MSc Computational Science
joint programme UvA/VU

A DIFFUSION-BASED MODEL OF SPATIAL INTERACTIONS IN *ASPERGILLUS* SPP. GERMINATION

INTERMEDIATE PRESENTATION JANUARY

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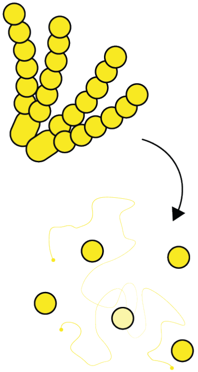
OUTLINE

INTRODUCTION

Hypothesis

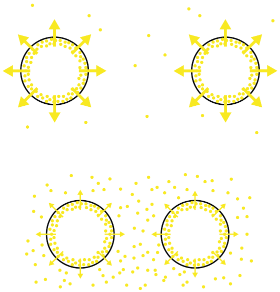
- Upon inoculation in an aqueous medium, a germination inhibitor diffuses away from the conidium.
  - Experiments have highlighted **1-octen-3-ol** as a likely candidate [1, 2, 3]
- Once its concentration at the spore falls below a certain threshold, the conidium breaks dormancy and enters a swelling phase.
  - It has been observed that in a **externally non-inhibited** spore swelling begins around **4 hours** from inoculation



INTRODUCTION

Hypothesis

- An increased spore density reduces the average probability of germination.
  - Densities above 10^5 spores/mL exhibit germination inhibition[3, 4]
- This could be caused by a reduction of the concentration gradient between the spore and the medium, which causes more inhibitor to stay in the spore.

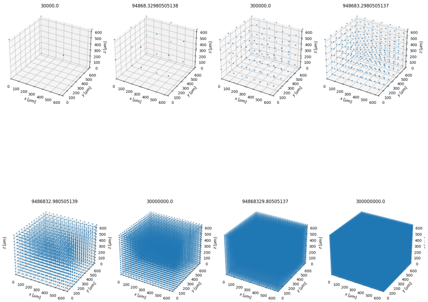


OUTLINE

SPORE DENSITY VS. CONCENTRATION AT SPORE

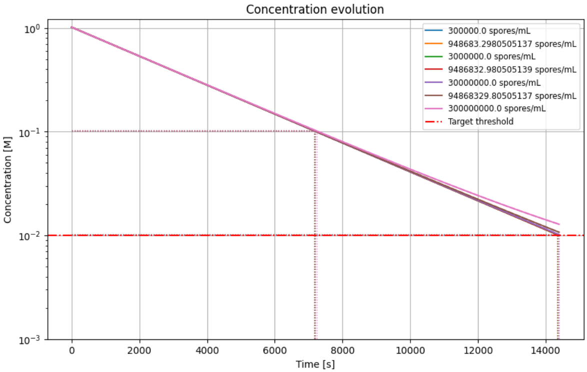
Experiment setup

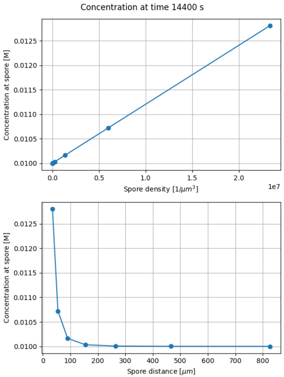
- Using a regular 3D grid of spores, a range of spore densities from 3×10^4 spores/mL to 3×10^8 spores/mL is simulated. The highest density corresponds to a spore spacing of about $15\ \mu$m, i.e. 3 spore diameters.
- The resulting concentrations at the spore locations are recorded for $t = 4$ h together with the corresponding spore densities and spore spacings.



SPORE DENSITY VS. CONCENTRATION AT SPORE

Functional relationship - plots





SPORE DENSITY VS. CONCENTRATION AT SPORE

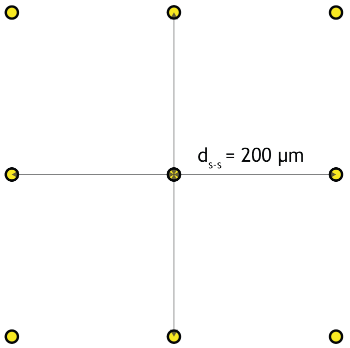
Functional relationship - observations

- The increase of residual inhibitor concentration c_s at 4 h evidently scales **linearly** with the spore density ρ_s.
- The linear fit is of the form

$$c_s(t = 4\,\mathrm{h}) = a\rho_s + b, \tag{1}$$

where $a \approx 1.2 \times 10^{-10}$ and $b \approx 0.01$.

