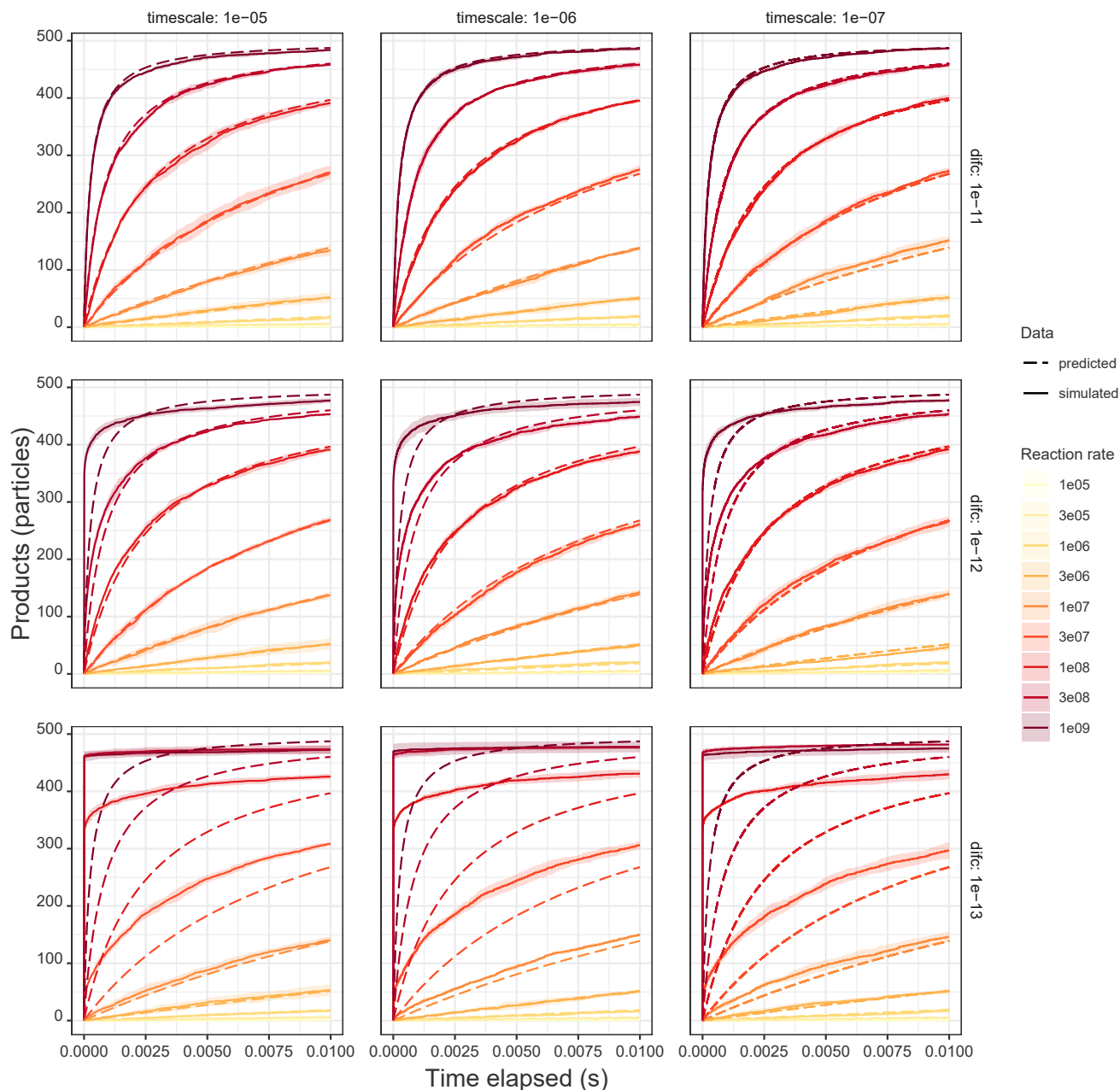


Reaction products from a two-particle reaction using AB-adjusted radii



Supplemental Figure 5: Summary of two-particle bimolecular products over time using the Andrews-Bray adjusted Smoluchowski method to calculate reaction radii.

Dashed lines represent the theoretical yield of products from a bimolecular reaction involving two particles over 0.01 seconds. Solid lines represent yield predicted in simulations using Cell4D (mean over 5 replicates). Theoretical yields were obtained from mass action kinetics using the equation $\frac{dA}{dt} = -k \times A^2$. Simulations used the Andrews-Bray adjusted Smoluchowski method. Line colors represent the rate constant of the reaction, with darker colors representing faster rates. Time step lengths of 0.1, 1, and 10 μs were used as simulation parameters, and particle diffusion constants of 1×10^{-11} to $1 \times 10^{-13} \text{ m}^2/\text{s}$ were investigated. For reactants with $1 \times 10^{-11} \text{ m}^2/\text{s}$ diffusion rate, the simulated product curve closely aligns with the theoretical yields at all reaction rates. For diffusion rates of $1 \times 10^{-12} \text{ m}^2/\text{s}$, simulations are accurate for reactions up to $1 \times 10^8 \text{ M}^{-1}\text{s}^{-1}$. For diffusion rates of $1 \times 10^{-13} \text{ m}^2/\text{s}$, simulations perform poorly.