Selecting surface treatments: "ready-made" strategies. Examples for the power industry.

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Abstract

Because of tremendous developments of surface treatments, databases and expert systems are necessary to help the designers. Several approaches are reviewed in this article, mainly for mono-treatments. The "EXPESURF" software for multi-layers is also introduced and illustrated in the case of power production devices.

Résumé

Les développements de traitements de surface ont conduit à la nécessité de bases de données et de systèmes experts pour guider les concepteurs. Plusieurs démarches possibles sont décrites dans cet article, essentiellement dans le cas des mono-couches, ainsi que le logiciel de sélection des multicouches « EXPESURF », qui est illustré dans le cas de dispositifs de production d'énergie.

I. INTRODUCTION

When designing surface treatments, a product engineer must select among many possible materials and processes, depending on shape, geometry, substrate material, forming processes, and finally assembly constraints.

Generally, such a decision process involves several knowledgeable and well-documented experts. Besides, experts often lack a complete view of all the possible options. Therefore, they could profitably query databases (1) and related software to select "good" materials" for their application, like CES, developed by Ashby et al. (2).

Surface treatments basically belong to four classes:

- Structural modifications, like shot peening or laser thermal treatment.
- Diffusion layers, like nitriding or boriding.
- Conversion layers, like phosphating or anodising.
- Coatings, like PVD/CVD coatings, electrochemical coatings or thermal spray coatings.

The following characteristics need consideration:

1) Not all the surface treatments generate a "layer", which in fact is a distinct compound from the substrate.
2) Most possible requirements do not express in a simple numerical way. For instance, marine corrosion resistance can be expressed through the salt brine test, but its reproducibility is sometimes questionable and the result obtained for one layer strongly depends on a small change of the substrate composition, the layer thickness, as well as the surface treatment parameters.
3) A surface treatment is defined at least by: the substrate, the layer (if any) and the process modifying the substrate or depositing the layer. These three items interact with each other (figure 1) and have to be expressed in a database, to produce a good selection software:

- The same chemical substance can be deposited through several techniques, which sometimes results in different properties. Think about alumina layers, which can be deposited either by thermal spray or obtained by aluminium anodising, with different microstructures.
- Some process may damage a substrate: a classical chemical vapour deposition process is likely to degrade a polymer substrate, following high temperature exposure.
- A given layer cannot be applied on any substrate: a change in the substrate may in turn impair the layer performance.

For such problems, an expert system approach (3)(sketched in figure 2) is often required.

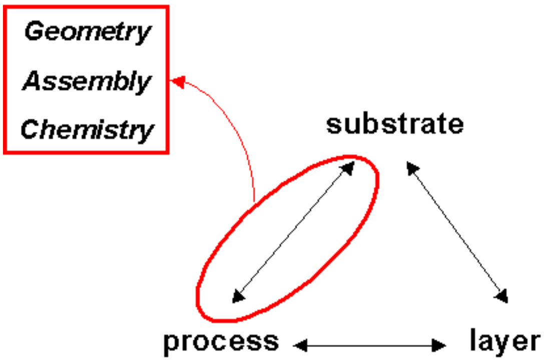


Figure 1: relationship between processes, substrates and deposited material in surface treatments

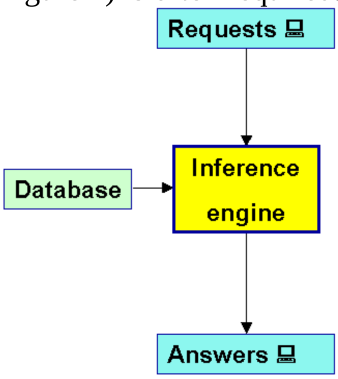


Figure 2: expert system definition

In part II, the previous surface treatments selection approaches are reviewed by assessing them according to: the way they include the afore mentioned interactions; their possible use for energy problems; the use of an expert system; the properties/requests they make possible.

In parts III and IV, a new expert system software is introduced and illustrated with examples dedicated to the power industry.

II. EXISTING APPROACHES

The general review presented in this paragraph can be found in an extended form in (4), chapter 2.

a) Systems for optical coatings

Starting from mathematical expressions derived from the Fresnel equations, the relationship between the electric and magnetic field on both sides of an infinite flat multi-layer system can be expressed, using basic optical properties (5,6). As a result, the reflectance and transmittance of a given multi-layer system are obtained.

