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Ethanol-to-butadiene: physicochemical properties of highly active Zn-Ta catalysts

AUTHORS
Guillaume POMALAZA / UNIVERSITÉ DE LILLE, 42 RUE PAUL DUEZ, LILLE
Franck DUMEIGNIL / UNIVERSITÉ DE LILLE, 42 RUE PAUL DUEZ, LILLE
Mickaël CAPRON / UNIVERSITÉ DE LILLE, 42 RUE PAUL DUEZ, LILLE

PURPOSE OF THE ABSTRACT

The automotive industry consumes large quantities of synthetic rubber for the manufacturing of tires [1]. Synthetic rubber entails, among other co-monomers, the polymerization of 1,3-butadiene (BD), a C4 diolefin [2]. At present, naphtha steam cracking for the production of ethylene supplies the large majority of BD, of which it is a byproduct [3]. For economic and sustainability reasons, on-purpose production of renewable BD has become a topic of interest [4]. The catalytic conversion of bioethanol, an abundant and promising feedstock [5], into BD offers an alternative to naphtha steam cracking [6,7]. However, this process is currently unable to compete with petroleum-based routes to ensure its economic viability [8]. Besides the influence of ethanol and BD prices, the catalytic performances remain too low: among other things, greater productivity and catalytic stability are needed [9]. Addressing these issues require improved catalytic design, which in turn depends on a thorough understanding of the relation between catalyst features and the chemical reactions taking place.

A catalysts' prescreening study showed that, of 48 different catalysts, the combination of zinc and tantalum supported on silica yielded the highest amount of BD from ethanol. We believed this catalytic system combined the right properties to achieve high yields. Since, the zinc-tantalum design has been optimized though improved synthesis methods, both in terms of chemical and physical properties. This led has to the highest BD productivity reported, with an initial production rate of 2.45 gBD.gcat-1.h-1, at 400 °C with a WHSVEtOH of 8 h-1 over a 6.1%Zn3.4%Ta-TUD-1 (mesoporous silica) catalyst [10]. Most notably, catalytic activity remained stable over 20 hours (Figure 1), especially when compared with the other best catalysts found in the literature (MgO-SiO2 and ZnY/deBEA).

In this presentation, we aim to trace back the sequential steps leading to the preparation of our optimized material in the context of catalyst design. This will be of value to researchers interested in the development of catalysts, most notably in the conversion of sustainable feedstocks such as bioethanol. Furthermore, we will discuss the characterization of the catalysts tested and present our contribution to the unraveling of the aforementioned relation between catalyst features and catalytic activity. Notably, the identification of Lewis acid sites as active sites in the production of C4 intermediate species was established using Fourier-transformed infrared (FTIR) with pyridine as chemical probe. Furthermore, the importance of a highly dispersed active phase, evidenced by transmission electron microscopy and X-ray photoemission spectroscopy, will be discussed. How these desirable properties are easily obtained with the synthesis method used will further be elaborated.

FIGURES

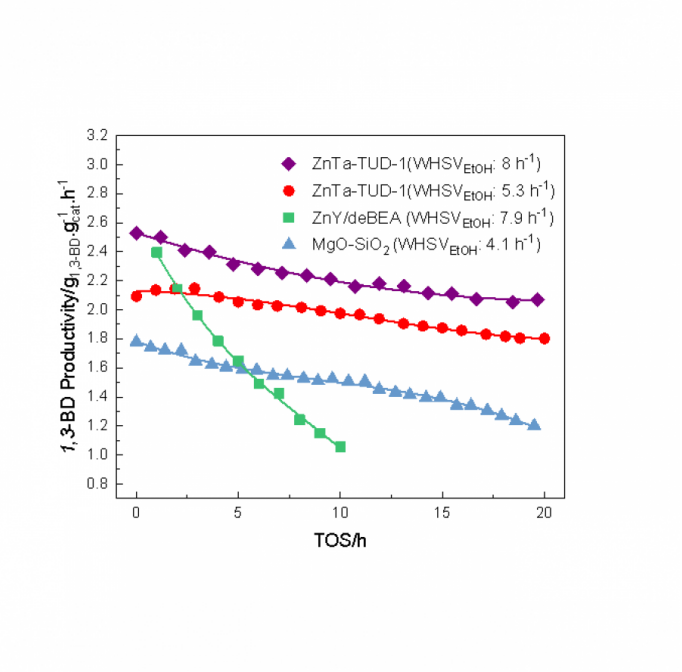

FIGURE 1
Comparative stability of most productive catalysts
Comparative stability of most productive catalysts

FIGURE 2

KEYWORDS

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