Property Model-based Tailor-made Design of Chemical-based Products

Computer-aided model-based methods and tools are increasingly playing important roles in chemical product design. They have the potential to very quickly search for and identify reliable product candidates that can then be verified through experiments. In this way, the time and resources spent on experiment are reduced leading to faster and cheaper to market the products. The tools also help to manage the solution of product design problems, which usually require efficient handling of model-data-knowledge from different sources and at different time and size scales.

The main contribution of this project is: (1) the development of a systematic model-based framework for chemical product design; (2) its implementation as a computer-aided tool based on a specially developed architecture; (3) the creation of product design template together with their algorithms, models, tools and data for various types of products. The goal has been to develop a chemical product simulator, similar in concept to a process simulator, which makes the product design and development easier and faster, and provide the way for unified and consistent product documentation. In the same way a typical process simulator works, the developed product simulator (VPPDLab) allows product designers to: (1) analyze chemicals based products by performing virtual experiments (product property and performance calculations); (2) predict the properties of products; and (3) create new product property and product performance models, when needed. However, unlike process simulators, VPPDLab can also be used directly for (4) design of chemicals based products using the design template for various types of products, such as, single molecule products, formulations, blends, emulsions and devices; and, (5) creation of new product design templates when the needed template for a desired product is not available. VPPD-Lab employs a suite of algorithms (such as database search, molecular and mixture blend design) and toolboxes (such as property calculations and property model consistency tests) for specific product property prediction, design, and/or analysis tasks.

In order to achieve the features mentioned above, several issues need to be addressed: the translation of consumer needs into target properties; property models and available data for each type of chemical products; design methods and algorithms; available computer-aided tools; the systematic framework for chemical product design and analysis and its implementation as architecture for VPPD-Lab. From many test problems, eight application examples are presented to illustrate the use of the software. For two of these examples, the prediction of product properties and the use of virtual experiments to test product performances are highlighted. Five examples illustrate the use of the product design templates with respect to five types of chemical products (molecular design, formulation design, emulsion design, blend design and device design).

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