The oldest systematic design methods for surface treatments are related to optical properties and are based on such physical laws. The user typically selects two or three materials he can vacuum-deposit in the form of high quality layers of well-controlled thickness. He specifies transmittance or reflectance vs. wavelength, as well as a maximum admissible error. The optimisation code relies on two components: proposition of combinations of layers (with given thicknesses) and evaluation of their match with the user's requirements (7). An example of multi-layer coating using such a technique is given in figure 3 in the case of an infrared filter (8).Such selection techniques might help design coatings for special glass products, e.g. for energy saving applications.

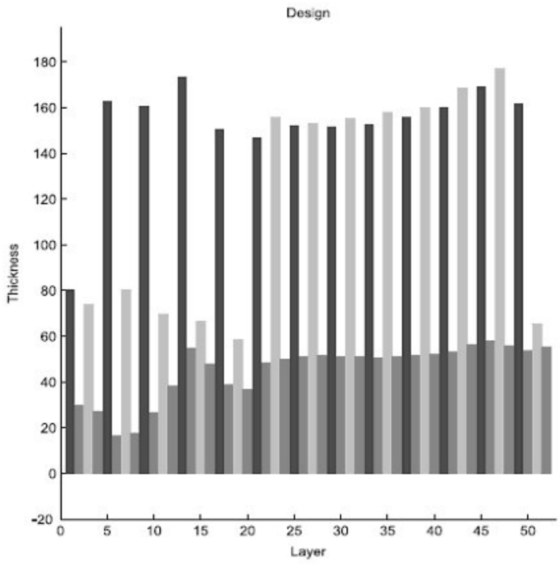


Figure 3: infrared filter (redrawn from (8))(black: MgF_2, dark grey: ZrO_2, light grey: SiC (thicknesses in nm)

b) Systems for tribological surface treatments

Friction and wear are of the greatest economical importance in all the industrial systems, due to the material loss, the energy loss and the reparation costs.

Fully predicting the wear resistance of any sliding pair from materials parameters is close to impossible, even if useful in case of moving parts like within bearings. In case of contacting materials sliding or rolling against each other, on a few simple rules like can be used:

- Minimising the expected friction coefficient of sliding pairs. If the values are unknown, the Rabonowicz's chart of metallic miscibilities is used (figure 4)(9), as well as the Ooi's citeria (10).
- Maximising the hardness/Young's modulus ratio to improve the accommodation (11).
- Applying the stress profiles derived from the theory of Hertzian contacts. For bulk materials, refer to (12). For mono-coated materials, refer for instance to Leroy and Villechaise (13) (figures 5 and 6: cylindrical contact).

The remaining pairs are "worth trying", even though selecting the proper material may call for some more experimental validation.

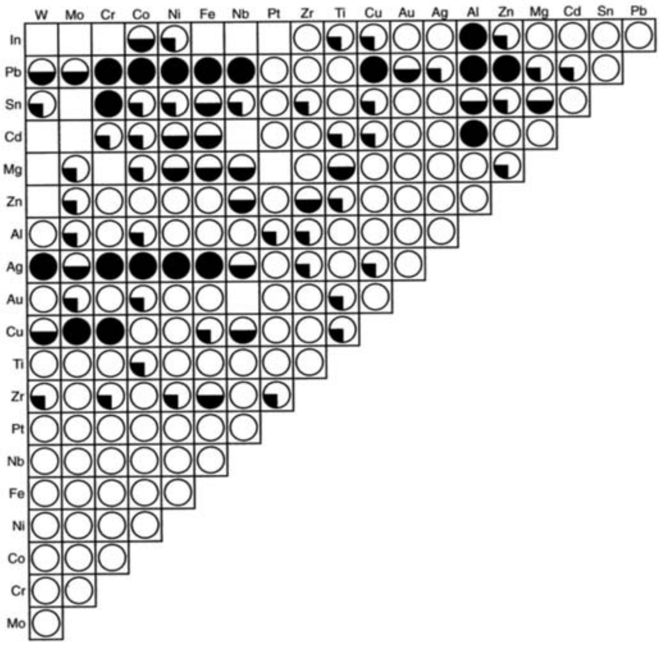


Figure 4: Rabinowicz's prediction of metallic mutual miscibilities. The blackest the circles, the least miscibles the materials and the lowest the friction (redrawn from (9)).

