REB, The Course
Class 7 Practice Assignment Calculations

Equation numbers correspond to the Class 7 Practice Assignment Solution.

Rates of the mechanistic steps:

$$r_j = k_{j,f} \prod_{i_r} [i_r]^{-\nu_{i_r,j}} - k_{j,r} \prod_{i_p} [i_p]^{\nu_{i_p,j}}$$

$$r_2 = k_{2,f} [E] \left[C\right] - k_{2,r} \left[E\text{-}C\right] \tag{5}$$

$$r_3 = k_{3,f} \left[E\text{-}C\right] \left[S\right] - k_{3,r} \left[S\text{-}E\text{-}C\right] \tag{6}$$

$$r_4 = k_{4,f} \left[S\text{-}E\text{-}C\right] \tag{7}$$

Rate of the apparent reaction:

$$r_{i,j_{non}} = \sum_{j'} \nu_{i,j'} r_{j'}$$

$$r_{P,1} = r_4 \tag{8}$$

Bodenstein steady-state approximations:

$$0 = \sum_{j'} \nu_{i_{RI},j'} r_{j'}$$

$$0 = -r_2 \tag{9}$$

$$0 = r_2 - r_3 + r_4 \tag{10}$$

$$0 = r_3 - r_4 \tag{11}$$

Catalyst conservation equation:

$$C_{cat,0} = C_{cat,free} + \sum_{i_c} \kappa_{i_c} C_{i_c}$$

$$E_0 = [E] + \left[E\text{-}C\right] + \left[S\text{-}E\text{-}C\right] \tag{12}$$

Most abundant intermediate inequalities:

$$\left[E\text{-}C\right] \gg [E] \tag{13}$$

$$\left[E\text{-}C\right] \gg \left[S\text{-}E\text{-}C\right] \tag{14}$$

Substitute (5) in (9) and rearrange.

$$\left[E\text{-}C\right] = \frac{k_{2,f}\left[C\right]}{k_{2,r}}[E] \tag{15}$$

Substitute (6) and (7) in (11) and rearrange, then substitute (15).

$$0 = k_{3,f}\left[E\text{-}C\right]\left[S\right] - k_{3,r}\left[S\text{-}E\text{-}C\right] - k_{4,f}\left[S\text{-}E\text{-}C\right]$$

$$\left[S\text{-}E\text{-}C\right] = \frac{k_{3,f}\left[E\text{-}C\right]\left[S\right]}{k_{3,r} + k_{4,f}}$$

$$\left[S\text{-}E\text{-}C\right] = \frac{k_{2,f}k_{3,f}}{k_{2,r}\left(k_{3,r} + k_{4,f}\right)}\left[S\right]\left[C\right][E] \tag{16}$$

Substitute (15) and (16) in (12) and solve for [E].

$$E_0 = [E] + \frac{k_{2,f}\left[C\right]}{k_{2,r}}[E] + \frac{k_{2,f}k_{3,f}}{k_{2,r}\left(k_{3,r} + k_{4,f}\right)}\left[S\right]\left[C\right][E]$$

$$[E] = \frac{E_0}{\left(1 + \frac{k_{2,f}}{k_{2,r}}\left[C\right] + \frac{k_{2,f}k_{3,f}}{k_{2,r}\left(k_{3,r} + k_{4,f}\right)}\left[C\right]\left[S\right]\right)} \tag{17}$$

Substitute (17) into (15) and (16) to get expressions for [E-C] and [S-E-C].

$$\left[E\text{-}C\right] = \frac{\frac{k_{2,f}}{k_{2,r}} E_0 \left[C\right]}{1 + \frac{k_{2,f}}{k_{2,r}} \left[C\right] + \frac{k_{2,f} k_{3,f}}{k_{2,r}\left(k_{3,r} + k_{4,f}\right)} \left[C\right] \left[S\right]} \tag{18}$$

$$\left[S\text{-}E\text{-}C\right] = \frac{\frac{k_{2,f} k_{3,f}}{k_{2,r}\left(k_{3,r} + k_{4,f}\right)} E_0 \left[C\right] \left[S\right]}{\left(1 + \frac{k_{2,f}}{k_{2,r}} \left[C\right] + \frac{k_{2,f} k_{3,f}}{k_{2,r}\left(k_{3,r} + k_{4,f}\right)} \left[C\right] \left[S\right]\right)} \tag{19}$$

