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Property Model-Based Chemcal Substitution and Chemical Formulation Design

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Chemical-based products including structured product formulations and single molecule products have proven to be a boon to mankind and have been a significant part of our economies. Our life and the changes around us cannot be imagined without the presence or involvement of chemicals. But like every coin has two sides, some chemicals constituting these products can also be a curse. This is primarily due to the hazardous environment-related properties that some of these chemicals possess and there are many more chemicals which have not been evaluated due to lack of resources for rigorous, experimental-based estimation methods [1]. Hence, there is a dire necessity to identify such chemicals which may be dangerous to the environment, toxic to human health and harmful for our fragile eco-system. Besides, in many cases, their corresponding chemical production processes generate harmful emissions, which also have severe impacts on the environment. The concern about the environment and human health has given rise to the REACH regulation implemented by the European Chemical Agency (ECHA), which compels European chemical companies to stop the use of hazardous substances and replace them with environmentally benign chemicals. Additionally, the decisions taken during chemical product design also have an impact on the process and product performance and are influenced by company strategy, availability of market and government policies [2]. 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, while still delivering the same or improved product functionality.

It is useful to start with making structured databases by collecting data from knowledge base, followed by the development of the predictive group-contribution property models and then the development of a general methodology for the model-based chemical substitution and chemical product design. The objective here is to quickly and reliably identify the promising candidates through model-based techniques and then to verify and evaluate their performance and applicability through experiments. In this way, the experimental resources are used for verification rather than for an inefficient, trial-and-error search used for practically all chemical products. Besides, when it is desired to come up with alternative substitutes for the undesirable chemicals, the trial an error based approach will have a very large search space. This could be avoided by having predictive models coupled with the desired target properties, making the identification of these substitutes easier. 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 product formulations or product formulations with improved product performance.

The model-based approach makes use of validated property models to identify the chemicals which need to be substituted, that is, the chemicals that meet the desired physico-chemical properties but not the regulatory (EH&S: environmental, health and safety) properties, and then to generate, evaluate and identify candidates that can replace them. The presentation will discuss the general methodology for chemical substitution, which caters to different problem definitions depending on the reason for substitution. The associated property modeling tools [3] will also be highlighted. A set of new group contribution-based models for a number of useful properties of amino acids will be presented. Through examples on substitution of chemicals from chemical-based products from various sectors namely cosmetics and personal care, pharmaceutical and food, with amino acids (as active ingredient or as additive) will be shown along with other well-known substitution problems. These examples will also highlight the role of property models in chemical substitution and chemical product formulation.

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