Project title:

Advanced web tools for promoting the application of nanotechnology and the safe use of nanomaterials in the plastic sector

Project Acronym: **NanoDesk**

Project Code: **SOE1/P1/E0215**

Report Title

E. A1c Decision making system based on Multi-criteria Decision Analysis (MCDA)

Coordinator and Responsible of the Document

ITENE

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EXECUTIVE SUMMARY

The objective of activity A1.3 is the development of a tool able to support the identification and selection of the most appropriate Engineered Nanomaterials (ENMs) that can be employed in the plastic sector to enhance specific properties of the compound. The tool, which is available both in Microsoft Excel format and as a multilanguage web application, consists in a decision-making system based on Multi-Criteria Decision Analysis. The most significant variables determining whether a nanomaterial is suitable for a specific use or application have been identified (selection criteria) and quantified, establishing a hierarchy and assigning them a punctuation. This system of criteria has been then implemented in a Microsoft EXCEL application with the use of Visual Basic (VB) programming language and as a web application available to Stakeholders in the NanoDesk online platform.

LIST OF ACRONYMS

ENM: Engineered Nanomaterial
MCDA: Multi-Criteria Decision Analysis
VB: Visual Basic

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1. OBJECTIVE OF THE TOOL

The project SUDOE NanoDesk is focused on the promotion of nanotechnology as a fundamental instrument for the development of new plastic materials. Studies have shown how the presence of nanomaterials provides the compounds with new properties of high added value with respect to the same material in bulk form, or permits the enhancement of already existing ones. However, in the selection of the most appropriate nanomaterial to be employed in a specific product, not only the benefits in terms of acquired or enhanced properties needs to be considered, but also the potential risks it poses both for the human health and the environment.

The main objective of the project is the development of a web-platform meant to encourage the diffusion in the market and the application of nanocomposites, but also to act as knowledge transfer structure. The idea is to provide the plastic market with an instrument capable to ensure the quality of the nanostructure polymers produced, guarantee the protection of human health and environment and foment the demand of products with enhanced properties in the plastic sector, increasing research and competitiveness.

Action A1.3 falls under this scope and aims at building a system for decision making to assist the companies of the plastic sector in the selection of the most appropriate nanomaterial to use, according to their needs. Based on Multi-Criteria Decision Analysis, (MCDA) A Microsoft EXCEL application has been designed using the Visual Basic (VB) language. The selection of the adequate nanomaterial is influenced by different factors, or variables. The target of our Tool is the entrepreneur trying to get in touch with nanotechnology applied to plastic products or eager to know more about the options available in the market. In order to make the tool available to all Stakeholders and interested users, the decision support system has been also integrated in the NanoDESK web platform.

The user will select the industrial sector he belongs to and the property he wants to improve or confer to the product by means of the use of nanomaterials. However, different factors can influence the selection, like price, availability in the market and hazardousness of the substance, all aspects which are directly taken care by the tool. These factors constitute the starting point to define a set of specific selection criteria and the application quantifies them, establishing a hierarchy and assigning a punctuation to each substance considered, and eventually suggests the user the best options for the industrial sector and product selected.

More details about the substances included, the selection criteria and the punctuation system will be given in the following sections.

2. MULTI-CRITERIA DECISION ANALYSIS

2.1. Definition of Multi-Criteria Decision Analysis (MCDA)

Multi-Criteria Decision Analysis, or MCDA, is a valuable tool that can be applied to many complex decisions. It is most appropriate to solving problems that are characterized as a choice among alternatives. The common purpose of these methods is to evaluate and choose among alternatives based on multiple criteria using systematic analysis to overcome the limitations of unstructured individual or group decision making.

MCDA methods use to proceed via the following steps:

1. Definition of the problem, based on stakeholders' inputs;
2. Generation of the alternatives through the help of stakeholders, including experts;

3. Formulation of criteria and subcriteria by which the alternatives must be judged, and development of hierarchies based on stakeholders' judgement;
4. Gathering of information about the relative importance of criteria, that is establishing the weights of the different criteria in the decision-making process;
5. Systematic choice of the appropriate alternatives by specifying well defined algorithms using criteria scores and weights.

2.2. Alternatives

In Table 1 the possible nanomaterials that can be used as filler for polymeric matrix that we selected as alternatives in our MCDA method are listed. More details about the reasons of the selection can be found in the Deliverable A1a.

Table 1: List of the alternatives considered in the decision-making process.