Substitute (7) in (8) and then substitute (19) in the resulting equation.

$$r_{P,1} = k_{4,f} \left[S\text{-}E\text{-}C\right]$$

$$r_{P,1} = \frac{\frac{k_{2,f} k_{3,f} k_{4,f}}{k_{2,r}\left(k_{3,r} + k_{4,f}\right)} E_0 \left[C\right] \left[S\right]}{\left(1 + \frac{k_{2,f}}{k_{2,r}} \left[C\right] + \frac{k_{2,f} k_{3,f}}{k_{2,r}\left(k_{3,r} + k_{4,f}\right)} \left[C\right] \left[S\right]\right)} \tag{20}$$

Substitute (17) and (18) in (14) and simplify.

$$\frac{\frac{k_{2,f}}{k_{2,r}} E_0 \left[C\right]}{1 + \frac{k_{2,f}}{k_{2,r}} \left[C\right] + \frac{k_{2,f} k_{3,f}}{k_{2,r}\left(k_{3,r} + k_{4,f}\right)} \left[C\right] \left[S\right]} \gg \frac{E_0}{\left(1 + \frac{k_{2,f}}{k_{2,r}} \left[C\right] + \frac{k_{2,f} k_{3,f}}{k_{2,r}\left(k_{3,r} + k_{4,f}\right)} \left[C\right] \left[S\right]\right)}$$

$$\frac{k_{2,f}}{k_{2,r}} \left[C\right] \gg 1$$

Delete the 1 in the denominator or (20).

$$r_{P,1} = \frac{\frac{k_{2,f}k_{3,f}k_{4,f}}{k_{2,r}\left(k_{3,r}+k_{4,f}\right)}E_0\left[C\right]\left[S\right]}{\left(\frac{k_{2,f}}{k_{2,r}}\left[C\right]+\frac{k_{2,f}k_{3,f}}{k_{2,r}\left(k_{3,r}+k_{4,f}\right)}\left[C\right]\left[S\right]\right)} \tag{21}$$

Substitute (17) and (19) in (14) and simplify.

$$\frac{\frac{k_{2,f}}{k_{2,r}}E_0\left[C\right]}{1+\frac{k_{2,f}}{k_{2,r}}\left[C\right]+\frac{k_{2,f}k_{3,f}}{k_{2,r}\left(k_{3,r}+k_{4,f}\right)}\left[C\right]\left[S\right]} \gg \frac{\frac{k_{2,f}k_{3,f}}{k_{2,r}\left(k_{3,r}+k_{4,f}\right)}E_0\left[C\right]\left[S\right]}{\left(1+\frac{k_{2,f}}{k_{2,r}}\left[C\right]+\frac{k_{2,f}k_{3,f}}{k_{2,r}\left(k_{3,r}+k_{4,f}\right)}\left[C\right]\left[S\right]\right)}$$

$$\frac{k_{2,f}}{k_{2,r}}\left[C\right] \gg \frac{k_{2,f}k_{3,f}}{k_{2,r}\left(k_{3,r}+k_{4,f}\right)}\left[C\right]\left[S\right]$$

Drop the term on the right from the denominator in (21) and simplify.

$$r_{P,1} = \frac{\frac{k_{2,f}k_{3,f}k_{4,f}}{k_{2,r}\left(k_{3,r}+k_{4,f}\right)}E_0\left[C\right]\left[S\right]}{\left(\frac{k_{2,f}}{k_{2,r}}\left[C\right]\right)}$$

$$r_{P,1} = \frac{k_{3,f}k_{4,f}}{\left(k_{3,r}+k_{4,f}\right)}E_0\ \left[S\right] \tag{22}$$