Supplementary data

1. The inversion method

This section shows how the inversion method for generating random numbers is used to generate random scavenging times in the hybrid simulations (reference 34 in the manuscript). The Smoluchowski rate constant given in equation 7 is used but the modified rate constant can be applied in the same way. Assuming that the probability of a radical surviving to time t is Ω, then the rate of the R+S reaction is

$$-\frac{d\Omega}{dt} = k(t) C_0 \Omega = 4\pi a D' \left(1 + \frac{a}{\sqrt{\pi D' t}}\right) C_0 \Omega \qquad (1).$$

And so

$$\Omega = \exp\left[-C_0 k_{D'} \left(t + 2a\sqrt{t/\pi D'}\right)\right] \quad : \quad k_{D'} = 4\pi a D' \qquad (2).$$

The reaction probability W is then

$$W = 1 - \Omega = 1 - \exp\left[-C_0 k_{D'} \left(t + 2a\sqrt{t/\pi D'}\right)\right] \qquad (3).$$

Which can be easily inverted so that t is expressed as a function of P as follows

$$t = \left(\frac{-a}{\sqrt{\pi D'}} + \left(\frac{a}{\pi D'} - \frac{\ln(1-P)}{C_0 k_{D'}}\right)^{1/2}\right)^2 \qquad (4).$$

And a similar equation can be written if the proposed correction is used in equation 9. Finally, it should be noted that the last equation does not include the possibility that $t = 0$, i.e. the radical will undergo a scavenging reaction immediately as it is introduced in contact with a scavenger particle. To take this into account, assume that the number of scavengers M in the volume V follows a Poisson distribution as follows

$$\Pr\{M = m\} = \frac{(C_0 V)^m}{m!} \exp(-C_0 V) \qquad (5).$$

The last equation will represent the zero-time survival probability Ω_0 if $V = 4\pi a^3/3$ and $m = 0$, and hence the zero-time reaction probability P_0 is

$$P_0 = 1 - \Omega_0 = 1 - \exp\left(-\frac{4}{3}\pi a^3 C_0\right) \qquad (6).$$

Which can be used in the simulation with a uniform random number between 0 and 1 to determine if the scavenging time is zero.

2. Example of the simulations

Another example of the simulations is included; the notations are the same as those in the article:

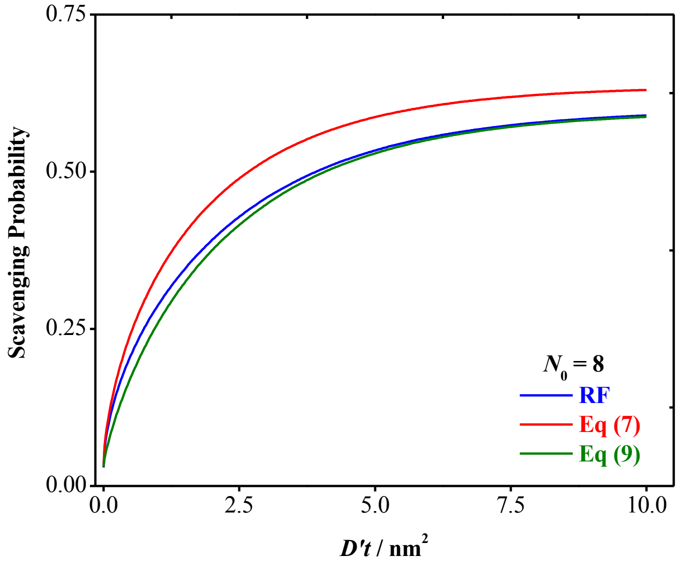

Figure 1. The scavenging probability in the S1 scheme for $N_0 = 8$.

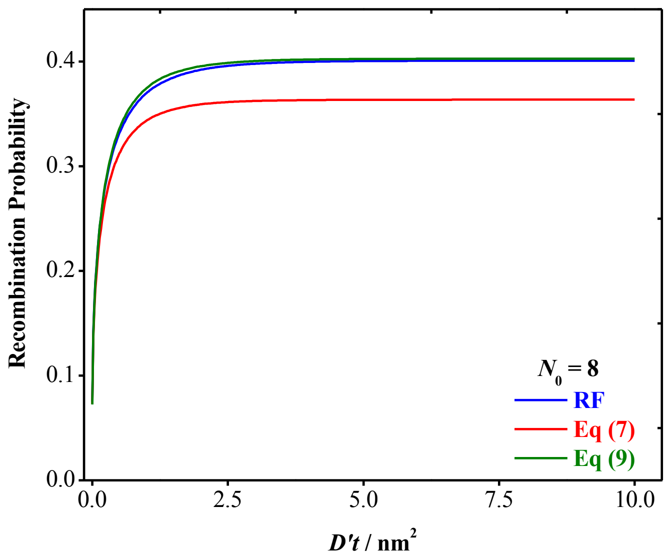

Figure 2. The recombination probability in the S1 scheme for $N_0 = 8$.

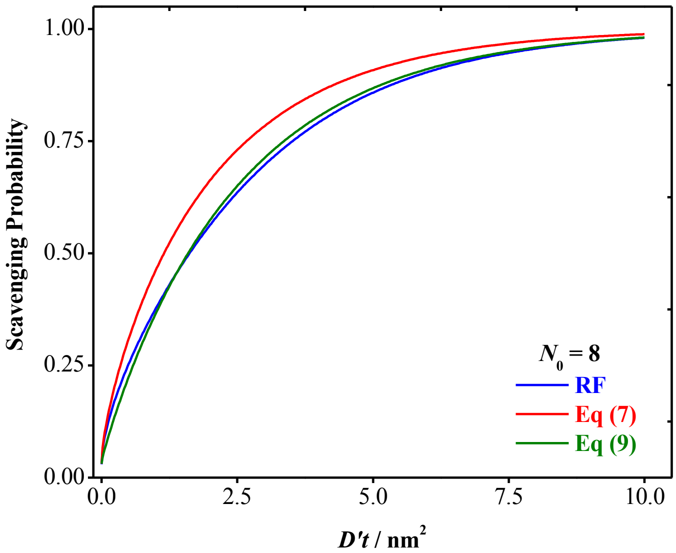

Figure 3. The scavenging probability in the S2 scheme for $N_0 = 8$.