MSc Computational Science
joint programme UvA/VU

MODELLING DIFFUSIVE SIGNALLING IN *ASPERGILLUS* SPP. GERMINATION INHIBITION

INTERMEDIATE PRESENTATION - MARCH

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OUTLINE

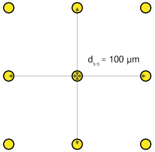
INTRODUCTION

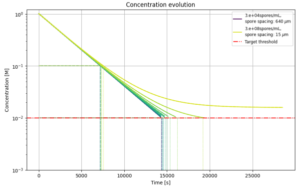
Sanity checks

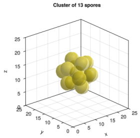
» The goal of the current experiments is to verify if

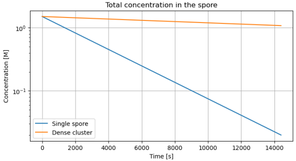
- the density-induced inhibitor saturation and
- the coverage-induced inhibitor decay deceleration

can be reproduced using **different model scales.**







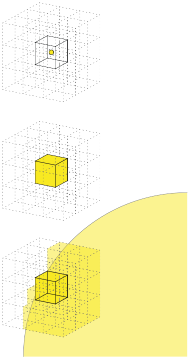


OUTLINE

OVERVIEW OF MODELS

Numerical models

- The diffusion process is simulated with the following discretisation scales:
  - **Macro-scale** (low resolution): a spore is infinitesimally small compared to the measured volumes with concentration.
  - **Spore-scale** (medium resolution): a spore is a inhibitor-releasing node on a lattice.
  - **Cell-wall scale** (high resolution): the spore is approximated by cubic volumes half the size of the cell wall.

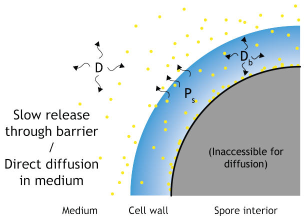


OVERVIEW OF MODELS

Analytical models

$$c(\vec{r}, t) = \frac{c_0 V}{(4\pi D t)^{3/2}} e^{-\frac{|\vec{r}|^2}{4Dt}} \quad (1)$$

- A drop of inhibitor in water diffuses **fast** (Equation 1).
- If the inhibitor permeates through the spore surface **much slower** than its diffusion in water, the **outside concentration is negligible** (Equation 2).
- However, if **densely-packed spores** release inhibitor, the **outside concentration is not negligible**.



$$c(\vec{r}, t) = c_0 e^{-\frac{t}{\tau}} \quad (2)$$

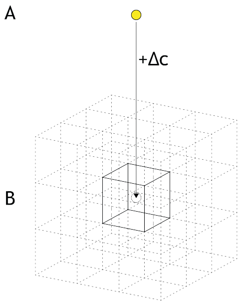
OVERVIEW OF MODELS

Analytical models

- Under the assumption that the sources have a **negligibly small volume** compared to the intermediate space,
- so they **do not obstruct** diffusion through the medium, but **only release** new concentration,
- the analytical solution is

$$c_{\mathrm{in}}(0,t) = (c_0 + c_{\mathrm{out}})\, e^{-\frac{t}{\tau}}, \tag{3}$$

where c_{out} is the cumulative contribution of all other spores to the concentration "just outside" the measured spore.



OVERVIEW OF MODELS

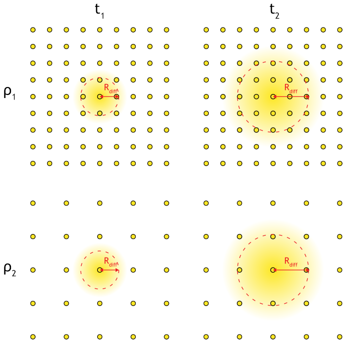
Analytical models

» The outside concentration can be computed from the spatial and temporal aggregation of concentrations from **discrete** sources within the diffusion radius $R_{\text{diff}} = \sqrt{4Dt}$:

$$c_{\text{out}} = \frac{AP_s c_0}{4\pi D^{3/2}} \sum_{|\vec{r}|^2 < R_{\text{diff}}} \int_0^t \tau'^{-3/2} e^{\left(\frac{P_s A \tau'}{V} - \frac{|\vec{r}|^2}{4D\tau'}\right)} d\tau', \quad (4)$$

or, in the **continuous** limit, as an integral multiplied by the spore density ρ_s:

$$c_{\text{out}} = \rho_s \frac{AP_s c_0}{4\pi D^{3/2}} \int_0^{R_{\text{diff}}} dr\, r^2 \int_0^t \tau'^{-3/2} e^{\left(\frac{P_s A \tau'}{V} - \frac{r^2}{4D\tau'}\right)} d\tau'. \quad (5)$$

