An Integrated Methodology for Emulsified Formulated Product Design

The consumer oriented chemical based products are used every day by millions of people. They are structured products constituted of numerous chemicals, and many of them, especially household and personal care products, are emulsions where active ingredients, solvents, additives and surfactants are mixed together to determine the desired emulsified product. They are still mainly designed and analysed through trial-and-error based experimental techniques, therefore a systematic approach, integrating model-based as well as experiment-based techniques, for design of these products could significantly reduce both time and cost connected to product development by doing only the necessary experiments, and ensuring chances for innovation. The main contribution of this project is the development of an integrated methodology for the design of emulsified formulated products. The methodology consists of three stages: the problem definition stage, the model-based design stage, and the experiment-based verification stage. In the problem definition stage, the consumer needs are translated into a set of target thermo-physical properties and into a list of categories of ingredients that are to be included in the formulation. In the model-based design stage, structured databases, dedicated algorithms and a property model library are employed for designing a candidate base case formulation. Finally, in the experiment-based verification stage, the properties and performances of the proposed formulation are measured by means of tailor-made experiments. The formulation is then validated or, if necessary, refined thanks to a systematic list of action. The problem definition stage relies on a robust knowledge base, which needs to systematically generate quantitative, useful input information for the model-based stage, starting from the consumer assessments. In the model-based stage, comprehensive chemical databases, consistent property models and a dedicated algorithm for the design of emulsified solvent mixtures are needed. Finally, for the experiment-based stage, an efficient planning of the experiments is required, together with the systematic generation of a list of actions to be taken, in case some of the experiments do not validate the candidate formulation generated in the previous stage. All the above mentioned issues are addressed in this PhD work: the necessary property models have been retrieved and organized in a model library; new property models have been developed for a set of thermo-physical properties of surfactants; a robust, systematic knowledge base has been developed in relation to emulsified formulated products; chemical databases have been improved and generated; and an algorithm for the model-based design of emulsified solvent mixtures has been developed. All these tools have been implemented as a new template in the virtual Product-Process Design laboratory software. To illustrate the application of the proposed methodology, three case studies have been developed. For one of these case studies, the whole methodology has been applied, while for the other two, only the first two stages and part of the experiment-based verification stage have been applied, that is, the experimental work has been planned, a list of actions has been generated, but no actual measurement has been taken.