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分离工程

萃取精馏溶剂的选择(Ⅰ)溶剂分子QSPR的人工神经网络模型

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摘要

在分子模拟的基础上选择萃取精馏溶剂首先要建立描述溶剂分子结构与其性质之间定量关系(QSPR)的数学模型。本文采用分子连接性指数(MCI)表示溶剂分子的二维拓扑结构,它不仅可以表示构成分子的原子或基团的种类与数目,而且还可以反映原子或基团之间相互连接的特征;而溶剂主要的性质指标,如选择性与溶解性,都是无限稀释活度因子γ∞的函数。由于分子结构与γ∞之间的关系十分复杂,所以利用人工神经网络(ANN)模型描述溶剂的QSPR。组建了具有广泛代表性的数据库,并采用BP算法对ANN模型进行训练,证明训练成熟的ANN模型可以更准确地计算γ∞,优于当前普遍使用的UNIFAC方法。

关键词

萃取精馏溶剂 定量的结构-性质关系 分子连接性指数 人工神经网络模型

分类号

Selection of solvents for extractive distillation（Ⅰ） Artificial neural network model for QSPR of solvents

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Abstract

In order to select the optimum solvents of extractive distillation on the basis of molecular simulation, a mathematical model must be firstly established for describing the quantitative structure-property relationships (QSPR) of the solvents.In this paper the molecular connectivity indexes (MCI) were used to express two-dimensional molecular topological structure, which could indicate not only the kind and number of atoms or groups composing the solvent molecule but also the inter-connective characteristics among them.The major solvent properties, such as selectivity and solubility were the functions of infinite dilution activity coefficients, γ∞.Because of the extraordinary complexity between molecular structure and γ∞, an artificial neural network (ANN) model was used for the QSPR.An appropriate database was established and the back-propagation (BP) algorithm was used to train the ANN model, and the well-trained ANN model proved to be more accurate in calculating γ∞ than the prevailing UNIFAC method.

Key words

extractive distillation solvent quantitative structure-property relationships molecular connectivity index artificial neural network model

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