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Mathematical modelling of siderophores-mediated iron acquisition and cross-feeding in bacterial communities

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The ability to acquire iron is a key determinant of survival, biofilm development and pathogenicity for most microorganisms. Many bacteria produce specialized siderophores that bind iron from the environment, making it available to cells under iron-limiting conditions. Fluorescent pseudomonads, for example, secrete pyoverdines (PVDs) as effective iron-chelating agents. Studies on iron chelation dynamics and cross-feeding models have demonstrated that the ability to produce siderophores and cross-feed provides a fitness advantage to certain species over those that cannot engage in this interaction.

This phenomenon has been empirically investigated in species such as the rhizosphere bacterium *Pseudomonas protegens* Pf-5 and *Pseudomonas aeruginosa* PA-01 which was carried out in a chemostat and batch cultures. However, most studies have not accounted for spatial heterogeneity settings. Unlike well-mixed and homogeneous environments, bacterial populations typically live and grow in spatially structured communities, such as colonies or biofilms on surfaces. We address this question in the present study.

Building on a previously introduced ordinary differential equations model of iron chelation dynamics and cross-feeding, we formulate a reaction-diffusion model for two related species. This approach leads to a highly non-linear system of partial differential equations. To solve it numerically, we use a finite difference method with implicit discretization in both space and time. Our findings indicate that siderophore production and cross-feeding confers a growth advantage even in spatially structured environments. Factors such as diffusion and the length of the spatial domain between the dual species significantly influence cross-feeding. Furthermore, the magnitude of the growth advantage also depends on the initial inoculation of the iron and substrate (carbon). The mathematical model allows for a better understanding of the complex interactions including quantification.

Keywords: siderophores, bacteria, pyoverdines, reaction-diffusion model, partial differential equations, ordinary differential equations, spatial domain, diffusion

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