Design of Experiment implementation in L'Oréal R&I laboratories and its link with the improvement of Environmental Profile of cosmetic products

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Abstract
We will present the way DOE are used in L'Oréal R&I laboratories for formula optimization. We will stress the statistical and process issues that can be encountered in the context of massive deployment of digital tools. And we will see how the corporate objectives for sustainable innovation will interfere with DOE applications.
Keywords: DOE, product development, process, sustainability, brakes and acceptance factors.

1. Introduction

Whether when developing a new prototype of product, or when finalizing a product to be put on the market, the recurrent task of formulators is to optimize formula, that is find the right recipe in order to reach specified values for end points .
These end points are relative to the Physical Chemical properties (eg viscosity) of the formula as well as of the final performance that will be perceived by the consumer (eg foam and conditioning effect for shampoo).
Thanks to a broad range of instrumental in vitro tests, it is possible to evaluate these properties in laboratories, on small quantities, and in short time.

In this context, Design of Experiment (DOE) is a perfectly well suited methodology to optimize formulas through the modification of the concentrations and nature of ingredients, and it has been applied successfully for many years. In order to optimize further the innovation process, it has been decided to massively deploy rapid and data driven tools, among which DOE, within formulation laboratories.

For the statisticians and data scientists that develop tools and process around DOE, it implies finding solutions robust enough to be broadly deployed, and agile enough to be accepted by all formulators, even those who might prefer to follow the usual assay-error iterative process.
This will be discussed in the first part of the presentation.

Since the end of 2013, L'Oréal has committed to a program of sustainable development called Sharing Beauty with ALL (SBWA). As a consequence for the Laboratories, the optimization of formula now requires the improvement of environmental or social criteria for each new formula. These SBWA

criteria are computed from the composition of the formula. As we will see in the second part of the presentation, this is both an opportunity and a challenge in the context of deployment of DOE.

2. The challenge of DOE deployment in R&I laboratories

2.1 Description of our environment

A recurrent task for formulators in Product Development Laboratories is to optimize formulas: given a consumer target (eg damage hair) and a technical context (eg design to cost for a specific market), the formulator must reach specified values for some end points through the modification of the concentrations and nature of ingredients.
Theses end points can be instrumentally measured, sensorially evaluated or computed.
Dedicated teams are developing tools so that all these end points can be measured or evaluated within laboratories, on small quantities, in short period of time.
Thanks to this, it is considered that DOE can be used on an everyday basis, for simple projects (adjusting a mere concentration) as well as for complex ones (determine a new skeleton for formula).
Thus, the vision is to deploy DOE as a routine tool. This implies that formulators must be able to perform it themselves.
To achieve that, we have developed a tool to allow formulators generate a DOE corresponding to their objective, model their results and find the best solution.
This tool must be performant from an algorithmic point of view, but it must also be user friendly and perfectly adapted to formulator's needs, in order to remove the hesitations about DOE.
This will be illustrated in two cases.

2.2 Concentration optimization

When all ingredients are chosen, and only the concentrations must be optimized, we are in the simple case of quantitative factor designs.
For most of cosmetics products, one of the ingredients is neutral relative to the responses (eg water) and can be used as filler, so we are in the case of independent factors.
Linear constraints occurs quiet often.
For acceptability reasons that will be explained, Space filling Designs are preferred to D-Optimal designs.
Interpretation is mainly based on response surfaces, due to the difficulty to interpret coefficients, especially in case of interaction.

Here are some technical issues we face, and that can be discussed:

- Does the "one that fits all" design exist
- What is the "good" number of experiments
- How do we model binaries responses
- How to narrow the experimental domain a posteriori, when entire domain could not be evaluated
- How to detect atypical data and handle them

2.1.2 Ingredients selection

When the exact nature of the ingredients is not yet fixed, formulators expect the DOE to help them select the most appropriate ingredients.
When it concerns only one alternative within the ingredients (eg: must select between surfactant A and surfactant B), we handle it has a qualitative factor.
But often, the objective is to select the best association between n type1 ingredients, and p type2 ingredients.
The main technical issue here is:

- How to address cases when the objectives are both select and optimize.

2. Sustainable Innovation

2.1 The Sharing Beauty With All Program

Sharing Beauty With All is the name of the L'Oréal program of sustainable development commitments, launched at the end of 2013, with objectives to be reached by 2020.
For example, 100% of products will have a demonstrable positive environmental or social benefit.
This means that social and environmental criteria will be just as important in evaluating future products as their efficacy or their contribution to the company's value creation.

The Group's Research & Innovation teams have therefore developed methods making it possible to calculate criterias:

- **Biodegradability percentage** is the capacity to be degraded by microorganisms in nature, as well as its water footprint. It is the ratio between the mass of organic ingredients in the formula, which are easily biodegradable, and the total mass of organic ingredients.
- The **Waterfootprint** measures the amount of water required for a product's manufacture and use. It incorporates two key parameters reflecting the environmental quality of the raw materials used: biodegradability and aquatic ecotoxicity.
- The Percentage of renewable raw material that are "**sustainably sourced",** that is that have a traceable supply that respects environmental and social regulations throughout the supply chain.
- The Percentage of renewable raw material processed using **Green chemistry**

The SBWA commitments also cover the production, with reducing CO2 emissions at plants and distribution centers, reducing water consumption per finished product and reducing the waste.

2.2 Impact on DOE implementation

Since 2013, the formulation laboratories must take the environmental criteria into account for each product development, whether new or in replacement.
The obvious way to integrate SBWA criteria in DOE is to handle them as responses, as it was already done with the price of the formula. By comparing responses surfaces for performance and SBWA, the formulator gets an overview of what can be achieved, and at which cost.

Beside, from a pedagogic point of view, SBWA criteria are good tool to learn how to interpret a DOE, as the link between factors (concentration) and SBWA response are straightforward to understand, still not as trivial as the price.
It is even possible to perform entirely in silico designs, in order to better select factors and boundaries in preparation of a DOE.
For these reasons, the SBWA program is a good ally for the deployment of DOE, and we do observe that formulators come to DOE thanks to this program.

In the other hand, it will be a challenge for R&I actors to keep innovating in a more and more normative context. The SBWA program makes the formulators revisit their technologies in order to find ways to improve the environmental profile of the products, while focusing on product performance. In the same way, statisticians and data scientists will have to think about new issues in the DOE field.
For example, in order to convince formulators to keep using DOE to explore formulation domains, even though some parts of the domain are not SBWA compliant, here are the technical issues we will have to solve:

- Performant algorithm to design SFD with non linear boundaries
- Non homogeneous designs in order to favor some part of the experimental domain

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