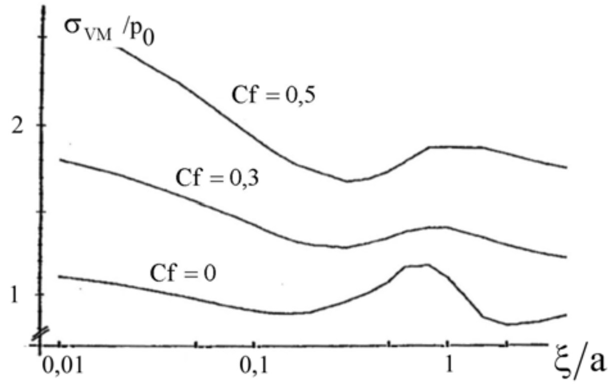


Figure 5: Von Mises' maximal stress σ_{vm} in the coating, normalised by the Hertzian pressure p_0 (redrawn from (13))(ξ : distance from the contact centre, a: half contact width, C_f :friction coefficient).

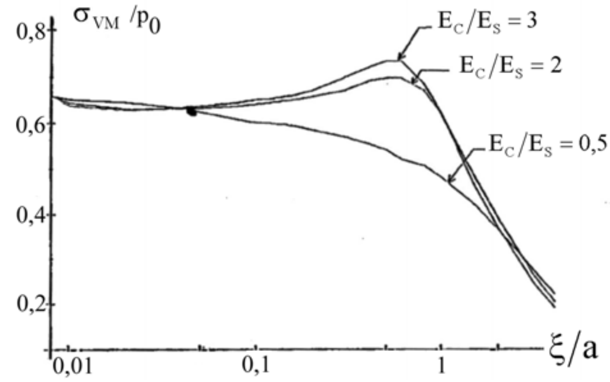


Figure 6: Von Mises' maximal stress in the substrate, normalised by the Hertzian pressure (13)(E: Young's modulus, C: coating, S: substrate. $C_f = 0{,}3$).

First, when it comes to select materials from a long list of "candidates", systematically implementing such principles in combination with a database proves useful, as attempted by Franklin et al. (11). This system is, however, not commercially available.

Galerie and co-workers (14) detail yet another approach in their surface treatments book. A few performance indices can be built to compare the performance of the plain substrate and the proposed surface treatment for well-defined tribological problems (14). These indices are ratios comparing the relevant properties of the treated surface and the substrate. A value < 1 means an improvement in the presence of the treatment. Treatments can then be compared in radar-like plots by comparing the areas of the obtained polygons.

Finally, a few computerised approaches have been proposed to deal with thermal stresses, arising in case of thermal expansion mismatch (difference of thermal expansion coefficient between a coating and a substrate) or thermal transients (15-17), with possible extensions to turbine blades, for instance.

c) Systems for anticorrosion surface treatments

Systems devoted to anticorrosion coatings are databases containing corrosion data on the surface treatments. In contrast to the previous softwares, they include few mathematical models, but more experimental results, owing to the unpredictability of corrosion resistance of any system in many diverse conditions. Most known systems are quite old (18-20). Due to the very local nature of atmospheric corrosion, certain systems are devoted to very limited cases (21).

d) Generalist systems

The above mentioned CES software contains a tool aimed at selecting surface treatments. Most surface treatment functionalities are represented in a binary fashion: corrosion resistance, wear resistance, friction reduction, superficial fatigue resistance, thermal/electrical resistance/conductance, … (2)

A few properties (layer thickness, hardness, deposition rate, deposition temperature) are given numerically, contrasting with the number-less approach shared by most generalist systems. This tool is no real expert system, as there is no actual “questionnaire” ; it allows neither eliminating treatments in terms of compatibility with a substrate proposed by the user nor building “performance indices”. Besides, the wide coatings possibilities offered by certain treatments are not considered: for instance, PVD is considered as one possible treatment with one set of attainable properties (2).

More powerful are the ST2S (22, 23) and Apticote-Isis tools (24). Both these systems allow selecting mono-layer coatings with respect to tribology, corrosion resistance, aesthetics, as well as electrical and thermal properties.

The main features of ST2S are:

- A child/parent structure of the database tree.
- A more sophisticated approach for “functional” properties.
- A more complete database (23).

On the other hand Apticote-Isis focuses more on tribological properties, based on an extensive description of contacts and loads (24).

Both systems are designed to automatically eliminate solutions that prove unsuitable for the substrate. None deals with the combinations of multiple successive treatments (multi-layers)(22-24).

