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Thermodynamic analysis of phenol hydrodeoxygenation reaction system in gas phase

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Abstract: In this study, the equilibrium mole fractions of the gaseous products for the hydrodeoxygenation (HDO) of phenol process were calculated using the Lagrange multipliers method. When CH4 was considered as a possible product, the thermodynamic analysis predicted that only methane and water would be present at equilibrium conditions. This result can be attributed to their lower Gibbs free energies, when comparing to other more complex HDO products. When methane was excluded, the thermodynamic study predicted the formation of benzene and cyclohexane. Experimental data of phenol HDO using 2%Pd/ZrO2 and 5%Ru/ZrO2catalysts were also conducted. For 2%Pd/ZrO2, the main products observed were benzene, cyclohexanone, cyclohexanol. For this situation, the best operational conditions to produce deoxygenated products are intermediate temperatures(≤600 K) and high H2/phenol ratio. However, for 5%Ru/ZrO2 catalyst, methane was also detected in addition to benzene, cyclohexanone, cyclohexanol. This confirms the difference of the two types of catalysts and the importance of selecting representative species when using the Lagrange Multipliers method in a thermodynamics analysis.