Overall:

MCH $\rightleftharpoons$ TOL + 3 H_2

Sequence:

MCH + s $\rightleftharpoons$ MCH·s (I)

MCH·s $\rightleftharpoons$ MCHe·s + H_2 (II)

MCHe·s $\rightleftharpoons$ MCHde·s + H_2 (III)

MCHde·s $\rightleftharpoons$ TOL·s + H_2 (IV)

TOL·s $\rightleftharpoons$ TOL + s (V)

Derivation:

From step-II, it may be written as

$$(-r_A) = k_2 \cdot C_{A\cdot s} - k_{-2} \cdot C_{D\cdot s} \cdot p_C \qquad \text{(rds)} \tag{1}$$

We need $C_{A\cdot s}$ and $C_{D\cdot s}$, so

From step-I, -III, -IV, and -V Eq. 2, Eq. 3, Eq. 4, and, Eq. 5 may be written, respectively

$$C_{A\cdot s} = K_A \cdot p_A \cdot C_s \tag{2}$$

$$C_{D\cdot s} = \frac{C_{E\cdot s} \cdot p_C}{K_3} \tag{3}$$

$$C_{E\cdot s} = \frac{C_{B\cdot s} \cdot p_C}{K_4} \tag{4}$$

$$C_{B\cdot s} = K_B \cdot p_B \cdot C_s \tag{5}$$

Where, K_B is adsorption equilibrium constant of toluene which is reciprocal to the desorption equilibrium constant for toluene

Using Eq. 4 with Eq. 5, it may shown that

$$C_{E\cdot s} = \frac{C_{B\cdot s} \cdot p_C}{K_4} = \frac{K_B \cdot p_B \cdot C_s \cdot p_C}{K_4} \tag{6}$$

Using Eq. 6 with Eq. 3, it may shown that

$$C_{D\cdot s} = \frac{C_{E\cdot s} \cdot p_C}{K_3} = \frac{K_B \cdot p_B \cdot C_s \cdot {p_C}^2}{K_3 \cdot K_4} \qquad (7)$$

$$(-r_A) = k_2 \cdot K_A \cdot p_A \cdot C_s - k_{-2} \cdot \frac{K_B \cdot p_B \cdot C_s \cdot p_c^3}{K_3 \cdot K_4}$$

$$(-r_A) = k_2 \cdot K_A \cdot p_A \cdot C_s \cdot \left(1 - \frac{k_{-2} \cdot K_B \cdot p_B \cdot {p_C}^3}{k_2 \cdot K_A \cdot K_3 \cdot K_4 \cdot p_A}\right) \qquad (8)$$

Now, $K = \frac{k_2 \cdot K_A \cdot K_3 \cdot K_4}{k_{-2} \cdot K_B}$, so Eq. 8 becomes as follows

$$(-r_A) = k_2 \cdot K_A \cdot p_A \cdot C_s \cdot \left(1 - \frac{p_B \cdot {p_C}^3}{K \cdot p_A}\right) \qquad (9)$$

<u>Site balance:</u>

$$C_T = C_s + C_{A\cdot s} + C_{B\cdot S} + C_{D\cdot s} + C_{E\cdot s} \qquad (10)$$

Inserting corresponding expressions in Eq. 10, it may shown that

$$C_T = C_s + K_A \cdot p_A \cdot C_s + K_B \cdot p_B \cdot C_s + \frac{K_B \cdot p_B \cdot C_s \cdot {p_C}^2}{K_3 \cdot K_4} + \frac{K_B \cdot p_B \cdot C_s \cdot p_C}{K_4}$$

$$C_T = C_s \cdot \left(1 + K_A \cdot p_A + K_B \cdot p_B + \frac{K_B \cdot p_B \cdot {p_C}^2}{K_3 \cdot K_4} + \frac{K_B \cdot p_B \cdot p_C}{K_4}\right)$$

$$C_s = C_T \cdot \left(1 + K_A \cdot p_A + K_B \cdot p_B + \frac{K_B \cdot p_B \cdot {p_C}^2}{K_3 \cdot K_4} + \frac{K_B \cdot p_B \cdot p_C}{K_4}\right)^{-1} \qquad (11)$$

Inserting Eq. 11 in Eq. 9 and writing $C_T \cdot k_2$ as *k*, it may shown that

$$(-r_A) = \frac{k \cdot K_A \cdot p_A \cdot \left(1 - \frac{p_B \cdot {p_C}^3}{K \cdot p_A}\right)}{\left(1 + K_A \cdot p_A + K_B \cdot p_B + \frac{K_B \cdot p_B \cdot {p_C}^2}{K_3 \cdot K_4} + \frac{K_B \cdot p_B \cdot p_C}{K_4}\right)}$$

<u>(Final form)</u>