III. THE EXPESURF SOFTWARE

The EXPESURF software developed at the ULB and the FUNDP presents the following features:

- It is a generalist software: it deals with all 4 classes of treatments mentioned in the introduction, which one can select to meet a wide range of properties such as corrosion and wear protection, aesthetics, hardness, electrical/thermal properties, fatigue resistance and weldability.
- It also checks data on the compatibility between substrate, layers and processes. In its database, “bond coat” layers can be sandwiched to improve the adherence between a layer and an underlying layer or substrate.
- It allows to select multi-layers, by partitioning requirements into small groups, each of which being addressed by a given layer. The definition of these groups is to be published elsewhere.

In order to achieve these characteristics, the EXPESURF software is composed of three main components: a relational database, memorizing substrate, layers and their processes, web-based interfaces for enriching the database and querying the system, and an inference engine, written in Prolog, for processing these queries.

This paper focuses on the practical application of the system. The complete description of the database and the selection procedure has been extensively described in (25). It can be summarized as follows: the inference engine is divided into three parts:

- Analysis of the properties that require a specific layer.
- Selection of each of these layers and their deposition process, taking into account the substrate, as well as the underlying layers.
- Classification of the matching treatments according to their ease of production in the industry.

IV. EXAMPLES FOR THE ENERGY INDUSTRY

In this section, a few examples derived from classical industrial applications are presented and the pertinence of the answers of the software is discussed, comparing them with widely accepted surface treatments.

a) Turbine blade protection against oxidation

Nickel superalloy turbine blades are exposed to oxidizing gases at high temperatures mandatory for a good efficiency (26).

In order to improve the oxidation resistance, the software can be queried for layers to deposit onto a superalloy substrate like IN600 and withstanding the aggressive operational conditions. The problem is entered into the user interface as follows:

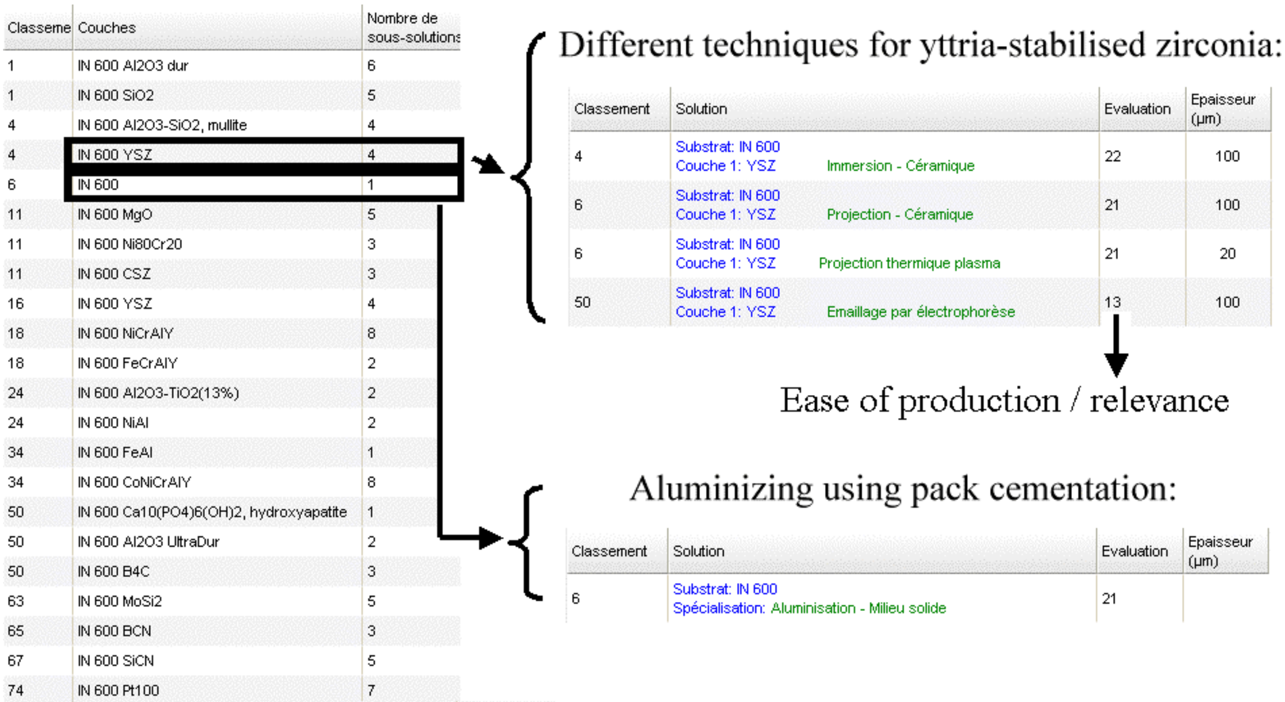
- Substrate: IN600.
- Cylindrical envelope of the substrate: 500 X 200 mm.
- Operating conditions: 950°C, oxygen.