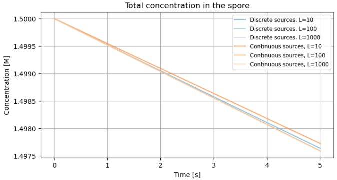


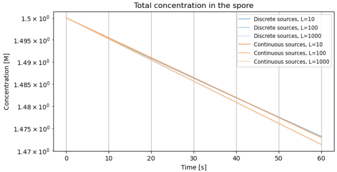
OUTLINE

SATURATION BEHAVIOUR

Discrete vs. continuous limit of spore grid

- At early times, the inhibitor released by neighbours has not reached too many spores.
- At late times, the inhibitor has reached so many spores that the continuous approximation becomes more accurate.
- So the continuous approximation (which can be more efficiently computed) is accurate enough for our purposes.



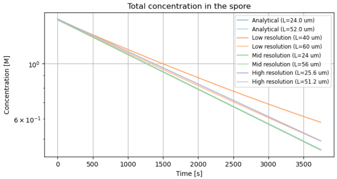


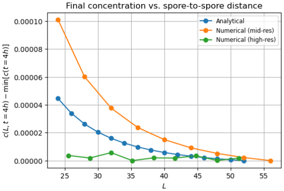
SATURATION BEHAVIOUR

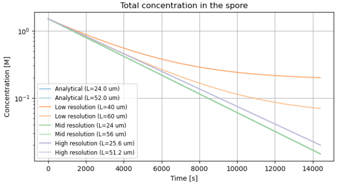
Model comparison

» The approach to saturation is different with each model:

- In the **high-resolution** scheme, the results are noisy, no significant saturation at high spore densities.
- In the **low-resolution** scheme, saturation happens quickly, likely due to the extreme coarseness of discretisation.
- In the **medium-resolution** scheme, there is saturation at high spore densities, as previous experiments showed.
- In the **analytical scheme**, the results are somewhat similar to the latter.



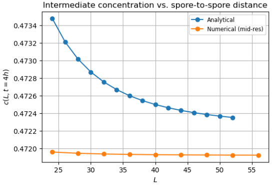


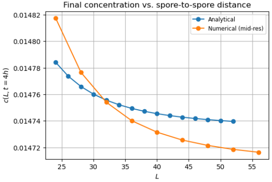


SATURATION BEHAVIOUR

Result discussion

- The **medium-scale** and the **analytical** solutions produce a qualitatively similar relationship between the spore-to-spore distance L and the concentration $c(L, t)$.
- However, their **approach to saturation** is different.
- The numerical scheme could be biased by a discretisation error — concentrations do not flow smoothly across the lattice.
- The analytical scheme could be biased by the assumption of a spatially non-interacting spore volume — which is inaccurate when spores are densely packed.
- But this narrows down the search for a clear formula.





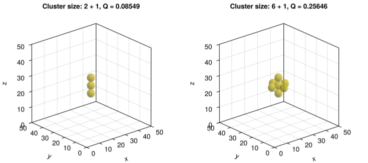
OUTLINE

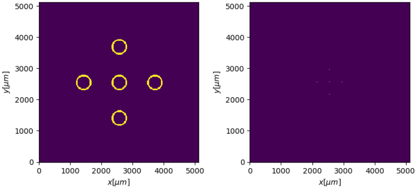
SPORE CLUSTER COVERAGE

Experiment setup

- Previously it was shown that the number of neighbours influences the inhibitor decay from the spore wall.
- However, **pulling the neighbours further away** did not influence diffusion significantly.
- It has been noted that the high-resolution model exhibits **numerical stability and accuracy issues**.
- Ongoing experiment: reproduce loose clusters (centre-to-centre distance increasing from $d = 2R$ to $d = 40R$) on
  - a medium-resolution lattice;
  - a low-resolution lattice

  and observe how the concentration decays.





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