An environmentally benign process for the efficient synthesis of cyclohexanone and 2-methylfuran

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Supporting Information

Thermodynamic Calculation

In this work, the equilibrium constant for the dehydrogenation of cyclohexanol (CHL) to cyclohexanone (CHN) is defined as followed:

$$K^0 = K_p K_\phi (P^0)^{-1} = \left(\frac{\chi_{CHN}\chi_{H_2}}{\chi_{CHL}}\right)_{eq} \left(\frac{\phi_{CHN}\phi_{H_2}}{\phi_{CHL}}\right)_{eq} \left(\frac{P^0}{P}\right)^{-1} \quad (1)$$

The equilibrium constant K^0 used in the present work is cited from reference.[1] K_p represents the equilibrium constant based on partial pressure. The typical reaction condition in this work is at atmospheric pressure, so $P^0 = P$. Here χ_i is the mole fraction of component i, and ϕ_i is the fugacity coefficient. K_ϕ is the fugacity coefficient ratio. The values of ϕ_i and K_ϕ can be calculated on the basis of the Redlich-Kwong equation of state.[2]

$$P = RT/(V-b) - a/T^{0.5}V(V+b) \quad (2)$$

The a and b are all constants in the Redlich-Kwong equation, which can be obtain from their critical properties.

$$a = 0.4278R^2T_C^{2.5}/P_C \quad (3)$$

$$b = 0.0867RT_C/P_C \quad (4)$$

When

$$Z = 1/(1-h) - (A^2/B)h/(1+h) \quad (5)$$

$$A^2 = a/R^2T^{2.5} = 0.4278T_C^{\ 2.5}/P_CT^{2.5} \quad (6)$$

$$B = b / RT = 0.0867 T_C / P_C T \qquad (7)$$

$$h = BP / Z \qquad (8)$$

are assumed, the fugacity coefficient ϕ_i is given by

$$\ln \phi = Z - 1 - \ln(Z - BP) - (A^2 / B) \ln(1 + BP / Z) \qquad (9)$$

The critical temperature T_C and pressure P_C of each component used in the present work is cited from reference.[3] Z is compressibility factor.

References

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