Control of encounter frequency on microbial dynamics and pesticide degradation from μm to cm scales

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I. Abstract

For µ-pollutants that are mainly degraded within cells, like 2,4-D, **contact** between microbes and pollutant is necessary for their degradation. In this case, the **distributions** of microbes and pollutants, as well as the **transport processes** affecting them, may be major controls of degradation.

Previous experiments have shown that water input leads to i) a strong increase in biodegradation of the herbicide 2,4-D, and at the same time ii) a dispersion, especially of bacteria, suggesting that **degradation increase could be caused by the dispersion of bacteria**.

To determine if the role of water inputs is rather **spatial** as suspected, or **physiological**, or both, we tested whether water-caused dispersion has the **theoretical capacity** to explain experimental results.

With a biological model calibrated on experiments without water input, we see that water-caused dispersion **can not explain** the increase of degradation. When modifying the biological model, we show that the model sensibility to its parameters **highly depends on the dispersion of bacteria**.

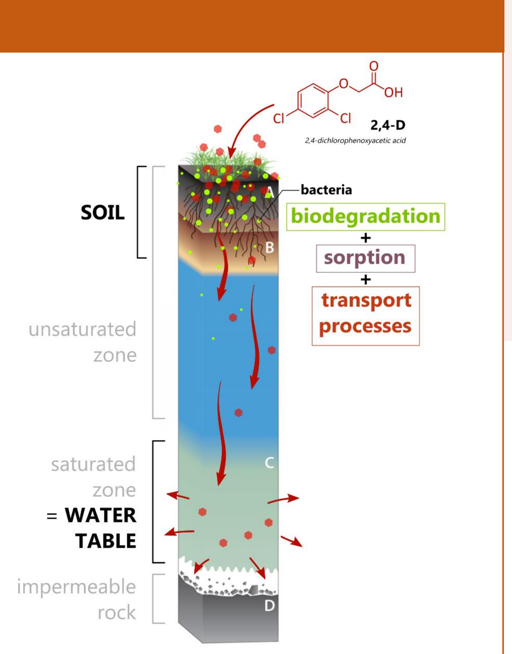
Moreover, bacterial dispersion has an **optimum**, which results from a **balance** between the depletion of substrate by biotic processes (biodegradation) and the depletion of substrate by abiotic processes (diffusion/dilution, adsorption…). This optimum strongly depends on some biological parameters such as degradation rate at low substrate concentrations, lag phase, or initial number of bacteria.

For achieving fitting the experimental data, these results point out that i) either the **dynamics** of dispersion are critical, or ii) a **physiological process** is missing in our model.

II. Context

Soil microorganisms perform several major desirable and undesirable ecosystem functions by degrading soil organic carbon. Yet, this microbial degradation is not fully understand, and particularly **how the encounter between bacteria and their substrate happens**.

