Development of a Systematic Methodology for Chemical Substitution using a Model-based Approach

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Consumer-oriented chemical products, encountered in everyday life, are structured products composed of one or more chemicals and are used by almost everyone. However, although these products are extremely useful in terms of functionality and bring substantial benefits to our lives and health, some of the chemicals constituting these products maybe hazardous to the environment and toxic to human health. Besides, in many cases, their chemical production processes generate harmful emissions, which have severe impacts on the environment. The concern about the environment and human health has given rise to the REACH regulation, which compels European chemical companies to stop the use of hazardous substances and replace them with environmentally benign chemicals. Also, the decisions taken during chemical product design have an impact on the process performance as well as product performance. Hence, undoubtedly there is a need to develop a systematic, model-based methodology that can help to find substitutes to existing chemicals in order to improve process economics, operability as well as the sustainability [1], while still delivering the same or improved product functionality.

The objective here is to quickly and reliably identify the promising candidates through model-based techniques and then to verify and evaluate them through experiments. In this way, the experimental resources are used for verification rather than trial-and-error search. The goal therefore is to investigate comprehensively the uses and properties of the chemicals of concern; develop a systematic framework to identify, compare and select safer alternatives to these including their corresponding manufacturing processes; and finally design safe chemical products or products with improved product performance.

The model-based approach makes use of validated property models [2] to identify the chemicals which need to be substituted, that is, the chemicals that do not meet the desired physico-chemical properties and EH&S (environmental, health and safety) properties, and then to generate, evaluate and identify candidates that can replace them. The presentation will highlight the developed methodology and the tools used for chemical substitution along with several case-studies on substitution of chemical compounds in products from cosmetics and personal care; food; pharmaceutical sectors. Several practical examples on substitution of chemicals from chemical-based products in various sectors, like cosmetics and personal care with amino acids (as an additive in a chemical product formulation) along with other well-known substitution problems from sectors like coatings and solvents, automobiles etc., together with the role of property models in chemical substitution, are highlighted.

References

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