Three-way reactions in MCell

The rate of reaction of a molecule that can engage in a three-way reaction with reactants I and J at concentrations ρ_I and ρ_J is $\kappa\rho_I\rho_J$. Suppose that a single molecules moves a distance R while sweeping out an interaction area of δA. Then the expected number of hits, assuming that the concentration of I and J is low, is

$$n_{\text{hits}} = R\,\delta A\,\rho_I \cdot R\,\delta A\,\rho_J$$

Thus, the expected number of hits for a molecule with a diffusion length constant of λ is

$$n = \int_0^\infty \rho_I\rho_J\delta A^2 R^2 \frac{4\pi R^2}{\pi^{3/2}\lambda^3} e^{-R^2/\lambda^2} dR = \frac{3}{2}\rho_I\rho_J\delta A^2\lambda^2$$

If we let p be the probability of reaction, then

$$\kappa\rho_I\rho_J\Delta t = p \cdot n = p \cdot \frac{3}{2}\rho_I\rho_J\delta A^2\lambda^2$$

Solving for p gives

$$p = \frac{\kappa}{6D\delta A^2}$$

If we let all three reactants move and react—let us number them 1, 2, and 3—then we matching the total rate gives

$$\kappa\rho_1\rho_2\rho_3\Delta t = \frac{3}{2}\rho_1\rho_2\rho_3\delta A^2\left(p_1\lambda_1^2 + p_2\lambda_2^2 + p_3\lambda_3^2\right)$$

and we can decide to let $p_1 = p_2 = p_3 = p$ to give

$$p = \frac{\kappa}{6\,(D_1 + D_2 + D_3)\,\delta A^2}$$

This solution also works for the cases where some of the reactants can't move (as D_i will be zero and will drop out of the equation).