An integrated approach for the design of emulsified products

Consumer oriented chemical based products, including emulsified ones, are structured products constituted by numerous chemicals, and they are used every day by millions of people. They are still mainly designed through trial-and-error based experimental techniques. 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. In this work we present 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 via a robust knowledge base. 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 actions. All these tools have been implemented as a new template in our in-house software called the Virtual Product-Process Design Laboratory and have been illustrated via a case study (a hand-wash detergent) where the complete methodology (all three stages) is for the first time applied.

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