Name	Formula
Titanium dioxide	TiO_2
Zinc oxide	ZnO
Silicon dioxide	SiO_2
Copper oxide	CuO
Aluminum oxide	Al_2O_3
Silver	Ag
Nanoclays	-
Carbon black	C
Graphene	C
Fullerenes	C
Single-walled nanotubes	C
Multi-walled nanotubes	C
Gold	Au
Calcium carbonate	$CaCO_3$

2.3. Determination of selection criteria and hierarchy

The choice of the appropriate nanomaterial to use in a specific industrial sector or for a specific product can be affected by a large number of variables, concerning both the role of the substance in the market and its hazardousness. The main selection criteria we chose belong to both classes and are listed in Table 2.

Table 2: Main selection criteria considered in the Multi-Criteria Decision Analysis.

Main criteria:
Inhalation toxicity

Freshwater toxicity (Daphnia)
European production per year (tons/year)
Price (€/kg)
Freshwater toxicity (Fish)
Oral toxicity

To this group belongs the most probable route of exposure of human to substances, inhalation, and the hazardousness of the material to the aquatic species more sensitive to water contamination (Daphnia and fish), since we want the companies of the plastic sector to make a safe use of nanomaterials. However, we want our approach to the industry to be realistic and to consider the needs of the different stakeholders. Therefore, we included in the main criteria also the price of the material and its availability in the market, since our objective is to provide the plastic industry with solutions which are affordable and easy to adopt.

In Table 3, a list of secondary factors influencing the selection of the nanomaterial, and which are taken into account in the MCDA, is shown. Among them the other, less likely, routes of exposure to ENMs for humans.

Table 3: Secondary factors included in the decision-making system.

Secondary factors:
Dermal toxicity
Genotoxicity
Cytotoxicity
Reproduction toxicity
Freshwater toxicity (Algae)
Soil toxicity (Worms)

Within each criterion or factor, it is possible to choose, for every substance, between five different qualitative levels (very high, high, medium, low, very low) plus the “not rated” option in case the information is not available in literature. (see Table 4 and Table 5).

2.4. Scoring system and relative weights

The criteria above are used to assign a score to the nanomaterial we included in our MCDA Tool.

The scoring system we applied is schematically represented in Figure 1. The main criteria determine the 90% of the punctuation, while the remaining 10% is given by the secondary criteria. The single criterion has its own weight, no matter if it is main or secondary. In the case of the main criteria, weights have been assigned based on the following list of priorities:

- human health;
- environmental safety;
- affordability of the product,

and keeping in mind that the sum of the weights must return one. To the secondary criteria have been assigned the same importance, which is simply 1/6.

Within the single criteria, we defined different levels and established the punctuations corresponding to each of them. These punctuations go from 0 to 90 in the case of the main criteria, and from 0 to 10 in the case of the secondary ones, where to higher scores correspond better properties. Main and secondary criteria with corresponding weights, levels and punctuations are listed in Table 4 and Table 5, respectively.

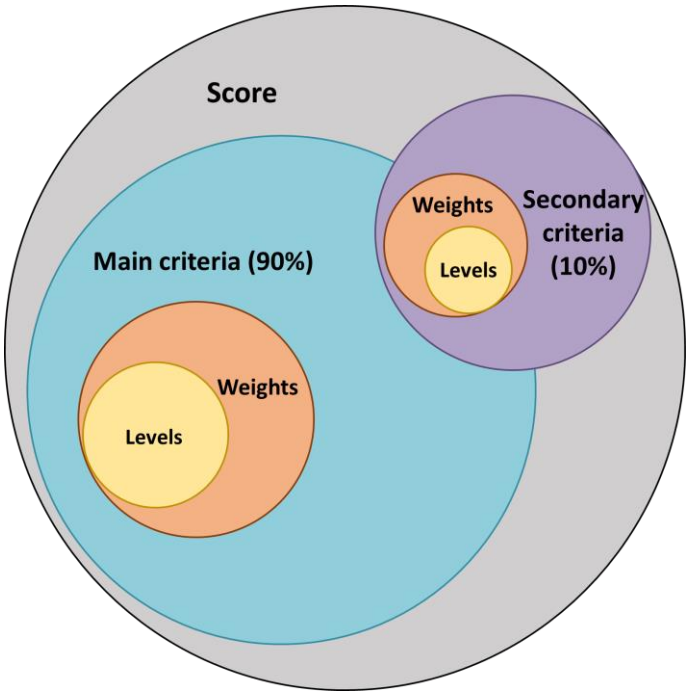

Figure 1: Schematic representation of the scoring system applied.

