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Surface reaction-diffusion kinetics on lattice at the microscopic scale
by Wei-Xiang Chew, Kazunari Kaizu, Masaki Watabe, et al.

Dear Dr. Muniandy,

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Surface reaction-diffusion kinetics on lattice at the microscopic scale

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ABSTRACT

Microscopic modeling of surface reaction-diffusion process can connect the local spatial-temporal effects to the macroscopic self-organized pattern often observed on cell membrane. As a microscopic modeling techniques, microscopic lattice method (MLM) is simple to implement and computationally less demanding. However, its accuracy and consistency in modeling surface reaction compared to continuum-based approaches have not been clarified in detail. This work examines the accuracy of MLM in modeling diffusion-influenced surface reaction based on the Spatiocyte simulation scheme. We derive the lattice-based bimolecular association rate for two-dimensional surface-surface reaction and one-dimensional volume-surface adsorption according to the Smoluchowski-Collins-Kimball model and random walk theory. By matching the time-dependent lattice-based and continuum-based rates, we obtain the expressions to determine the MLM parameters from the physical constants. We found that the voxel size need to be at least 0.6% larger than the molecule size to simulate surface reaction on the triangular lattice accurately. This value is smaller compared to the 5% requirement on the square lattice. We also demonstrate the capability of Spatiocyte scheme by simulating a reaction-diffusion model that involve all dimensions: three-dimensional diffusion in the cytoplasm, two-dimensional diffusion on the cell membrane and one-dimensional cytoplasm-membrane adsorption. The contribution of 2D reaction pathway to the overall reaction rate has been studied at different reactant diffusivity, reactivity and concentration.