage has been a premier focus of the research on nanomaterials development, as it is the fundamental step where the design of the product is defined, the functionality is shaped, the reliability empowered and an important contribution to the sustainability implications is determined (Dahl, Maddux, & Hutchison, 2007; Hutchison, 2008; Patete et al., 2011). In order to guarantee a responsible supply of nanomaterials many synthesis processes have been developed to take their sustainability impacts

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into consideration. In this way, the principles of green chemistry (Anastas & Warner, 1998) and engineering (Anastas & Zimmerman, 2003) started being integrated into this life-cycle stage (Anastas & Warner, 1998; Eckelman, Zimmerman, & Anastas, 2008; Gilbertson, Zimmerman, Plata, Hutchison, & Anastas, 2015; Hutchison, 2008; Patete et al., 2011).

Indeed, these innovative approaches account for such principles by increasing energy efficiency, using renewable and less hazardous materials, increasing speed reactions and ensuring safer operating conditions (Dahl et al., 2007; Gawande, Shelke, Zboril, & Varma, 2014; Nadagouda et al., 2014; Patete et al., 2011; Varma, 2013; 2014; Virkutyte & Varma, 2013). At the same time, they succeed to produce nanoparticles with desired uniform size and shape. To assess the implementation of green chemistry principles by the synthesis protocols, it is necessary to account for a number of evaluation criteria in an integrated manner. This suggests the appropriateness of using MCDA methods whose role is to provide and justify decision recommendations in the presence of multiple conflicting points of view. More specifically, there is currently a demand for classification methods that can be used to assign a preference-oriented performance class to the synthesis processes for nanomaterials, showing how "green" they actually are (Bergeson, 2013; Gilbertson et al., 2015; Mata, Martins, Costa, & Sikdar, 2015).

This paper proposes an MCDA model for classifying synthesis protocols into a set of pre-defined and ordered green chemistry-based classes and exemplifies its application for the silver nanoparticles, particles of silver at the nanoscale. The methodology that supported the model development implements the paradigm of Ordinal Regression (ORDREG) (Jacquet-Lagrèze & Siskos, 2001) (or preference disaggregation, Doumpos & Zopounidis, 2011) by inferring compatible models composed of an additive value function and extrapolating class thresholds from the assignment examples provided by nanotechnology experts. Then, these models are used to suggest an assignment for the remaining protocols. This work has been conceived as a complementary strategy to the one advanced by Cinelli et al. (2015) where Dominance-based Rough Set Approach (DRSA) (Błaszczyński, Słowiński, & Szelag, 2011; Greco, Matarazzo, & Słowiński, 2001) was employed to the same problem and provided a classification model based on decision rules.

The proposed integrated approach combines a few procedures whose properties were found to be useful to support sustainability assessment and it contributes to the preference learning process that is hallmark of MCDA. First, the method is able to integrate the expert knowledge, being usable even in case the provided preference information is inconsistent. This is achieved by automatic identification of all maximal sets of consistent assignment examples. Second, it effectively deals with both qualitative and quantitative criteria by applying general value functions. Third, the approach constructs a representative model that indicates which factors are most important for the classification. This model differentiates also the intra-criterion attractiveness with possibly non-convex or non-concave shape of a marginal value function. Fourth, it quantifies how green the synthesis protocols are by performing aggregation of alternatives' evaluation on all considered criteria. Fifth, thanks to the applied threshold-based classification procedure, the underlying decision aiding process is intuitive and transparent even for the non-experts in MCDA field. Sixth, the delivered recommendation is easily interpretable and justifiable due to the decomposition of overall values into marginal ones. The latter provide thorough insight into each protocol's strengths and weaknesses. Finally, the method builds on the synergy of ORDREG methods. In this way, it provides means for verifying the certainty of an assignment suggested by a single representative model against the outcomes of Robust Ordinal Regression (ROR) (Corrente, Greco, Kadziński, & Słowiński, 2013; Greco, Mousseau, & Słowiński, 2008) and Stochastic Ordinal Regression (SOR) (Kadziński & Tervonen, 2013a; 2013b) derived from all classification models compatible with all maximal sets of consistent assignment examples. ROR indicates which assignments are possible using Linear Programing (LP) techniques, whereas SOR estimates the probability of such possibility with Monte Carlo simulation. In this way, the constructed recommendation can be deemed robust.

By exhibiting all these features when reporting results of the case study, the paper aims to show that the proposed method is able to effectively support not only the development and assessment of nanoparticle synthesis, but also other decision making contexts oriented toward sustainability. Overall, this paper has the following objectives:

- Propose (Section 2) and test (Section 3) a new methodology based on ORDREG for classification of synthesis processes of silver nanoparticles based on green chemistry principles implementation.
- Highlight the practical learning derived from the use of MCDA in this applied research. Throughout the paper, we illustrate how MCDA is a ductile process that allows structuring a complex and undefined problem, define the alternatives to be assessed, the evaluation parameters and shape a robust decision support model.

2. Methodology

An important issue in nanotechnology is the development of production processes for nanomaterials, since they have a pivotal role in determining the properties of the ensuing product, its reliability and the impacts that it can have from a sustainability perspective (Duan, Wang, & Li, 2015; Sengul, Theis, & Ghosh, 2008). The processes that received major attention in the last decade are those performed with more responsible, green and sustainable approaches, integrating the principles of green chemistry and green engineering in the nanosynthesis practice (Dahl et al., 2007; Duan et al., 2015; Gilbertson et al., 2015; Mata et al., 2015; Nadagouda et al., 2014; Patete et al., 2011; Varma, 2013; 2014).

So far bacteria, fungi, plants, plants extracts, yeasts and algae have been employed to produce nanomaterials, receiving the label of bio-inspired reduction approaches and employing several principles of green chemistry, including renewable materials use, synthesis at ambient temperature and pressure as well as safe processing conditions (Das & Marsili, 2011; Korbekandi, Iravani, & Abbasi, 2009; Stark, Stoessel, Wohlleben, & Hafner, 2015; Virkutyte & Varma, 2013). Understanding and assessing how "green" these bio-inspired processes are is hampered by several challenges, including (i) the need to account for impacts criteria of different type (e.g., quantitative, qualitative, fuzzy) (Eason, Meyer, Curran, & Upadhyayula, 2011; Mata et al., 2015; Naidu, 2012), (ii) high uncertainty in input dataset (Hischier, 2014; Mata et al., 2015; Meyer & Upadhyayula, 2014), and (iii) limited capacities of conventional tools to provide a comprehensive and justifiable performance of each process (Bates, Larkin, Keisler, and Linkov, 2015; Eason et al., 2011; Tsang, Bates, Madison & Linkov, 2014).

MCDA has been specifically developed to tackle these types of challenges (Cinelli, Coles, & Kirwan, 2014; Munda, 2005), especially in cases where the problems are ill-defined, which is another peculiar characteristic of sustainability assessment of nanosynthesis. Such problem framing justified the use of MCDA in the case study, to develop a classification model for the performance evaluation of synthesis of nanomaterials with respect to implementation of the green-chemistry principles. The research objective was achieved through the application of the MCDA process, tailored to this decision making problem. Fig. 1 summarizes the procedure. Its phases are described in detail in the following sections.