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Ligand-Receptor Binding Kinetics in Surface Plasmon Resonance Cells: A Monte Carlo Analysis JACOB CARROLL, Center for Soft Matter and Biological Physics & Physics Department, Virginia Tech, MATTHEW RAUM, Baker Hughes, Blacksburg, Va, KIMBERLY FORSTEN-WILLIAMS, Biomedical Engineering, Duquesne University, UWE TÄUBER, Center for Soft Matter and Biological Physics & Physics Department, 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 thus a mean-field rate equation description is appropriate. This approximation ignores the spatial fluctuations and temporal correlations induced by local rebinding events, which become prominent for slow diffusion rates and high binding rates. We report detailed Monte Carlo simulations of ligand binding kinetics in an SPR cell subject to laminar flow. We extract the binding dynamics by means of the techniques employed in experimental analysis that are motivated by the mean-field approximation. We find major discrepancies in a wide parameter range between the thus extracted rates and the known input simulation values. These results underscore the crucial quantitative importance of spatio-temporal correlations in binary reaction kinetics in SPR cell geometries, and demonstrate the failure of a mean-field analysis of SPR cells in the regime of high association rates, where the spatio-temporal correlations due to diffusive transport and ligand-receptor rebinding events dominate the dynamics of SPR systems.

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