

Process safety assessment of semibatch nitration of naphthalene with mixed acid to 1-nitronaphthalene

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June 13, 2021

Abstract

In this study, different calorimetric and analytical techniques were used to evaluate the thermal behaviour of the preparation of 1-nitronaphthalene through the nitration of naphthalene with mixed acid. Differential scanning calorimetry and adiabatic calorimetry revealed that 1-nitronaphthalene lacks thermal decomposition characteristics. The results of reaction calorimetry, high-performance liquid chromatography, and the density function theory method were combined to analyse the reaction mechanism. An expanded Stoessel criticality diagram was developed to evaluate the process safety of the semibatch nitration reaction. The results revealed a higher degree of risk than that obtained when using the traditional Stoessel criticality diagram. Kinetics parameters of the reaction were investigated.

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