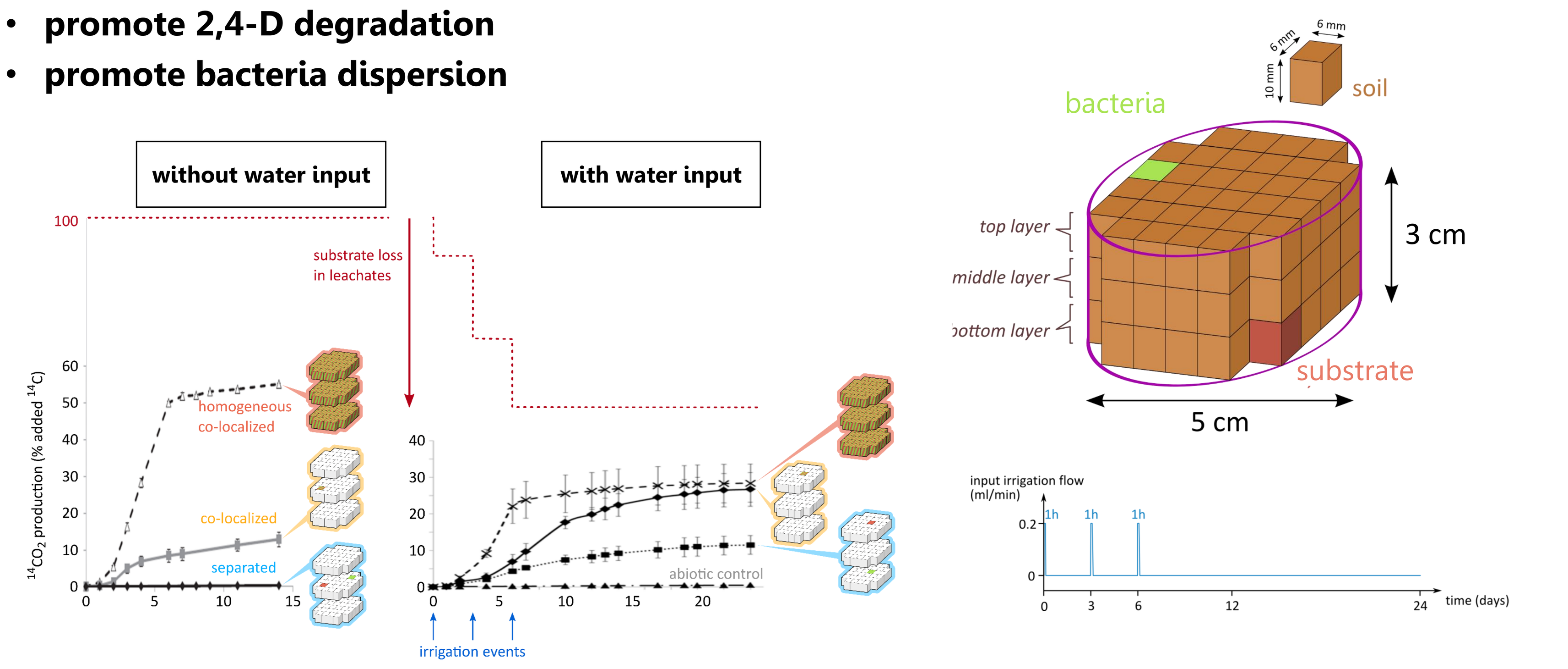
Mobile organic µ-pollutants such as 2,4-D pesticide are mainly prevented from reaching the water table through **adsorption on soil particles** or **microbial degradation**. This last process requires contact between degraders (as bacteria) and 2,4-D. This **spatiotemporal access** is achieved through transport mechanisms such as **diffusion** and **advection** that strongly interact with biological and chemical processes by reshaping the distributions of pollutants and microbes.



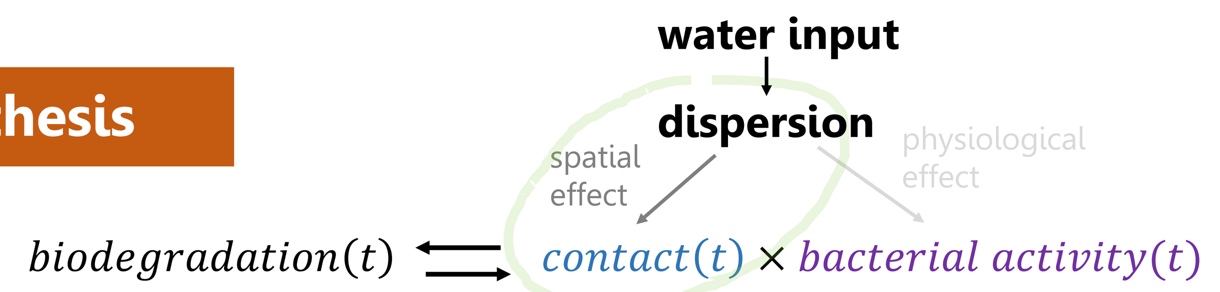
III. Starting point and aim

The importance of transport is stressed out by several observations and is significant in the following cm-scale material experiment previously performed on the degradation of 2,4-D in natural repacked soils under controlled advection and diffusion conditions (Pinheiro *et al*, 2015 ; Pinheiro *et al*, 2018).

