SEPARATION SCIENCE & ENGINEERING

苯或甲苯萃取己内酰胺和甲基己内酰胺分配系数的测定和预测

龚行楚，吕阳成，骆广生

State Key Lab of Chemical Engineering, Department of Chemical Engineering, Tsinghua University, Beijing 100084, China

摘要　　To get high purity caprolactam is a challenging task in the chemical fiber industry. To date, reports on the prediction of the distribution of caprolactam and its derivative chemicals have been few. In this study, the extraction of caprolactam with toluene as the extractant and N-methyl caprolactam with benzene and toluene as the extractants has been carried out. By defining new UNIFAC groups and calibrating related interaction parameters, a UNIFAC method was introduced to predict the equilibrium concentration of caprolactam and methyl caprolactam in toluene or benzene extraction processes. The calculated results fit very well with the experimental data. Using the UNIFAC model, the selectivity of extractants can be predicted.

关键词　　extraction　UNIFAC model　caprolactam　benzene　toluene

分类号

Distribution coefficient of caprolactam and methyl caprolactam using benzene or toluene as extractants: Experiments and prediction

GONG Xingchu, LÜ, Yangcheng, LUO Guangsheng

State Key Lab of Chemical Engineering, Department of Chemical Engineering, Tsinghua University, Beijing 100084, China

Abstract

  To get high purity caprolactam is a challenging task in the chemical fiber industry. To date, reports on the prediction of the distribution of caprolactam and its derivative chemicals have been few. In this study, the extraction of caprolactam with toluene as the extractant and N-methyl caprolactam with benzene and toluene as the extractants has been carried out. By defining new UNIFAC groups and calibrating related interaction parameters, a UNIFAC method was introduced to predict the equilibrium concentration of caprolactam and methyl caprolactam in toluene or benzene extraction processes. The calculated results fit very well with the experimental data. Using the UNIFAC model, the selectivity of extractants can be predicted.

Key words　extraction　UNIFAC model　caprolactam　benzene　toluene

通讯作者　龚行楚 gsluo@tsinghua.edu.cn