教师个人主页

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论文成果

Integrated solvent-process design methodology based on COSMO-SAC and quantum mechanics for TMQ (2,2,4-trimethyl-1,2-H-dihydroquinoline) production

论文类型： 期刊论文

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关键字： Solvent design; Process design; COSMO-SAC; Quantum mechanics; 2,2,4-trimethyl-1,2-H-dihydroquinoline

摘要： TMQ (2,2,4-trimethyl-1,2-H-dihydroquinoline) is an important antioxidant because of relatively low price and ease of application in rubber production technologies. However, due to the limited experimental data and unclear reaction mechanism, the quality of the TMQ product needs to be improved in industry processes. To this end, a systematic solvent-process design methodology is proposed in this paper to identify promising reaction solvents to increase the yield and selectivity of TMQ. In this methodology, group contribution methods and COSMO-SAC (COnductor-like Screen MOdel for Segment Activity Coefficient) are employed to predict TMQ and the solvent properties including activity coefficients. An improved dynamic process model formulated as a set of ordinary differential equations is applied to calculate the composition of each product. In the process model, the missing reaction kinetic parameters are obtained by DFT calculation. Finally, a computer aided solvent-process design model and a case study is formulated for the design of the reaction solvents to increase the yield and selectivity of TMQ products. (C) 2020 Elsevier Ltd. All rights reserved.

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