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Ligand binding kinetics in surface plasmon resonance devices: A Monte Carlo simulation analysis JACOB CARROLL, UWE TAUBER, Virginia Tech — Surface plasmon resonance (SPR) chips are widely used to measure association and dissociation rates for the binding kinetics between two species of chemicals, e.g., cell receptors and ligands. It is commonly assumed that ligands are spatially well mixed in the SPR region, and hence a mean-field rate equation description is appropriate. This approximation however ignores the spatial fluctuations as well as temporal correlations induced by multiple local rebinding events, which become prominent for slow diffusion rates. We report detailed Monte Carlo simulations of ligand binding kinetics in an SPR cell subject to laminar flow. We extract the binding and dissociation rates by means of the techniques frequently employed in experimental analysis that are motivated by the mean-field approximation. We find major discrepancies in a wide parameter regime between the thus extracted rates and the input simulation values. These results underscore the crucial quantitative importance of spatio-temporal correlations in binary reaction kinetics in SPR cell geometries.

Jacob Carroll
Virginia Tech

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