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Chemical-Based Formulation Design: Virtual Experimentation

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This paper presents a software, the virtual Product-Process Design laboratory (virtual PPD-lab) and the virtual experimental scenarios for design/verification of consumer oriented liquid formulated products where the software can be used. For example, the software can be employed for the design of the active ingredient-solvent mixture and/or their verification in terms of the product function. These consumer products are still primarily designed, developed and/or tested through experiment-based trial and error approaches. However, using the powerful methodologies and tools developed within the process system engineering community, it is possible now to replace, at least, some of the experimental steps with efficient and validated model-based approaches. For example, the search space can be significantly reduced through computer-aided screenings of the active ingredient (AI), the solvent mixture, the additives and/or their mixtures (formulations). Therefore, the experimental resources can focus on a few candidate product formulations to find the best product.

The virtual PPD-lab allows various options for experimentations related to design and/or verification of the product. For example, the selection and verification of the functions of the AI; the design of solvent mixtures for the delivery of the AI; the stability test of the liquid formulated product; the selection of additives such as aroma compounds to be added to the products to enhance their quality; the generation of a list of candidate formulations; the addition of the missing chemicals to an incomplete formulation and the verification of the final product.

The software is based on a framework that allows quick implementation of different design/verification work-flows and their associated models, methods, tools and data. The software contains a suite of databases with data of AIs used in different products (such as insect repellents), solvents classified in terms of special characteristics (such as solubility in water), and additives classified in terms of their application (such as aroma agents, wetting agents and preservatives). In addition, the software has built-in intelligence through implemented knowledge-bases related to transforming product attributes (consumer needs) to a set of physical-chemical properties; templates (work-flows) for specific product types are also available; guidance for property model (such as pure component properties and mixture properties) selection and adaptation is provided; the selection and use of models for product verification is also possible (such as stability of liquid and evaporation of the solvent after application of the product). Finally, the software has a collection of algorithms (such as CAMD, mixture design, model adaptation). All of the above helps to perform virtual experiments by blending chemicals together and observing their predicted behaviour.

The paper will highlight the application of the virtual PPD-lab in the design and/or verification of different consumer products (paint formulation, hair spray, sunscreen lotion, insect repellent lotion). The results of the virtual experimentations will be illustrated through the (initial) base case designs that were obtained and their verification through real experiments and/or available product data analysis.

Theme: Synthesis and Design