

Bio Jet Fuels Production from Lignocellulosic Biomass: Butyl Levulinate a Promising Molecule Towards the Development of Sustainable Aviation Fuels.

Doctorant·e

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Abstract

In the context of the aviation sector, which poses significant challenges due to the complexity and stringent standards of fuel, our research proposal gains particular relevance. We aim to develop an integrated approach that fully valorizes lignocellulosic biomass into jet fuels, thereby contributing to the sustainable development of society. Lignocellulosic biomass is a renewable resource that can be used as feedstock to produce high-value materials and chemicals, such as jet fuel. This type of biomass valorization includes many transformation steps, for which the kinetics and the thermal risk of the chemical reaction are not necessarily known. This work focuses on a specific compound: butyl levulinate (BL). This compound can be obtained from lignocellulosic biomass and can be transformed into gamma-valerolactone (GVL) via hydrogenation. The GVL is a vital platform molecule that can serve as a feedstock to produce substitutes for fossil fuels like gasoline, diesel, and jet fuels. The main objectives of this research are: 1) To develop a robust and reliable kinetic model for BL hydrogenation to produce GVL. Here, we seek to develop a kinetic model experimentally in different thermal modes of operation, i.e., isothermal, isoperibolic, and adiabatic. This model type not only predicts kinetics and the corresponding heat-flow rate but also allows the assessment of the thermal risk related to the chemical reaction. The experiments for developing this kinetic model were performed in the calorimeter reactor Mettler-Toledo RC1. 2) The complete valorization of lignocellulosic biomass targets the industrial scale. Therefore, the continuous production of GVL from BL should be assessed. In that sense, we studied the thermal stability of the continuous production of GVL from BL in a CSTR reactor (continuous stirred tank reactor). 3) One of the intriguing aspects of our research is the potential use of butyl levulinate (BL) as a fuels additive. We have conducted a thorough assessment of the suitability of BL as a kerosene additive, aiming to understand how its addition affects the combustion efficiency and operating limits in a gas turbine combustion chamber. The results obtained concerning the kinetic model showed that the Non-Competitive Langmuir-Hinshelwood models predict the experimental data of concentration and temperature for BL hydrogenation with good accuracy. The thermal risk analysis, linked to BL hydrogenation, showed that the energy released during the reaction is relatively low, $dH_{hyd} = -35.28 \text{ kJ/mol} \pm 1.00 \text{ kJ/mol}$, and subsequently the thermal stability study showed that for values of $Ua > 1500 \text{ W/m}^3/\text{K}$ in a continuous reactor, the risk of thermal instabilities is low. The evaluation of BL as a kerosene additive showed that adding up to 20% of BL into Kerosene does not significantly change the physical properties, neither the combustion efficiency nor the operating limits in the operating conditions considered during the combustion assessment.