A Systematic Methodology for Property Model-Based Chemical Substitution from Chemical-based Products

In this paper, a general model-based methodology for chemical substitution, which takes into account different problem definitions depending on the objective for substitution, is presented. The associated property models and modeling tools are also described. The application of the methodology is shown through an example on substitution of a chemical from a chemical-based product. It is about finding a substitute for a non-biodegradable surfactant used in products from the cosmetics and personal care sector. Amino acid based surfactants are found to be particularly viable substitute candidates. However, this example requires the development of a set of new group contribution-based models for a number of useful properties of amino acids, which are also presented. Besides this, several other known substitution problems are solved using the developed methodology.

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