REB, The Book
Example 4.8.3 Calculations

Equation numbers match those in the Example 4.8.3 Solution

Rates of the mechanistic steps:

$$r_2 = k_{2,f}[E]\left[S\right] - k_{2,r}\left[E{-}S\right] \tag{4}$$

$$r_3 = k_{3,f}\left[E{-}S\right] \tag{5}$$

Rate expression for the apparent rate of generation of reagent P:

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

$$r_{P,1} = r_3 = k_{3,f}\left[E{-}S\right] \tag{6}$$

Bodenstein Steady-State Approximations or Quasi-Equilibrium Expressions

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

$$0 = r_2 - r_3 = k_{2,f}[E]\left[S\right] - k_{2,r}\left[E{-}S\right] - k_{3,f}\left[E{-}S\right] \tag{7}$$

$$0 = -r_2 + r_3 = -k_{2,f}[E]\left[S\right] + k_{2,r}\left[E{-}S\right] + k_{3,f}\left[E{-}S\right] \tag{8}$$

Enzyme Conservation Equation

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

$$E_0 = [E] + \left[E{-}S\right] \tag{9}$$

Solving equation (7) for $\left[E{-}S\right]$

$$\left[E{-}S\right] = \frac{k_{2,f}[E]\left[S\right]}{k_{2,r} + k_{3,f}} \tag{A}$$

Substituting in equation (9) and solving for $[E]$

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

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

$$[E] = E_0 \frac{k_{2,r} + k_{3,f}}{k_{2,r} + k_{3,f} + k_{2,f}\left[S\right]} \tag{10}$$

Substituting in equation (A)

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

$$\left[E{-}S\right] = \frac{k_{2,f}E_0\left[S\right]}{k_{2,r} + k_{3,f} + k_{2,f}\left[S\right]} \tag{11}$$

Substitute equation (11) in equation (6)

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

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