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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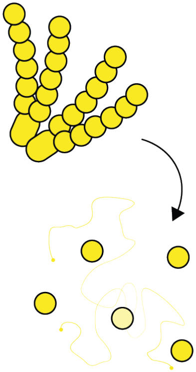
OUTLINE

INTRODUCTION

Hypothesis

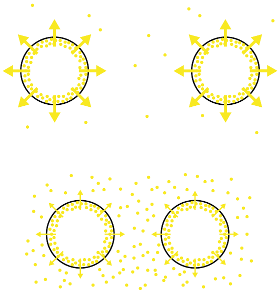
- Upon inoculation in an aqueous medium, a germination inhibitor diffuses away from the conidium.
  - Experiments have highlighted **1-octen-3-ol** as a likely candidate [1, 2, 3]
- Once its concentration at the spore falls below a certain threshold, the conidium breaks dormancy and enters a swelling 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

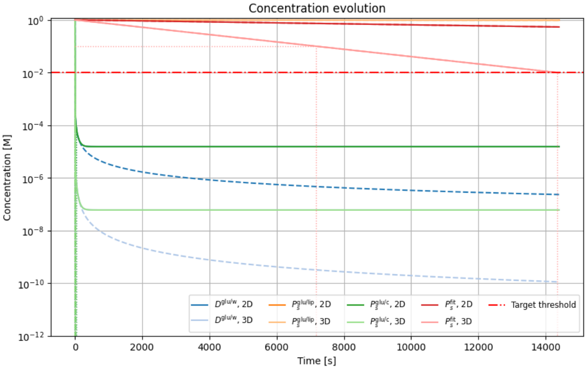
SINGLE-SPORE EXPERIMENTS

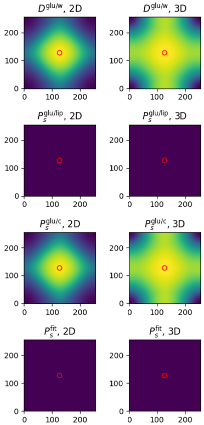
Overview

- Lattice size of $L = 256 \times 5\,\mu\text{m} = 1280\,\mu\text{m}$
- Initial concentration of $c_0 = 1.018\,\text{M}$
- $t_{\text{max}} = 4\,\text{h}$
- List of experiments
  1. Superficial release with D of glucose in water (2D)
  2. Superficial release with D of glucose in water (3D)
  3. Slow release with P_s of a lipid bilayer membrane (2D)
  4. Slow release with P_s of a lipid bilayer membrane (3D)
  5. Slow release with P_s of a CNF film (2D)
  6. Slow release with P_s of a CNF film (3D)
  7. Slow release with analytically fitted P_s (2D)
  8. Slow release with analytically fitted P_s (3D)
- Fitted permeation constant is $P_s = 2.675 \times 10^{-8}\,\text{cm/s}$

SINGLE-SPORE EXPERIMENTS

Results



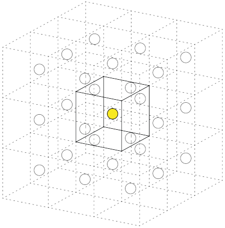


OUTLINE

MULTI-SPORE EXPERIMENTS

Assumptions

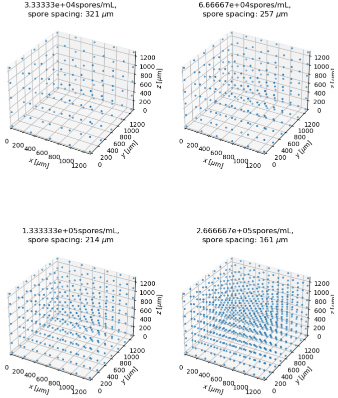
- Spores assumed to be arranged in a regular three-dimensional grid.
- Assuming a large inoculum, in which the central part exhibits characteristic germination behaviour and the boundaries are irrelevant.
- Therefore, the grid can be considered infinite.
- Since the spores **repeat periodically**, it suffices to simulate a **single spore** in a **volume of variable size** L and a triply periodic boundary.



MULTI-SPORE EXPERIMENTS

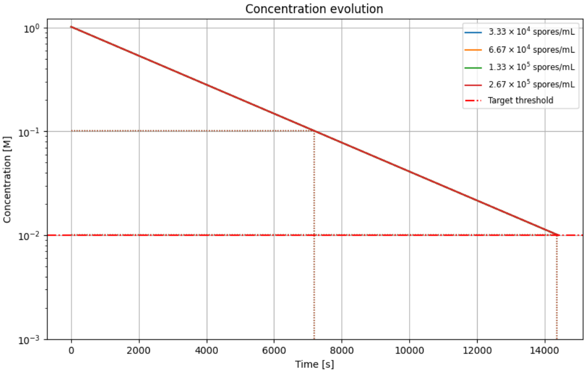
Experiment setup

- The size L of the simulation volume depends on the spore density.
- In [4] a difference in germination is observed between 5000 spores and 40000 spores in a $150\ \mu$L medium.
- 4 densities are chosen for the experiment:
  - 5000 spores$/150\ \mu$L $\approx 0.33 \times 10^4$ spores$/$mL
  - $10\,000$ spores$/150\ \mu$L $\approx 0.67 \times 10^4$ spores$/$mL
  - $20\,000$ spores$/150\ \mu$L $\approx 1.33 \times 10^5$ spores$/$mL
  - $40\,000$ spores$/150\ \mu$L $\approx 2.67 \times 10^5$ spores$/$mL
- Spore spacings of 315, 250, 200 and $160\ \mu$m respectively.
- The simulations are run for $t_{\max} = 4$ h.



MULTI-SPORE EXPERIMENTS

Results



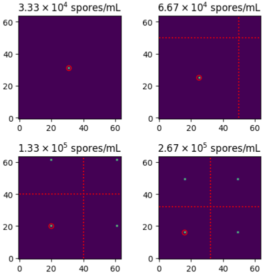
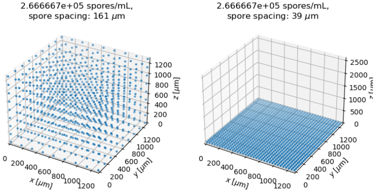


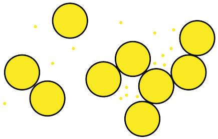
Figure: Concentrations at $t = 4$ h. The boundaries are aligned with the largest lattice for comparison, i.e. smaller lattices are repeated.

MULTI-SPORE EXPERIMENTS

Discussion

- No observable saturation effects at $t = 4$ h for any of the given spore densities $\rightarrow$ the space around each spore is too large to become saturated.
- To observe saturation, higher local densities are necessary. These are present when:
  - the spores densify at the bottom of the medium due to gravity;
  - isolated pockets form between spores due to their irregular distribution / aggregation.
- Next experiments:
  - Rectangular grids of spores at the bottom of a 3D volume;
  - Irregular distributions / aggregation studies with spherical spores.





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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.