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Co-solvent free conversion of biomass-originated levulinic acid to γ -valerolactone: from molecular level to process design

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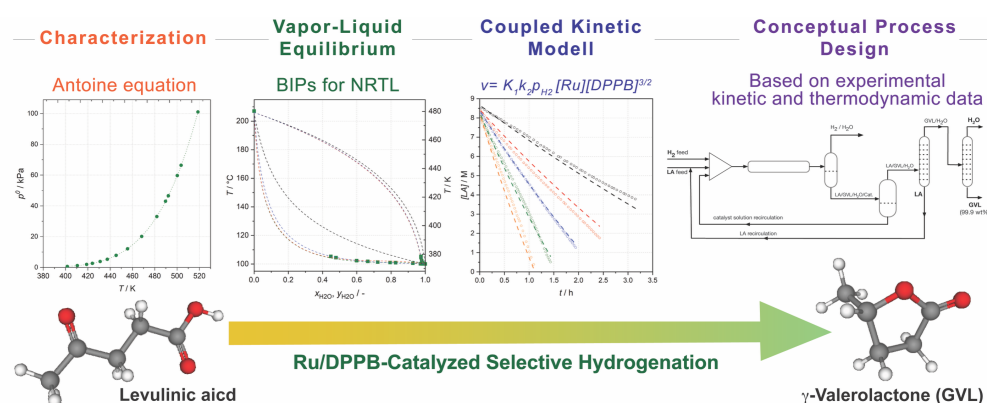
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The global efforts to replace fossil-based resources for the chemical industry demand new and innovative strategies for the green production of fuels and platform molecules, among which γ -valerolactone (GVL) stands out as a promising C₅-platform molecule.¹

We showed that GVL can be readily obtained via catalytic hydrogenation of levulinic acid (LA) in the presence of a catalyst *in situ* generated from Ru(acac)₃ and 1,4-bis(diphenylphosphino)butane (DPPB). While numerous investigations have been carried out to develop selective catalyst systems, no experimentally derived kinetic and thermodynamic data-based conceptual process design has been reported for the homogeneous phosphine-modified Ru-catalyzed transformation of LA to GVL. Thus, we aimed to determine the kinetic parameters and demonstrate the continuous production of GVL from LA using our recently published concept of “from Molecular Level to Process Design (MoLePoD)”.²

It was found that the concentration-time profiles of LA followed almost perfect linear trends up to more than 70% conversion, suggesting a formal kinetic order of zero for LA in the rate-determining step. Using a newly developed Coupled Kinetic Model (CKM), it was shown that the rate-determining step is the activation of molecular hydrogen to form the active catalyst for the reduction of LA, leading eventually to the formation of GVL and H₂O. Furthermore, temperature-dependent measurements provided the corresponding activation parameters of $\Delta H_{app}^\ddagger = 113.5 \pm 8.5 \text{ kJmol}^{-1}$ and $\Delta S_{app}^\ddagger = +53.1 \pm 20.2 \text{ Jmol}^{-1}\text{K}^{-1}$, respectively.³



Our contribution will discuss the development of the conceptual process design for GVL production, including vapor-liquid equilibria study, mechanistic study using deuterium isotope labeling, and reaction kinetic measurements.

1 Mika, L. T.; Cséfalvay, E.; Németh, Á. *Chem. Rev.* **2018**, *118*, 505–613.

2 Árvai, C.; Horváth, A. K.; Komka, K.; Mika, L. T. *Chem. Eng. J.* **2025**, *511*, 161550.

3 Árvai, C.; Horváth, A. K.; Tóth, I.; Szilágyi, A.; Mika, L. T. *Submitted for publication on January 21, 2026.*