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Efficient ant colony optimization for computer aided molecular design: case study solvent selection problem

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Abstract

In this paper, we propose a novel computer-aided molecular design (CAMD) methodology for the design of optimal solvents based on an efficient ant colony optimization (EACO) algorithm. The molecular design problem is formulated as a mixed integer nonlinear programming (MINLP) model in which a solvent performance measure is maximized (solute distribution coefficient) subject to structural feasibility, property, and process constraints. In developing the EACO algorithm, the better uniformity property of Hammersley sequence sampling (HSS) is exploited. The capabilities of the proposed methodology are illustrated using a real world case study for the design of an optimal solvent for extraction of acetic acid from waste process stream using liquid-liquid extraction. The UNIFAC model based on the infinite dilution activity coefficient is used to estimate the mixture properties. New solvents with better targeted properties are proposed.

Keywords: Ant Colony Optimization, Group contribution method, Computer aided molecular design, Hammersley Sequence Sampling, Oracle penalty function, UNIFAC

1. Introduction

Solvents are used for a variety of purposes in process industries. They are extensively used as process materials, as extracting agents, and as process liquids in process industries, pharmaceutical industries, and solvent based industries. Waste solvents are main source of pollution to air, water, and soil. Therefore, it is empirical to use environmentally benign solvents without compromising the process performance. Moreover, there are some solvents that must be