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Adiabatic hydrogenation of Alkyl Levulinates to Gamma-valerolactone

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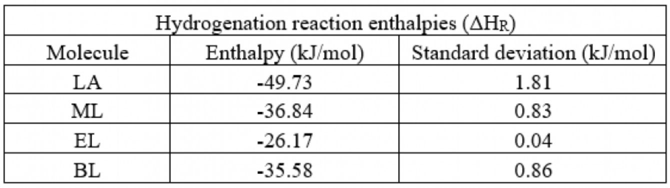
PURPOSE OF THE ABSTRACT

The use of biomass as a raw material has increased due to environmental concerns and fossil-based raw material depletion. In order to avoid concurrence with the food industry, the use of 2nd generation biomass, specifically lignocellulosic biomass (LCB), has increased [1][2]. From the valorization of LCB, several platform molecules can be obtained. Among these platform molecules, gamma-valerolactone (GVL) can be considered as one of the most relevant nowadays [3].

It has been shown that the catalytic hydrogenation of levulinic acid (LA) and alkyl levulinates (AL) over Ru/C is the most efficient method for GVL production [4]. Some studies [5] showed that the risk of thermal runaway is not negligible for such a system. This study aims to find a correlation between the structure of AL and thermal risk parameters, such as the time for maximum adiabatic rate (TMRad) and highest adiabatic temperature (?Tad) [6]. While ?Tad represents the severity of the risk and it is linked to the reaction enthalpy, TMRad is used to represent the probability of the risk and is linked to the kinetics of the reaction.

In the first stage, we have studied the hydrogenation of LA, Methyl (ML), Ethyl (EL) and Butyl (BL) levulinates to measure their reaction enthalpies (Table 1). From these measurements, one can notice that LA hydrogenation is the most exothermic reaction system. Since thermal risk also depends on kinetics, and to evaluate this parameter, experiments in adiabatic conditions were carried out (Figure 1). Based on reaction enthalpies and kinetics, the risk of thermal runaway seems to decrease with bigger levulinate structures. We are developing a kinetic model in adiabatic mode to find the relationship between these thermal risk parameters and the molecule structure. To the best of our knowledge, such a study has not been done yet.

FIGURES



Hydrogenation reaction enthalpies (ΔH_R)		
Molecule	Enthalpy (kJ/mol)	Standard deviation (kJ/mol)
LA	-49.73	1.81
ML	-36.84	0.83
EL	-26.17	0.04
BL	-35.58	0.86

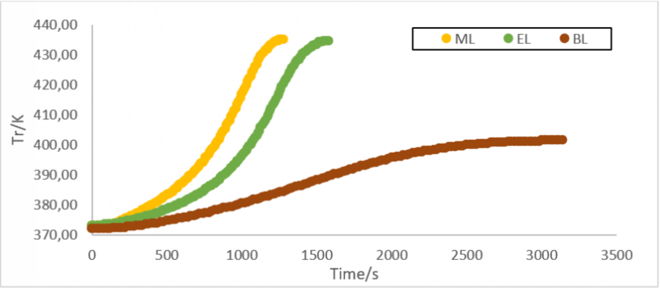


FIGURE 1

Hydrogenation Enthalpies for LA and AL

Table 1

FIGURE 2

Temperature evolution for alkyl levulinates on adiabatic conditions

Figure 1

KEYWORDS

Calorimetry | Hydrogenation | Adiabatic | Kinetic Model

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