For every criterion, we included the "Not rated" level, to account for the cases in which the information is not available. However, as it can be seen from the tables, different punctuations have been assigned to this level depending on the criterion considered. For example, we assigned a score of 33 over 90 to the fact of not knowing the price of a substance, but the value drops down to 11 when we are dealing with toxicity levels, since not knowing the toxicity of a product can have very serious consequences on human health and environment and cannot be considered the same as not knowing if a product is expensive or not.

Table 4: Scoring system relative to the main criteria considered. To a darker colour corresponds a better quality and consequently a higher score.

Main Criterion	Weight	Levels	Punctuation (0-90)
Inhalation toxicity	0,5	Very high	0
		Not rated	11
		High	22,5
		Toxic	45
		Low	67,5
		Non toxic	90
Freshwater Toxicity (Daphnia)	0,2	Very high	0
		Not rated	11
		High	22,5
		Toxic	45

		Low	67,5
		Non toxic	90
European production (tons/year)	0,1	0-100	0
		100-500	22,5
		Not rated	33
		500-1000	45
		1000-5000	67,5
		5000-10000	90
Price (€/kg)	0,1	>500000	0
		50000-500000	22,5
		Not rated	33
		5000-50000	45
		500-5000	67,5
		0-500	90
Freshwater toxicity (fish)	0,06	Very high	0
		Not rated	11
		High	22,5
		Toxic	45
		Low	67,5
		Non toxic	90
Oral toxicity	0,04	Very high	0
		Not rated	11
		High	22,5
		Toxic	45
		Low	67,5
		Non toxic	90

Table 5: Scoring system relative to the secondary criteria considered. To a darker colour corresponds a better quality and consequently a higher score.

Secundary criterion	Weight	Levels	Punctuation (0-10)
Dermal toxicity	1/6	Very high	0

		Not rated	1,5
		High	2,5
		Toxic	5
		Low	7,5
		Non toxic	10
Genotoxicity	1/6	Very high	0
		Not rated	1,5
		High	2,5
		Toxic	5
		Low	7,5
		Non toxic	10
Citotoxiciry	1/6	Very high	0
		Not rated	1,5
		High	2,5
		Toxic	5
		Low	7,5
		Non toxic	10
Toxic for reproduction	1/6	Very high	0
		Not rated	1,5
		High	2,5
		Toxic	5
		Low	7,5
		Non toxic	10
Freshwater toxicity (algae)	1/6	Very high	0
		Not rated	1,5
		High	2,5
		Toxic	5
		Low	7,5
		Non toxic	10
Soil toxicity (worms)	1/6	Very high	0
		Not rated	1,5

		High	2,5
		Toxic	5
		Low	7,5
		Non toxic	10

At this point, evaluating the score of the nanomaterials included in the MCDA Tool is straightforward. We applied the weighted arithmetic sum method which consists in the following equation:

$$S_k = \sum_i w_i p_i + \sum_j w_j p_j \, ,$$

with the index *i* running over the six different main criteria, the index *j* running over the six secondary criteria and where:

- *S* is the total score of the nanomaterial,
- w_i and p_i are respectively the weight and punctuation of the *i-th* main criteria,
- w_j and p_j are respectively the weight and punctuation of the *j-th* secondary criteria.

The first term in *S* gives a value between 0 and 90, while the second one between 0 and 10, such that the score *S* returns is a number between 0 and 100 which is the total score of the nanomaterial.

3. THE MICROSOFT EXCEL TOOL

The MCDA has been integrated in an Excel tool programmed in the Visual Basic language. The application is structured to be user friendly and proceeds via only four simple steps, two of them optional, consisting in four questions the user is invited to answer to provide us with the necessary information to perform the analysis. The two mandatory ones are:

1. the industrial sector he is interested in (e.g. food packaging, constructions, electronics, automotive, sport and wellness…),
2. the property he wants to enhance or confer to the polymer by means of nanotechnology (e.g. enhance mechanical properties, antibacterial properties, improved resistance or stiffness, self-cleaning properties…).

If the user has available information on the polymeric matrix he wants to embed the nanomaterial in, or already knows the product is going to manufacture (for example films if he is in the food packaging sector, or pipes if he works with constructions), he can introduce it in the application. All the answers can be easily provided by the user by selecting an option from multiple selection drop down lists. The lists are interdependent, which means that the property selectable by the user will depend on the industrial sector picked and so will the properties and the products.

After answering the four questions, the Tool looks in our database for the most appropriate nanofiller. The data on the nanomaterials used in the different industrial sectors of the plastic market, the properties they are capable to enhance or confer and the polymeric matrix they use to be embedded in have been retrieved through a deep and thorough analysis of bibliographic sources, especially books about the use of nanopolymers and peer reviewed articles published on specialized journals. In **¡Error! No se encuentra el origen de la referencia.** the structure of the Tool is shown.

