

Integrated Computer-aided Framework for Sustainable Chemical Product Design and Evaluation - DTU Orbit (09/11/2017)

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This work proposes an integrated model-based framework for chemical product design and evaluation based on which the software, VPPD-Lab (The Virtual Product-Process Design Laboratory) has been developed. The framework allows the following options: (1) design a product using design templates, such as, single molecule products, formulated products, blended products, emulsified products and devices; (2) analyze the product by performing virtual experiments (product property and performance calculations); (3) create and add new product property and product performance models; (4) create new product design templates when the desired template is not available. The product design templates follow the same common steps in the workflow for a product type but have options to employ product specific property models, data and calculation routines, if necessary. This paper highlights the application of the templates for three case studies: (i) the design of a refrigeration cycle, (ii) a mixture/blend design problem involving lubricant design and (iii) a tailor-made product design of jet-fuels (blended chemical products).

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