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:

\[
K^0 = K_p K_{\phi}(P^0)^{-1} = \left( \frac{X_{CHN} X_{H2}}{X_{CHL}} \right) \left( \frac{\phi_{CHN} \phi_{H2}}{\phi_{CHL}} \right) \left( \frac{P^0}{P} \right)^{-1} \tag{1}
\]

The equilibrium constant \(K^0\) used in the present work is cited from reference.\textsuperscript{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 \(\chi_i\) is the mole fraction of component \(i\), and \(\phi_i\) is the fugacity coefficient. \(K_{\phi}\) is the fugacity coefficient ratio. The values of \(\phi_i\) and \(K_{\phi}\) can be calculated on the basis of the Redlich-Kwong equation of state.\textsuperscript{2}

\[
P = RT/(V - b) - a / T^{0.5}(V + b) \tag{2}
\]

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

\[
a = 0.4278 R^2 T_c^{2.5} / P_c \tag{3}
\]

\[
b = 0.0867 RT_c / P_c \tag{4}
\]

When

\[
Z = 1/(1 - h) - (A^2 / B)h / (1 + h) \tag{5}
\]

\[
A^2 = a / R^2 T_c^{2.5} = 0.4278 T_c^{2.5} / P_c T_c^{2.5} \tag{6}
\]
are assumed, the fugacity coefficient \( \phi_i \) is given by

\[
\ln \phi_i = Z - 1 - \ln(Z - BP) - (A^2 / B) \ln(1 + BP / Z)
\]

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