These experiments show that short water input events
- **promote 2,4-D degradation**
- **promote bacteria dispersion**



Hypothesis



IV. Results: exploring advection (biology is set according to Babey *et al*, 2017)

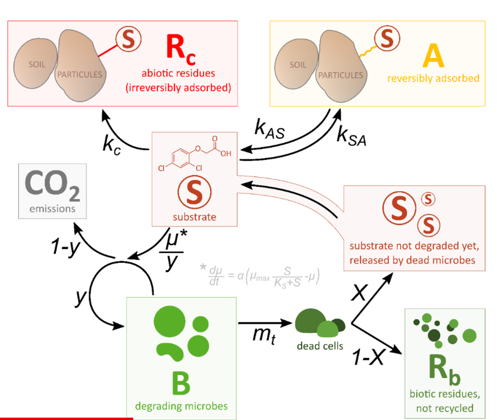
Experimental method

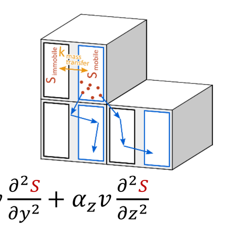
- **virtual experiment** (System of Ordinary/Partial Differential Equations)

(relations in concentration)

- $\frac{\partial S}{\partial t} = -k_{S\to A}S + k_{A\to S}A - k_c S - \frac{1}{y}\mu_{(S)}B + m_t\chi B$
- $\frac{\partial A}{\partial t} = k_{S\to A}S - k_{A\to S}A$
- $\frac{\partial R_c}{\partial t} = k_c S$
- $\frac{\partial B}{\partial t} = \mu_{(S)}B - m_t B$; $\frac{\partial \mu}{\partial t} = \propto \left(\mu_{max}\frac{S}{K_S+S} - \mu\right)$ *Monod model with delay*
- $\frac{\partial CO_2}{\partial t} = \frac{(1-y)}{y}\mu_{(S)}B$
- $\frac{\partial R_b}{\partial t} = m_t(1-\chi)B$

- $\frac{\partial S}{\partial t} = D\frac{\partial^2 S}{\partial x^2} + D\frac{\partial^2 S}{\partial y^2} + D\frac{\partial^2 S}{\partial z^2}$
- $\frac{\partial S}{\partial t} = -v\frac{\partial S}{\partial z} + \alpha_x v\frac{\partial^2 S}{\partial x^2} + \alpha_y v\frac{\partial^2 S}{\partial y^2} + \alpha_z v\frac{\partial^2 S}{\partial z^2}$



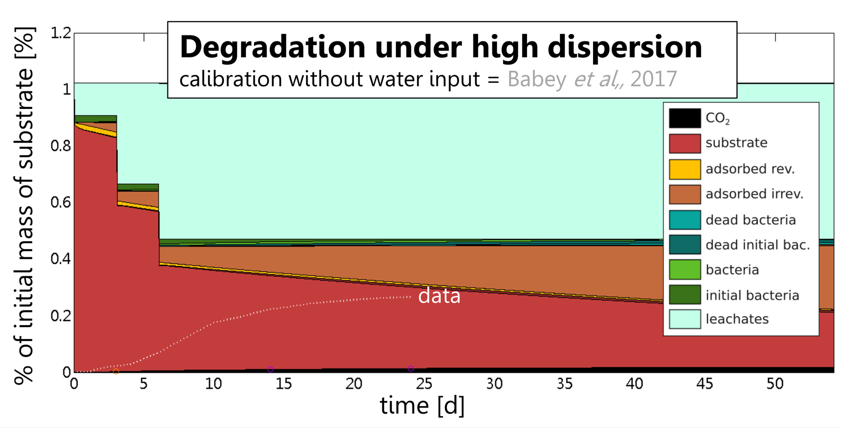


Results

- Huge **discrepancy** between model and data
- Similar results with modeling a simplified 1D-advection or a one-shot initial spreading instead..

$\frac{m_{S_{consumed}}}{m_{S_{t=0\ not-leached}}}$	~~Advection~~ ✗		**Advection** ✓	
	experiment	model	experiment	model
Colocalized	12,9 ±1,9 %	13 %	**22,3** ±8 **%** (+ 55% in leachates)	**< 8 %** (+ 55% in leachates)
Separated	0,3 ±0,1 %	0,2 %	**9,2** ±7 **%** (+ 55% in leachates)	**< 1 %** (+ 55% in leachates)

With a biological model calibrated without water input, dispersion of bacteria has a **negative effect** on degradation.

