The proper rearrangement of distillation sequences can approach the most suitable structure of the chemical separation process according to considerations of cost. This study suggests two meta-heuristic techniques: Ant colony algorithm and Harmony search algorithm. The overall synthesis problem is formulated as an implicit mixed-integer linear programming (MILP) problem. Four cases including 3-components case, 4-components case, 5-components case and 6-components case for separation are illustrated. The shortcut model DSTWU was simulated. Percents of light key and heavy key are determined. Ninety-eight percent pure substrate can be obtained for these optimizations. Either Ant colony algorithm or Harmony search algorithm can address at the exact optimum point but Ant colony algorithm proposes the better value and is more robust than Harmony search algorithm. As a result, it was found that the system of 3-components can separate at 97.02-99.45% purity, 4-components at 95.46-99.96%, 5-components at 91.96-99.19%, and 6-components at 92.88-99.26% purity; respectively. After application of heat-integrated distillation sequences, the system of 3-components can reduce the cost at 0.1772%, 4-components at 0.5068%, 5-components at 0.4255% and 6-components at 0.3310%; respectively.

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