

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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Experiment results

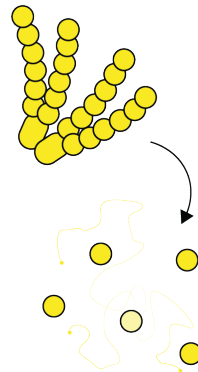
Discussion

# 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

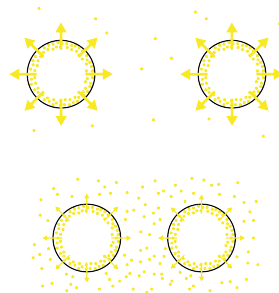


# INTRODUCTION



## 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.



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# SINGLE-SPORE EXPERIMENTS



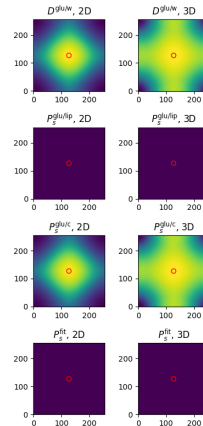
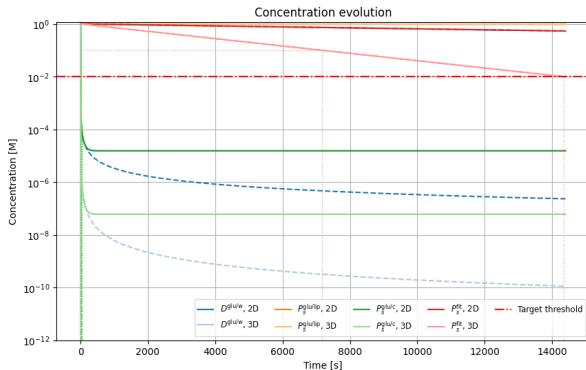
## Overview

- » 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



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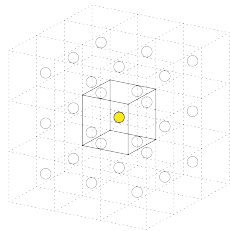


# MULTI-SPORE EXPERIMENTS



## 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.

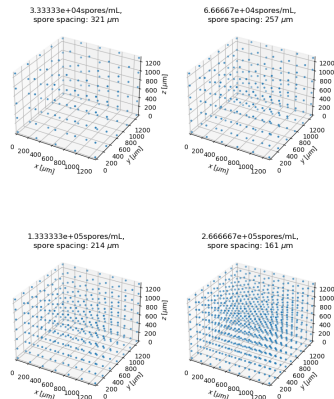


# MULTI-SPORE EXPERIMENTS



## 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  $\mu\text{L}$  medium.
- » 4 densities are chosen for the experiment:
  - 5000 spores/150  $\mu\text{L} \approx 0.33 \times 10^4$  spores/mL
  - 10 000 spores/150  $\mu\text{L} \approx 0.67 \times 10^4$  spores/mL
  - 20 000 spores/150  $\mu\text{L} \approx 1.33 \times 10^5$  spores/mL
  - 40 000 spores/150  $\mu\text{L} \approx 1.33 \times 10^5$  spores/mL
- » Spore spacings of 315, 250, 200 and 160  $\mu\text{m}$  respectively.
- » The simulations are run for  $t_{\text{max}} = 4$  h.



# MULTI-SPORE EXPERIMENTS



## Results

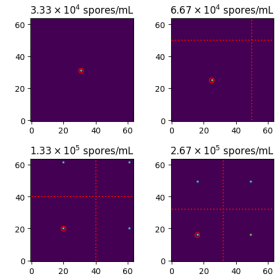
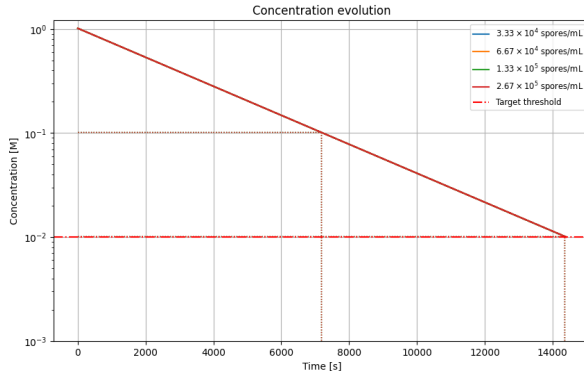


Figure: Concentrations at  $t = 4$  h.  
The boundaries are aligned with the largest lattice for comparison, i.e. smaller lattices are repeated.

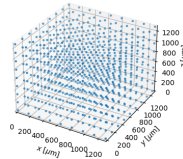
# MULTI-SPORE EXPERIMENTS



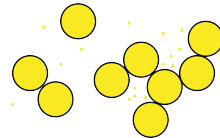
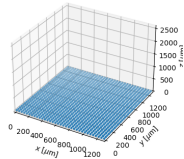
## Discussion

- » 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.

2.666667e+05 spores/mL,  
spore spacing: 161  $\mu\text{m}$



2.666667e+05 spores/mL,  
spore spacing: 39  $\mu\text{m}$





- [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>.