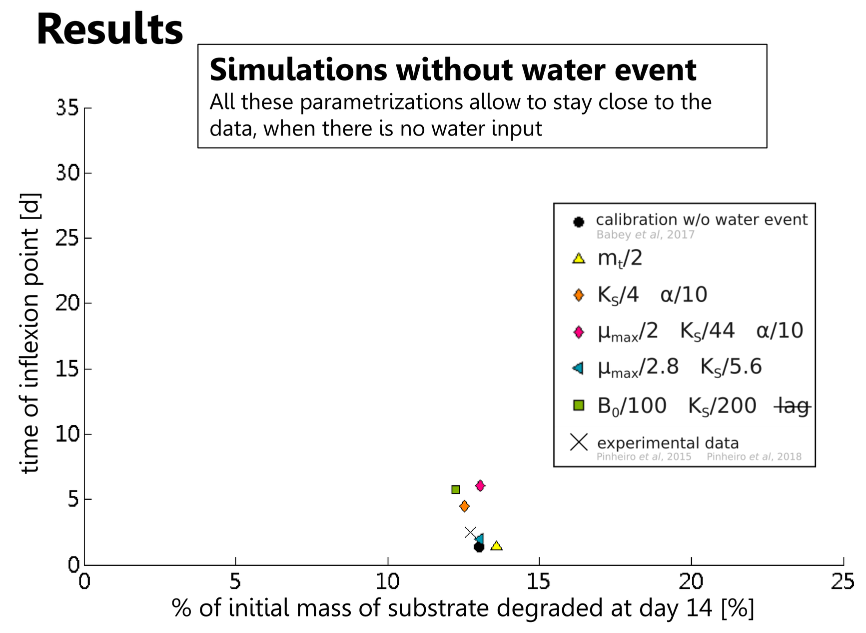


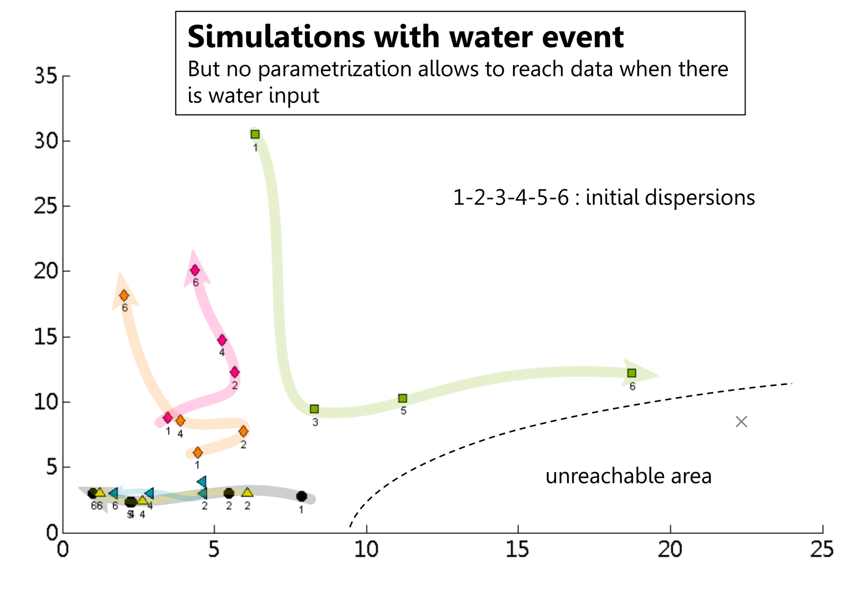
V. Results: exploring biological activity

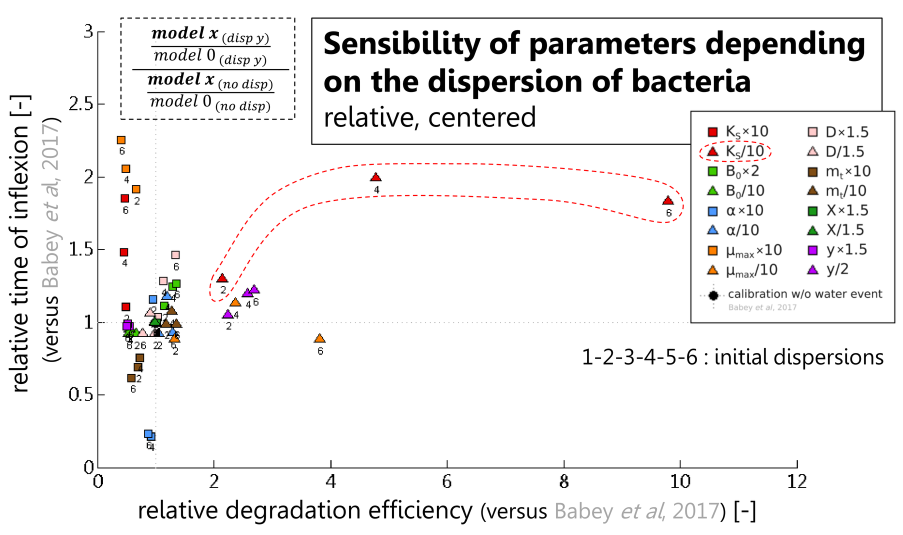
Experimental method

- Mimicking advection in a basic way (through an **initial dispersion** of bacteria and substrate and a **leaching** of substrate) and exploring various parametrizations of the biological part of the model

