APPENDIX

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SUPPORTING INFORMATION FOR KINETIC STUDY OF NICKEL AND COPPER MONO/BIMETALLIC CATALYSTS IN HYDROGENATION OF METHYL LEVULINATE TO GAMMA-VALEROLACTONE

Kinetic chart of k_1 and k_2 from Ni and NiCu catalysts

Note that the data points selected represent where the rates are the most constant, which leads to the most linear plots – applies to Figure A1 and A2.

Rate constants (k_1 and k_2) are plotted according to the second-order rate law due to good fit and correlation. Figure A.1(a, b, c) and A.2(a, b, c) were plotted as 1/concentration by time for both ML and HPA.

Due to the simultaneous production and consumption of HPA, the quantity of the intermediate product was calculated from the amount of ML converted and the concentration of GVL produced in as shown in equation below:

HPA conc. (mol) = (starting ML) – (current GVL + current HPA)

The rate constant k_2 was calculated by the rate in which HPA was consumed. However, as the HPA was both produced and consumed simultaneously, the HPA concentration obtained in the equation is an assumption that was deduced from the 100 % selectivity in converting ML to GVL.

The activation energy was obtained from the rearranged Arrhenius equation in Figure A.1(d) and A.2(d)

$$\ln k = \frac{-E_a}{RT} - \ln A \qquad \text{(ln A = intercept on y-axis)}$$
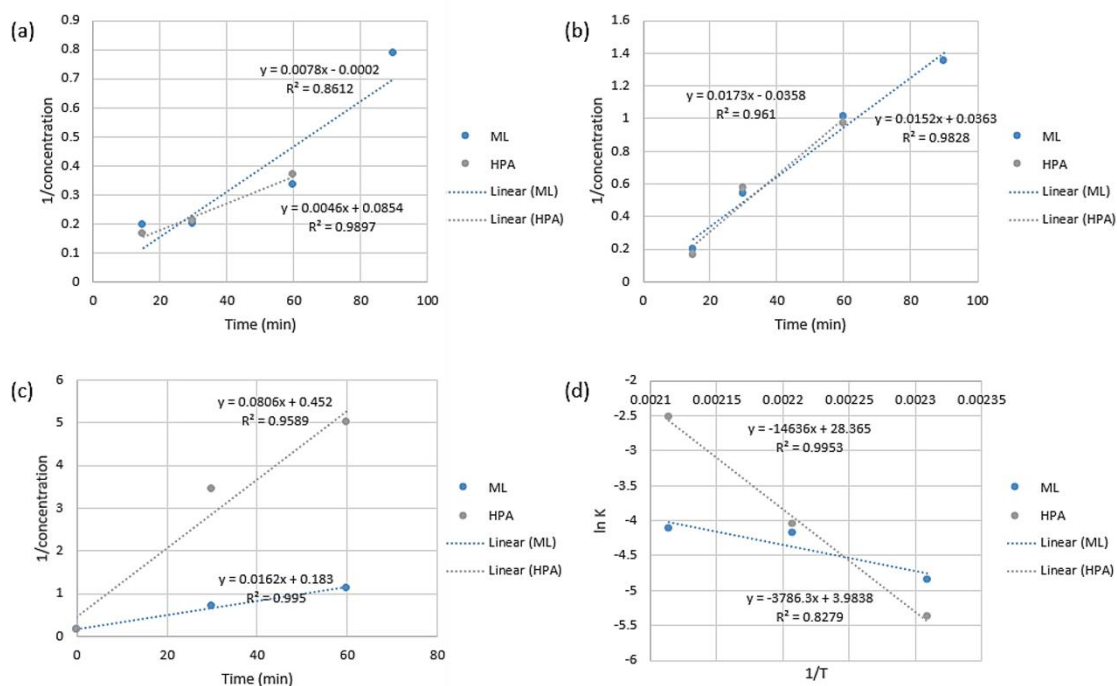
Figure A.1 Kinetic chart of k_1 and k_2 Ni catalyst at the temperatures of (a) 160 °C (b) 180 °C and (c) 200 °C and (d) the Ea calculation plot of ln k by 1/T
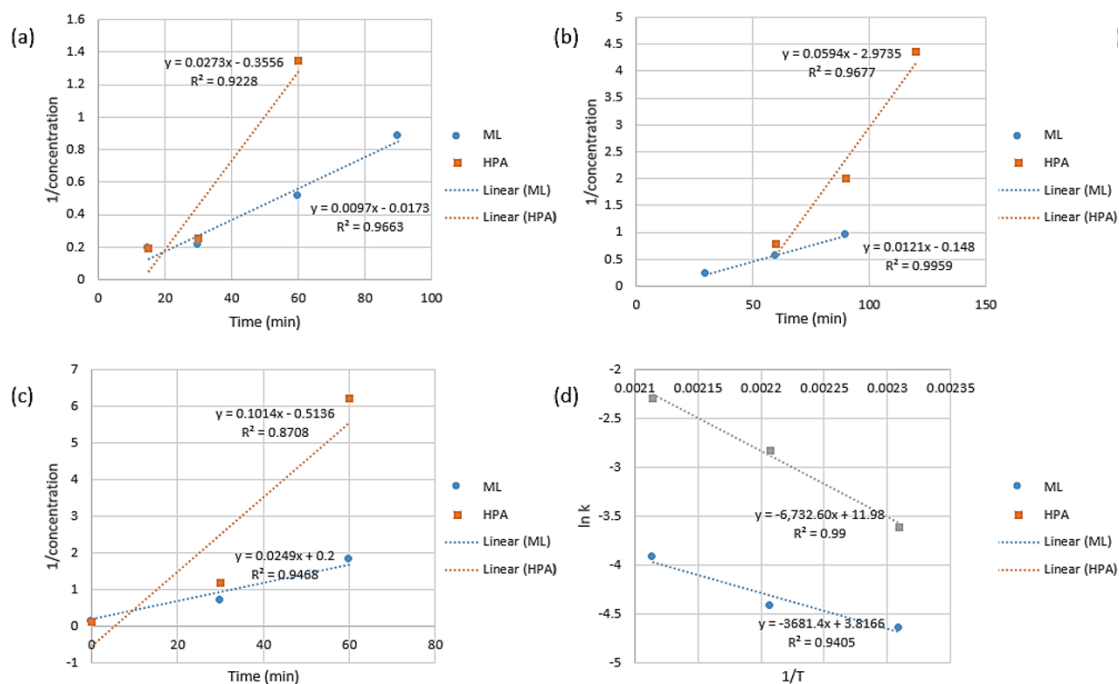
Figure A.2 Kinetic chart of k_1 and k_2 NiCu catalyst at the temperatures of (a) 160 °C (b) 180 °C and (c) 200 °C and (d) the Ea calculation plot of ln k by 1/T