UNIVERSITY OF AMSTERDAM

Abstract

Faculty of Science Informatics Institute

Master of Science in Computational Science

Modelling Diffusive Signals for the Germination of Aspergillus Conidia

by Boyan Mihaylov

The germination rate of Aspergillus conidia is known to be influenced by the inducing carbon source in the medium and by an auto-inhibitor produced by the spores. This thesis assesses the plausibility of diffusion-driven mechanisms timing the action of these signals until germination is enabled. To this end, computational models of spores releasing inhibitor molecules are constructed on multiple scales, first simulating the depletion of inhibitor from a single spore, then exploring the effect of increasing densities of spores and eventually examining the diffusive outflow in a dense spore cluster in closer detail. This leads to several observations: that the commonly considered inhibitor 1-octen-3-ol is depleted too fast, unless a strong cell wall adsorption or continuous synthesis slow down its decrease; that increasing spore densities lead to an ambient inhibitor saturation flattening the permeation-driving gradient; and that dense spore packings do not lead to substantial inhibitor retention, unless their contact area is large. Finally, germination probability models incorporating induction and inhibition are proposed, representing heterogeneities in the spores through random variables. Parameter estimation through global and local optimisation highlights a promising model which fits experimental data under biologically sensible parameters. In this model, an inhibitor falls below a critical value and an inhibitor-dependent inducing signal rises above an inhibitor-dependent threshold to trigger germination. In an attempt to explain data with both endogenously driven and exogenously controlled inhibition with 1-octen-3-ol, no appropriate parameter combination is found, leading to the supposition that the in-vivo inhibition is more complex than a saturation of the medium with the volatile organic compound.