Results

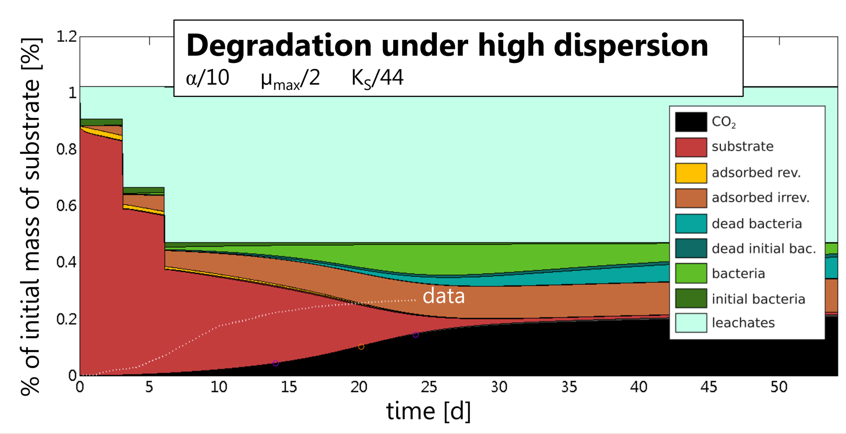


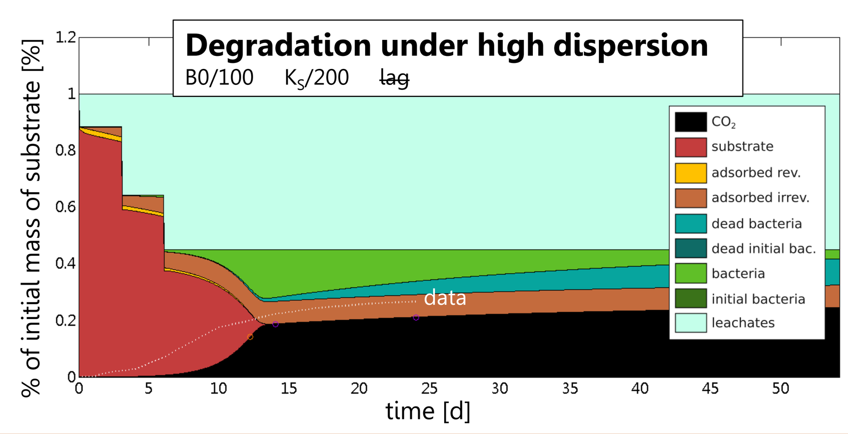




Results
- the experimental data **are not reachable** in this model
- dispersion **reveals** sensibility of parameters
- some parameters (K_S…) **strongly interact** with dispersion

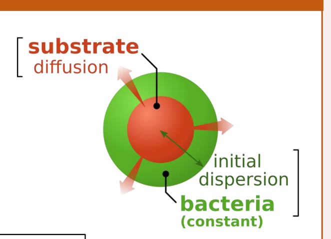
These results suggest that: i) either the initial dispersion of bacteria is a poor way to mimic advection, and so **dynamics** of dispersion are critical ; or ii) the model is **missing a process** (active density-inhibition, O_2 limitation…)