84 (layer, process) pairs are proposed to solve this problem. The user first accesses a list of the possible treatments to solve his problem. By clicking on any of them, all eligible processes appear (figure 7). The layers are selected to match the requested properties, while the processes are selected or eliminated according to:

- The geometry / accessibility of the surface.
- Whether the requested properties are not altered by the process itself. For instance, most corrosion protections require a coating that is impermeable enough. Processes leading to thin porous layers are thus automatically eliminated, even if the layer exhibits a good intrinsic resistance to oxidation.

Many classical coatings for such a problem are proposed (alumina, silica, yttria-stabilised zirconia (YSZ), …). Taking, for instance, YSZ, the proposed processes are immersion coating, thermal spray, plasma spray and electrophoretic coating. The latter got a lower evaluation, because it is a less standard product.

Solution 6 in figure 7 is solely “IN600”. This means that no coating (in the sense of layer obtained without reaction with the substrate) is proposed. By clicking on this solution, it appears that the proposed solution is in fact aluminising, which is also a classical solution for this kind of problem.



Classeme	Couches	Nombre de sous-solutions
1	IN 600 Al2O3 dur	6
1	IN 600 SiO2	5
4	IN 600 Al2O3-SiO2, mullite	4
4	IN 600 YSZ	4
6	IN 600	1
11	IN 600 MgO	5
11	IN 600 Ni80Cr20	3
11	IN 600 CSZ	3
16	IN 600 YSZ	4
18	IN 600 NiCrAlY	8
18	IN 600 FeCrAlY	2
24	IN 600 Al2O3-TiO2(13%)	2
24	IN 600 NiAl	2
34	IN 600 FeAl	1
34	IN 600 CoNiCrAlY	8
50	IN 600 Ca10(PO4)6(OH)2, hydroxyapatite	1
50	IN 600 Al2O3 UltraDur	2
50	IN 600 B4C	3
63	IN 600 MoSi2	5
65	IN 600 BCN	3
67	IN 600 SiCN	5
74	IN 600 Pt100	7

Classement	Solution		Evaluation	Epaisseur (µm)
4	Substrat: IN 600 Couche 1: YSZ	Immersion - Céramique	22	100
6	Substrat: IN 600 Couche 1: YSZ	Projection - Céramique	21	100
6	Substrat: IN 600 Couche 1: YSZ	Projection thermique plasma	21	20
50	Substrat: IN 600 Couche 1: YSZ	Emaillage par électrophorèse	13	100

Classement	Solution	Evaluation	Epaisseur (µm)
6	Substrat: IN 600 Spécialisation: Aluminisation - Milieu solide	21	

Figure 7: proposed materials for protection of IN600 against high temperature oxidation.

Note that the database can be customised. In this example, the expert user can implement bond coats for coatings that fail to adhere to a given substrate. This allows the software to propose an undercoat between layers like YSZ and the substrate.

b) Turbine blade thermal protection, using a thermal barrier coating

Another requirement for turbine blades is to reduce the temperature in the superalloy substrate to increase its durability. This can be obtained using a low thermal conductivity coating. Inspecting the solutions of figure 7, coatings like molybdenum silicide or silicon carbo-nitride are ineligible due to their high thermal conductivity.

When asked to add an excellent thermal insulation barrier to the previous oxidation protection, EXPESURF again comes up with a few insulating oxide mono-layers identical to those of the previous example. It also yields other solutions like multi-layers, as in figure 8, where a bottom coat serves as protection against oxidation beneath a top coat which is porous, but both resistant to oxidation and thermally insulating. This illustrates how the software separates complex requirements, so that specific layers respond to specific requirements, like building blocks of a surface multi-treatment. EXPESURF interface also briefly explains the role of each part of the multi-treatment (figure 9).