- In relation to spore-to-spore distance, a significant saturation is observed for distances below 200 μm.

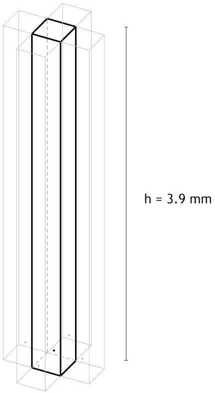


OUTLINE

LATTICE BOTTOM SPORE ARRANGEMENT

Experiment setup

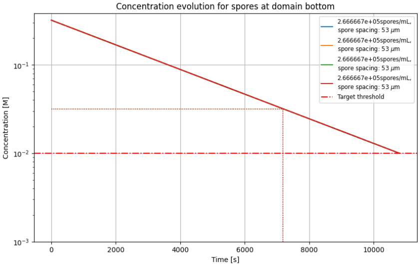
- Spores sink to the bottom of the medium due to gravity.
- Typically[4] it takes 1 h for spores to sink to the bottom of a well (150μL medium $\rightarrow h = 3.9$ mm of medium).
- It is assumed that while spores settle the inhibitor diffuses homogeneously like in the 3D grid scenario, so the simulations of the 2D lattice bottom array start with a concentration $c_0 = c(t = 3600\text{s})$.
- The lattice is periodic along the x and the y dimensions but has a Neumann boundary condition at $z = 0$ and $z = h$, (zero derivative of $c(x, y, z)$ normal to the boundary).
- Spore densities from the first multi-spore experiment (5000, $10\,000$, $20\,000$, and $40\,000$ spores per 150μL)



LATTICE BOTTOM SPORE ARRANGEMENT

Experiment results

- No significant difference in final concentrations, just like in the homogeneous 3D grid counterpart experiment.
- Local density at lattice bottom is compensated by fast diffusion in the large overhead space.



OUTLINE

NEXT STEPS

- Do not terminate simulations at $t_T = 4$ h but continue them until the threshold of 10 mM is reached $\rightarrow$ find effective threshold times t'_T.
- Find the functional relationship between the spore density ρ_s and t'_T.
- Find an analytical solution for multi-spore diffusion. Current derivation leads to

$$c(x, y, z, t) = AP_s \frac{c_0^2 V_s}{(4\pi D)^{3/2}} e^{-\frac{P_s At}{V_s}} \sum_{i=0}^{M} \int_0^t \frac{1}{\tau'^{3/2}} \exp\left(-\frac{P_s A \tau'}{V_s} - \frac{r_i^2}{4D\tau}\right) d\tau', \tag{2}$$

  Verify by comparing with numerical solutions.
- Model high-resolution oval spores.
- Look into plausible spatial distributions of spores (Brownian coagulation).

BIBLIOGRAPHY I

[1] Gilma Silva Chitarra et al. “1-Octen-3-ol inhibits conidia germination of Penicillium paneum despite of mild effects on membrane permeability, respiration, intracellular pH, and changes the protein composition.”. In: *FEMS microbiology ecology* 54 1 (2005), pp. 67–75. URL: https://api.semanticscholar.org/CorpusID:24273006.

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[3] Erika Herrero-García et al. “8-Carbon oxylipins inhibit germination and growth, and stimulate aerial conidiation in Aspergillus nidulans.”. In: *Fungal biology* 115 4-5 (2011), pp. 393–400. URL: https://api.semanticscholar.org/CorpusID:33687383.

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[4] Maryam Ijadpanahsaravi et al. "The impact of inter- and intra-species spore density on germination of the food spoilage fungus Aspergillus niger.". In: *International journal of food microbiology* 410 (2023), p. 110495. URL: https://api.semanticscholar.org/CorpusID:265268197.