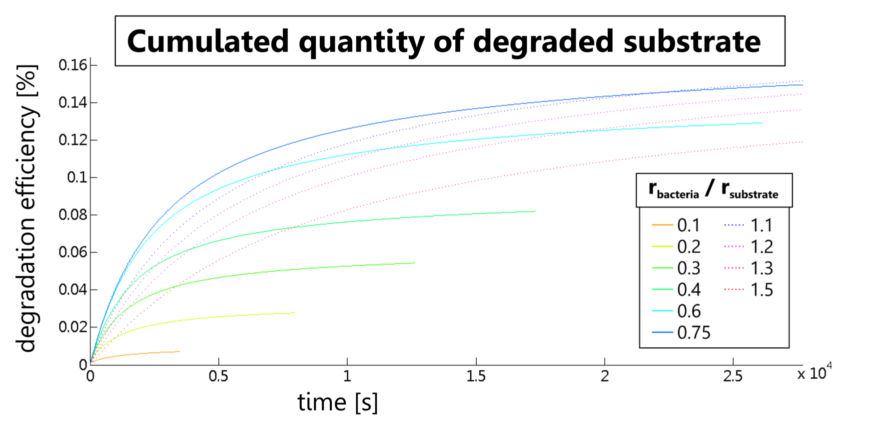


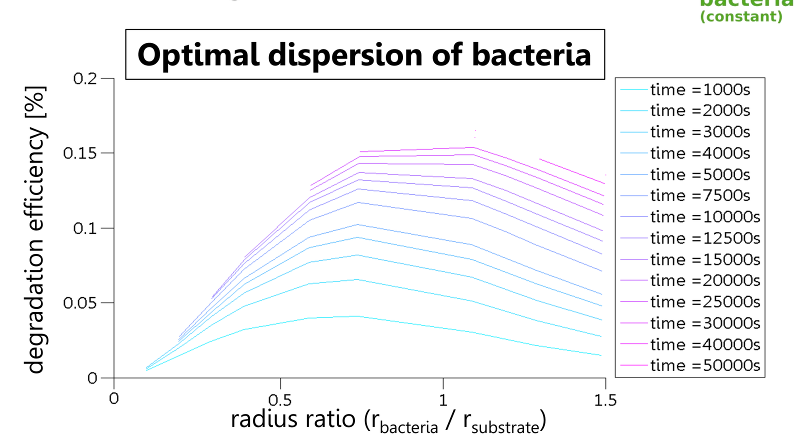


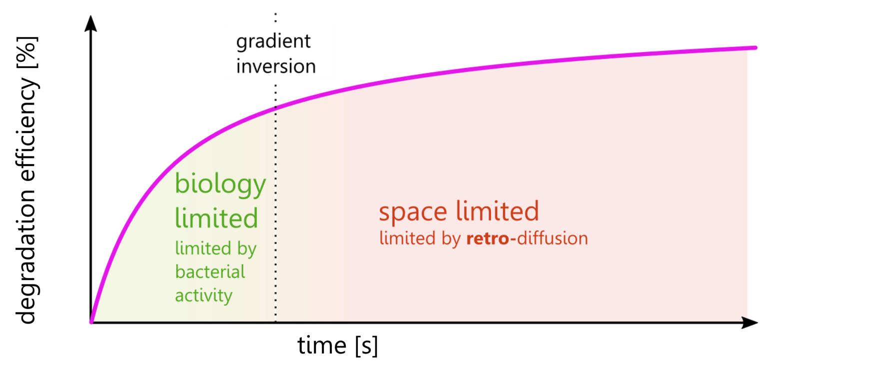
VI. Formalizing the role of bacteria dispersion

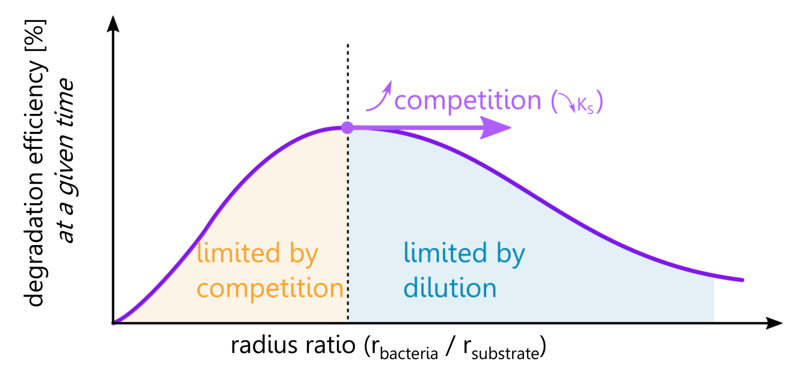
In order to interpret these results, we aim now at formalizing the impact of bacteria dispersion on the degradation. In a first case we use the following simplified model. This allowed us to postulate first tracks of interpreting the shape of the following curves. These first ideas are currently under investigation.











Contact probability between bacteria and their substrate is directly related to **substrate concentration**. There is a **balance** for bacteria between **avoiding substrate dilution** and **avoiding competition for substrate**.

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