MSc Computational Science
joint programme UvA/VU

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

INTERMEDIATE PRESENTATION DECEMBER

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December 20, 2024

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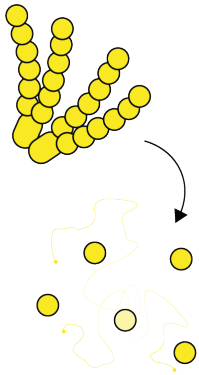
OUTLINE


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
- An increased density of spores drives the local inhibitor concentration high, reducing overall germination.
  - Densities above 10^5 sporesl/mL exhibit germination inhibition[3, 4]



OUTLINE

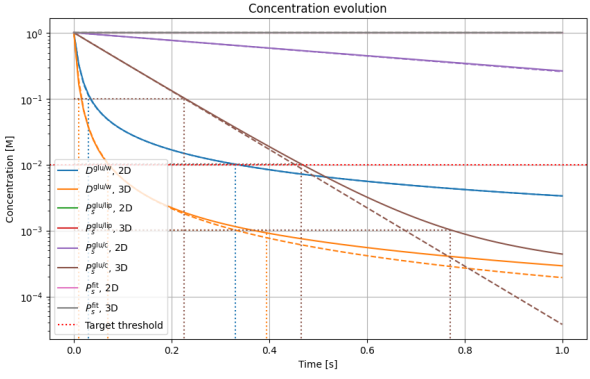

EXPERIMENT COMPILATION

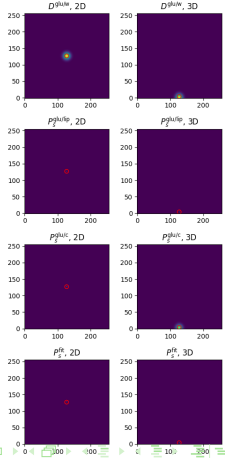
Overview

- Lattice size of $L = 256 \times 5\,\mu\text{m} = 1280\,\mu\text{m}$
- Initial concentration of $c_0 = 1.018\,\text{M}$
- $t_{\max} = 4\,\text{h}$
- 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 $P_s = 1.17 \times 10^{-7}\,\text{cm/s}$

EXPERIMENT COMPILATION

Results





OUTLINE


MULTI-SPORE EXPERIMENTS

Assumptions

- Volume of medium used in experiments [4]: $150\ \mu$L
- 96-well suspension culture plate used in experiments has well diameters of ≈ 7 mm, area of $\approx 38.48\ \text{mm}^2$
- The height of the medium is therefore $h \approx 3.9$ mm

MULTI-SPORE EXPERIMENTS

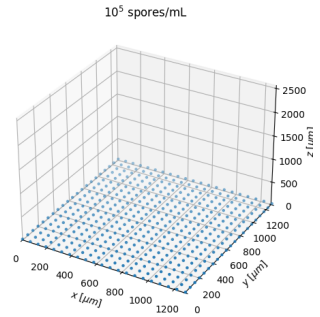
Setup

- For an optimal algorithm parallelisation, powers-of-2 grid sizes are beneficial
- Therefore, as a start, a lattice of $L \times W \times H$ can be used where

$$L = W = Ndx = 256 \times 5\,\mu\text{m} = 1280\,\mu\text{m}, \quad (1)$$

$$H = 2Ndx = 512 \times 5\,\mu\text{m} = 2560\,\mu\text{m} = 2.56\,\text{mm} \quad (2)$$

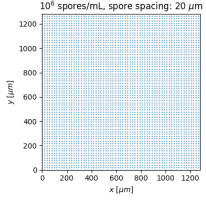
- Spores are assumed to be at the bottom of the lattice, with a slight buffer height (e.g. 20 μm) to allow a bit of diffusion underneath
- Boundary is periodic in x and y, impermeable in z (Neumann boundary condition)

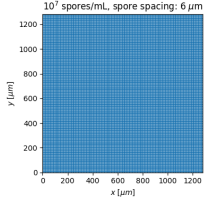


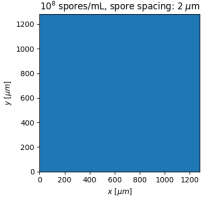
MULTI-SPORE EXPERIMENTS

Spore arrangement

- Square grid ordering
  - easy to implement
  - fits in a regular volume
  - only allows densities up to 10^7 spores/mL







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[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.

[2] Gilma Silva Chitarra et al. “Germination of Penicillium paneum Conidia Is Regulated by 1-Octen-3-ol, a Volatile Self-Inhibitor”. In: *Applied and Environmental Microbiology* 70 (2004), pp. 2823 –2829. URL: https://api.semanticscholar.org/CorpusID:19828197.

[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.