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A general concern shared by everyone, wherever they live, whatever their social rank, whatever their age, is to be neat and to live in a clean environment. Maintaining or restoring cleanliness is usually among the top priorities of everyone and a significant amount of time and money is involved in the cleaning processes. The real breakthrough for soaps and detergents appeared during the early 1940s with the introduction of “built” detergents in the United States; since then, a great variety of products appeared on the market to help people address the cleaning tasks. Today, cleaning products are becoming increasingly more sophisticated, for various reasons; mainly the technological progress (dishwashers, washing machines, *etc.* are nowadays in almost every house in the developed world) and the evolution in lifestyle (consumers need more refined products to deliver superior performances on a wider spectrum of soils with a minimum of efforts and time commitment)[1]. Among the many raw materials used in a formulated cleaning product like liquid soaps and detergents, surfactants are by far the most important and needed ingredients. They are present in every cleaning or conditioning product and several factors are important in the choice of the surfactant system[2]. Some of the applications of surfactants in cleaning products are improving the cleaning activity, improving mildness, boosting foaming properties, making the product antimicrobial active and in forming the emulsion[3]. The design of these emulsified liquid formulated products has quite a few degrees of freedom: in addition to the nature of the three main components (water, oil and surfactant), decisions also need to be made on the influence of electrolytes, alcohols and other additives on the final product. As a consequence of this and of consumer assessments, the number of components in a commercial emulsified product is often quite high. Consequently, the design of these formulated products has been considered more of an art, in which a successful “magic recipe” is worth a lot of development time and money[4].

The above problem definition matches perfectly with the general definition of a product (formulation) design problem: given a set of desired (target) product attributes, determine a set of blends (a mixture of chemicals) that satisfy the desired attributes, and, from them, select the most appropriate candidates for final validation by experiments[5]. The development of a systematic model-based methodology to quickly and reliably reduce the search space and within it, to identify a set of candidates (to be afterwards experimentally validated and, if necessary, refined for further improvement) can then make the design and development of these products less costly, so that the product itself can be introduced to the market earlier, while using the experimental resources mainly for verification of the product.

A systematic model-based step-by-step methodology for design of emulsion based chemical products has been developed, which employs a hierarchical approach consisting of seven sequential steps, starting with the identification of the needs to be satisfied by the product; then building up the formulation by adding one-by-one the different classes of chemicals needed; and finally determining the composition of the formulated product. Based on the ingredients chosen and the target properties, their compositions on the formulation are adjusted. The choice of ingredients is ordered, so that the most advantageous active ingredients are identified first, followed by the dispersed and continuous phase solvents, then the emulsifiers and finally the additives. The selection is carried out considering effectiveness, safety, toxicity and cost of each candidate. A specially developed database of different types of chemicals (ingredients) and a library of property models help in evaluating, screening and defining the candidate formulations. This model-based methodology is intended to be generic, in the sense that many different emulsified products can be designed through this procedure once the needs-property relations are established, appropriate structured databases for all the categories of ingredients are accessible and the property prediction models are applicable (to estimate the needed properties when their data are not available in the database). The concepts of the methodology have been tested on the design of an emulsified sunscreen lotion[6].

In this work, an extended and more generic version of the methodology is presented and the main steps are illustrated through a case study involved with the design of an emulsified hand wash product. The focus of the application of the methodology presented here is on the definition of consumer assessment and their translation into measurable target properties, as well as on modelling of some of the critical properties, such as, properties of surfactants (acting in a hand wash product both as active

ingredients and emulsifiers at the same time) in order to estimate their effectiveness so that the most effective can be selected. These properties have been modelled through the development of a classical group-contribution (GC) method, based on the GC^+ approach. The work-flow methodology and all the related tools will be implemented into "The Virtual Process-Product Design Laboratory[7] software.

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