Contents lists available at ScienceDirect

Chemical Engineering Research and Design

journal homepage: www.elsevier.com/locate/cherd

Synthesis of isopropyl acetate by acetone method and its reaction mechanism

Zhang Junmei[a], *Zhu Ahui*[a], *Xu Wenhui*[c], *Li Daoxian*[c], *Zhang Yanhua*[c], *Duan Zhenya*[b], *Wang Yan*[b,*]

[a] *College of Chemical Engineering, Qingdao University of Science and Technology, Qingdao 266011, Shandong, China*
[b] *College of Electromechanical Engineering, Qingdao University of Science and Technology, Qingdao 266061, Shandong, China*
[c] *Shandong Xinhua Pharmaceutical Company Limited, Shouguang 262700, Shandong Province, China*

ARTICLE INFO

Article history:
Received 25 March 2021
Received in revised form 3 July 2021
Accepted 3 August 2021
Available online 8 August 2021

Keywords:
Ketene
Acetone esterification
Isopropenyl acetate
Quantum chemistry
Reaction mechanism and kinetics

ABSTRACT

Isopropenyl acetate, an important chemical raw material intermediate, has an extremely wide range of applications in chemicals, materials and medicine. In this paper, acetone and ketene are used as raw materials to synthesize isopropenyl acetate under acidic conditions. The process conditions were studied through experiments with one variable, and the effects of the catalyst activity and dosage, the reaction time and the reaction temperature on the yield of isopropenyl acetate were investigated. The optimal reaction conditions were obtained, and macroscopic kinetic equations of esterification reaction was obtained by fitting the experimental data. The mechanism of the reaction was studied by quantum chemistry. The results of experimental and theoretical research can provide theoretical guidance for further expanding experiment and industrial quantitative production.

1. Introduction

Isopropenyl Acetate (IPA) can be used as hydrogen acceptor (Fujita et al., 2013), wood improver (Nagarajappa and Pandey, 2016), and is often used as the high purity solvent and fine chemical intermediate for skin relaxed series products in medicine. Its downstream products acetylacetone and acetylacetone calcium, magnesium, zinc, nickel and other salts are widely used in the production of PVC heat stabilizer, flame retardant, resin crosslinking agent, catalyst, hot wire reflective glass film and transparent conductive film forming agent (Hu et al., 2021; Lak et al., 2020; Yang et al., 2019; Wu et al., 2020; Sarkar et al., 2020).

At present, the industrial synthesis of isopropyl acetate is mainly by the esterification of ketene and acetone. The esterification catalysts include sulfuric acid, polyphosphoric acid, acetylsulfonylacetic acid, naphthyl disulfonic acid and strong acid cation exchange resin (Peng et al., 2007), etc. Among them, fuming sulfuric acid has been widely used due to its low price, high reaction rate and less by-products.

Ketene can only be preserved at −80 °C, and it is easy to polymerize to form diketene at room temperature, so it is very difficult to prepare and use in laboratory. Therefore, there are few related report on the preparation of isopropyl acetate esterification of ketene and acetone. In the industrial production, the production of isopropyl acetate is batch reaction process based on stirred tank reactor with great labor intensity, low productivity, low automatic level. In order to optimize the industrial production process, update automatic level and realize continuous production, it is necessary to study the production process conditions, reaction principle and kinetics to provide necessary basic data.

With the development of computer, quantum chemical calculation has been widely used, and gradually applied to various fields, and it achieved a very good effect, especially in reaction mechanism, drug design and reaction rate constant calculation (Kotev et al., 2020; Arathala et al., 2020; Shao et al., 2020; Martinez-De la Hoz et al., 2016; Lu et al., 2020; Zhang et al., 2020; Huang et al., 2020; Tang et al., 2020; Vitkovskaya et al., 2020). Acetone esterification is a complex reaction process including ketene gas diffusion, gas-liquid mass transfer and reaction. It is necessary to further explain the reaction process by means of quantum chemistry to study the microscopic reaction mechanism of this esterification reaction. Finally, a description of

* *Corresponding author.*
E-mail address: ctdyz369@163.com (Y. Wang).
https://doi.org/10.1016/j.cherd.2021.08.003