Figure 2: The NanoDESK MCDA Tool.

Once the button is clicked, the application runs and returns a list of up to three nanomaterials, which represent the best option on the market for the chosen industrial sector, property, product and polymeric matrix. An example is shown in Figure 3.

It is important to stress that both the database of the nanomaterials ranked through the decision-making scoring system and the database behind the tool containing the information on products, applications and polymeric matrices, is something that we expect to evolve and widen within the project and in its afterlife period too, thanks to the experience and knowledge we expect to acquire in the development of the project and to the direct contact with experts of the plastic industry.

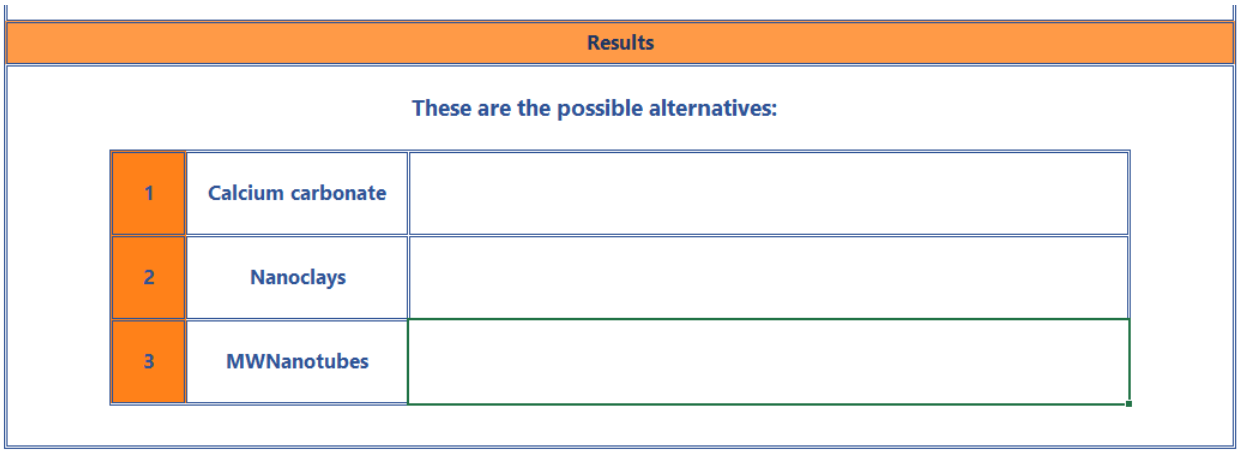

Figure 3: Example of list of results returned by the NanoDESK Tool.

4. THE WEB APPLICATION

The NanoDESK decision support tool described in the previous section, is the first one of a set of applications that are going to be included in the NanoDESK web platform, which aims at acting as a knowledge transfer structure, encouraging the diffusion in the plastic market and the application of nanocomposites, providing stakeholders with an instrument capable to ensure the quality of the nanostructure polymers produced, guarantee the protection of human health and environment and foment the demand of products with enhanced properties in the sector.

All the functionalities described in Section 4 have been implemented in this online application available at *http://dsstool.sudoenanodesk.europeanprojects.net/#* and directly accessible from the project website *http://sudoenanodesk.europeanprojects.net*.

The technical specifications of the tool are listed below:

- For the **backend (or server part)** an open source software to develop dynamic web framework in the **PHP**[1] language called **CodeIgniter**[2] has been used;
- The **frontend (or client part)** has been programmed using **JavaScript(AngularJS)**[3], **CSS**[4] and **HTML5**[5];
- For the **database,** has been used **MySQL**[6].

Figure 4 shows an example of analysis made using the NanoDESK tool. The design is very clean and user friendly, the user is called to answer to same questions detailed in Section 4 and the results is a list of up to three nanomaterials considered by our system the best ones for the product and property selected. The ranking of the proposed substances is also shown in order to give the user an idea of their adequateness level.

[1] PHP: a server-side scripting language designed primarily for web development but also used as a general-purpose programming language.
[2] https://www.codeigniter.com/
[3] JavaScript(AngularJS): a JavaScript-based open-source front-end web application framework
[4] CSS (Cascading Style Sheets): a style sheet language used for describing the presentation of a document written in a markup language.
[5] HTML5: fifth and current version of a markup language used for structuring and presenting content on the World Wide Web.
[6] MySQL: an open-source relational database management system.

