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Computer-aided product design (CAPD) is a method for the generation and selection of novel pure, mixed and blended chemical products [1]. In CAPD, the chemical product is generated and selected based on defined structure, property and process/application constraints. Several challenges exist for CAPD, including the accuracy of the property estimation, molecular structure generation, inclusion of sustainability, process and application targets and needs in the problem formulation. CAPD has been widely utilized for the synthesis of several types of products, such as solvents, polymers, fuels and formulated products [2]. However, for product design problems where the process needs and sustainability possess demanding constraints, the complexity of the problem is increased as the relation between product property, sustainability and process criteria is difficult to mathematically define.

In this work, a generic computer-aided framework for chemical product design is presented through a systematic framework. A CAPD problem for the generation of novel pure, mixed and blended chemical products is formulated and solved through the application of four sequential steps. In step (1), the product design problem is defined together with the process and/or application boundaries. In step (2), the CAPD problem is formulated through property constraints for pure, mixed and blended products, process/application constraints and objective function. The property constraints are carefully selected for the thermo-physical property needs and the process/application needs. Process/application and property needs are connected through an analysis of the property influence on the process/application models and thermodynamic relations. The sustainability is considered through product and process/application performance, economics and environmental impact. In step (3), the CAPD formulation is converted into a mixed-integer nonlinear program (MINLP) by set-up of constraints, objective and boundaries defined in step (2). In step (4), the MINLP is solved through a decomposed approach [3]. The decomposed approach breaks down the MINLP problem into a sub-set of programs to manage the complexity: mixed-integer linear program (MILP) for molecular generation, linear program (LP) for property constraints, non-linear program (NLP) for mixture/blend property constraints, and NLP for process constraints and objective function. This approach ensures that the optimal chemical product can be found through systematic generation and screening of alternatives based on the problem definition. The framework is implemented into a GAMS-based tool.

The application of the framework is demonstrated through sustainable working fluid design for a heat pump cycle. Working fluids used in heat pumps are continuously regulated due to the environmental issues, such as ozone depletion or global warming potential. Many of the currently used working fluids are soon to be phased out [4]. The design of novel working fluids is a challenging task as retro-fitting as well as re-designing demand increased sustainability and minimal trade-off with system performance. In the CAPD formulation, the product properties are related to the needs of heat pump cycle and its components through sensitivity analysis of the thermodynamic models and energy balances of the system. Furthermore, simple models are included for efficient assessment of the sustainability and design criteria of both the cycle and its components. It will be demonstrated that the working fluid product designed is optimal with respect to the sustainability and the heat pump cycle performance.

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