Classement	Solution	Evaluation	Epaisseur (µm)
23	Substrat: IN 600 Couche 1: Ni80Cr20 Projection thermique plasma Couche 2: Al2O3-SiO2, mullite Projection thermique à la flamme	20	60
39	Substrat: IN 600 Couche 1: Ni80Cr20 Projection thermique High-Velocity OxyFuel Couche 2: Al2O3-SiO2, mullite Projection thermique à la flamme	19.5	60

Figure 8: thermal barrier coating selection

Materiel	Proprietes	Couche(s)
Al2O3-SiO2, mullite	Isolation thermique, Oxygéné (milieu oxydant)	Couche 2
Ni80Cr20	Oxygéné (milieu oxydant)	Couche 1
IN 600		Substrat

Figure 9: “explanation” of the role of the individual layers in a multi-treatment

c) A burner with high temperature corrosion in the presence of sulphur

Coal-fired thermal power plants are becoming increasingly efficient and environment-friendly. However, coal contains sulphur, which forms SO_2 or SO_3 during combustion. NaCl, another impurity, reacts with the sulphur oxides to form Na_2SO_4, which melts onto the metal surface (27). Therefore, a protective coating might be of interest for a stainless steel burner. The software can help the engineer at an early stage of the materials design, since the material corrosion resistance is listed for several kinds of atmospheres.

Let us first consider a small component described by the following problem:
- Substrate: AISI 304 stainless steel.
- Cylindrical envelope of the substrate: 100 X 100 mm.
- Operating conditions: 900°C, sulphur-containing atmosphere (high concentration).

The proposed treatments are:
- Pack aluminizing
- Ni80Cr20, NiAl, FeAl, FeCrAlY or CoNiCrAlY, using high velocity oxy-fuel (HVOF) and/or plasma spray
- NiCrAlY, using HVOF, plasma spray, electroless nickel plating or electroplating
- Alumina, using chemical vapour deposition (CVD) or plasma-enhanced CVD.
- $MoSi_2$, using plasma spray, HVOF, detonation gun, CVD or magnetron sputtering.
- Platinum, which appear in last position due to its cost, using electroplating or magnetron sputtering.

Aluminising is suitable as it produces Fe-Al compounds that resist to such a corrosion (27). The nickel-based layers are also a classical solution (27). MoSi2 (28) and alumina (29) are also sometimes mentioned in the literature for very similar problems.

When it comes to a complete burner, certain treatments should be avoided because of the device dimensions. In the interface, the cylindrical envelope has to be increased to 10 000 X 10 000 mm. It can also be of interest to limit this search to treatments that can be applied “in situ”, which can be requested via the interface.

Many solutions are discarded, like aluminising, requiring too large ovens to accommodate the dimensions of the piece. Likewise PVD and CVD disappear for the synthesis of Pt and MoSi2 coatings.

HVOF and plasma spray finally remain eligible, as well as localised forms of electroplating. Indeed, there exist portable devices enabling such treatments.

V. CONCLUSIONS

Systematic approaches for selecting surface treatments were reviewed. In the past, researchers from different fields focused on very specific problems, such as the selection of: optical coatings, tribological coatings and anticorrosive coatings. Depending on the application, these systems differ in the number of possibly selected treatments (optical: low) and the presence of an extensive database (corrosion and tribology). They also differ in the kind of selection criteria they use, from the most logical to the most empirical:
- Optical: physical modelling.
- Tribological: simple eliminatory criteria or rules of thumb.
- Corrosion: experimental results.

Later on, other researchers proposed procedures aimed at selecting mono-treatments able to meet multiple requirements. Even if they proved efficient, there remains a need for selection method covering multiple treatments as well.

In this paper, the relevance of a new software is discussed. It allows selecting treatments with respect to multiple criteria, which can be split into distinct treatments/layers, if they cannot be met with a mono-layer selection. It also eliminates treatments that are unsuitable for the substrate, in terms of chemistry, shape or post-treatments requirements. The system does not focus on a few treatments: it contains a database with a wide choice of thin or thick coatings, as well as substrate transformations. These aspects were illustrated using such classical examples as coal burners and turbine blades.

The system can be used as a learning tool as well as assistance for exploring treatments in new fields of applications. To increase its appeal, its database should be continuously improved (wear modes, corrosive media, …) and more exclusion criteria with respect to the coating/substrate compatibility should be introduced. Finally, one could complete it with specific tools with advanced exclusion model-based criteria.

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