RSC Reaction Chemistry & Engineering

Esterification of propanoic acid with 1,2-propanediol: Catalysis by cesium exchanged heteropoly acid on K-10 clay and kinetic modelling

Devendra P. Tekale and Ganapati D. Yadav*

Supplementary Information

Adsorption of 1,2-PDO (A) on the vacant surface site S is given by

$$A + S \rightleftharpoons AS \quad (1)$$

Similarly, adsorption of propanoic acid (B) on the vacant surface site is represented as

$$B + S \rightleftharpoons BS \quad (2)$$

Having adsorbed on surface, reaction of AS with BS on adjacent sites leads to formation of monoester of propionic acid (ES) and water (WS) on the catalytic sites

$$AS + BS \rightleftharpoons ES + WS \quad (3)$$

Second molecule of adsorbed propionic acid (BS) reacts with the adsorbed monoester (ES) on the adjacent site, as follows to give the diester; 1,2-propanedioldipropanoate (FS) and water (WS).

$$ES + BS \rightleftharpoons FS + WS \quad (4)$$

Desorption of product species is given by

$$ES \rightleftharpoons E + S \quad (5)$$

$$FS \rightleftharpoons F + S \quad (6)$$

$$WS \rightleftharpoons W + S \quad (7)$$

Total concentration of the sites, C_t can be expressed as

$$C_t = C_S + C_{AS} + C_{BS} + C_{ES} + C_{FS} + C_{WS} \quad (8)$$

or

$$C_t = K_A C_A C_S + K_B C_B C_S + K_E C_E C_S + K_F C_F C_S + K_W C_W C_S \quad (9)$$

or, the concentration of vacant sites,

$$C_S = \frac{C_t}{(1 + \mathrm{K_A C_A} + \mathrm{K_B C_B} + \mathrm{K_E C_E} + \mathrm{K}_F \mathrm{C_F} + \mathrm{K_W C_W})} \quad (10)$$

If the surface reaction (4) is controlling the rate of reaction, then the rate of conversion of A is given by the equation

$$-r_A = -\frac{dC_A}{dt} = k_3 C_{ES} C_{BS} = k_3 K_2 C_{AS} C_{BS}^2 / C_{WS} \quad (11)$$