VPPD Lab - The Chemical Product Simulator - DTU Orbit (08/11/2017)

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In this paper, the development of a systematic model-based framework for product design, implemented in the new product design software called VPPD-Lab is presented. This framework employs its in-house knowledge-based system to design and evaluate chemical products. The built-in libraries of product performance models and product-chemical property models are used to evaluate different classes of product. The product classes are single molecular structure chemicals (lipids, solvents, aroma, etc.), blended products (gasoline, jet-fuels, lubricants, etc.), and emulsified product (hand wash, detergent, etc.). It has interface to identify workflow/data-flow for the inter-related activities between knowledge-based system and model-based calculation procedures to systematically, efficiently and robustly solve various types of product design-analysis problems. The application of the software is highlighted for the case study of tailor made design of jet-fuels. VPPD-Lab works in the same way as a typical process simulator. It enhances the future development of chemical product design.

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