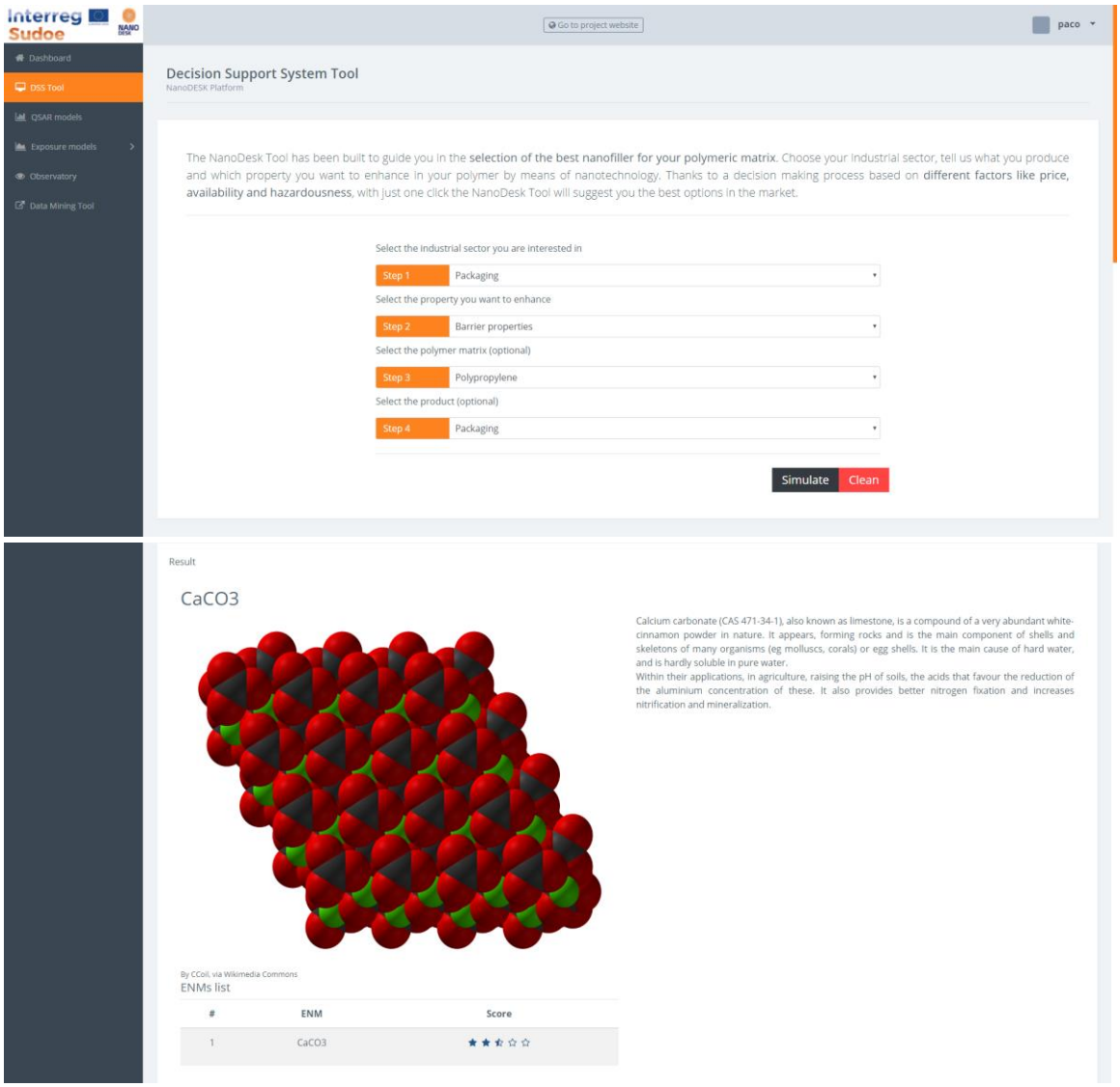

Figure 4: Example of analyses performed using the NanoDESK decision making tool.

5. CONCLUSIONS

During Action A1.3 we built a decision-making system with the objective of assisting the companies of the plastic sector in the selection of the most appropriate nanomaterial to embed in a polymer depending on their specific needs. The most influential parameters for the selection have been defined, taking into account the protection of human health and the environment and also the role of the different substances in the plastic market. Successively a hierarchy has been assigned to them. The system, based on MCDA has been included in a Microsoft EXCEL application programmed using Visual Basic. This tool, which is straightforward to use, has been also integrated in the NanoDESK web-platform to assist the stakeholders of the plastic sector in getting in touch with the benefits of nanotechnology in a safe, simple and convenient way.