

Design of an Emulsion-based Personal Detergent through a Model-based Chemical Product Design Methodology - DTU Orbit (09/11/2017)

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An extended systematic methodology for the design of emulsion-based Chemical products is presented. The methodology consists of a model-based framework involving seven sequential hierarchical steps: starting with the identification of the needs to be satisfied by the product and then adding one-by-one the different classes of chemicals, until a formulation is obtained, the stability of which as an emulsion is finally checked with appropriate models. Structured databases, appropriate pure component as well as mixture property models, rule-based selection criteria and CAMD techniques are employed together to obtain one or more candidate formulations. A conceptual casestudy representing a personal detergent is presented to highlight the methodology.

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Authors: Mattei, M. (Intern), Hill, M. (Ekstern), Kontogeorgis, G. (Intern), Gani, R. (Intern)

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