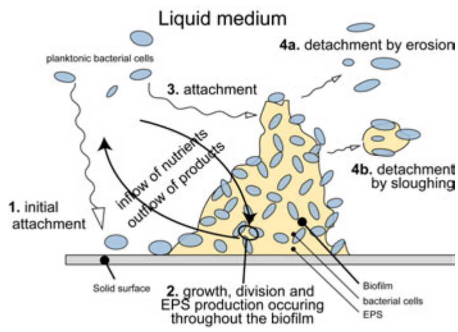
Dynamic Multidimensional Modeling of Structure and Activity in Multispecies Multisubstrate Biofilm Systems

– a Particle Based Approach –

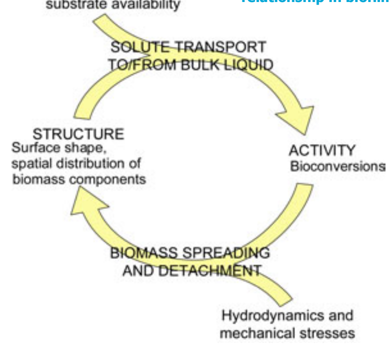


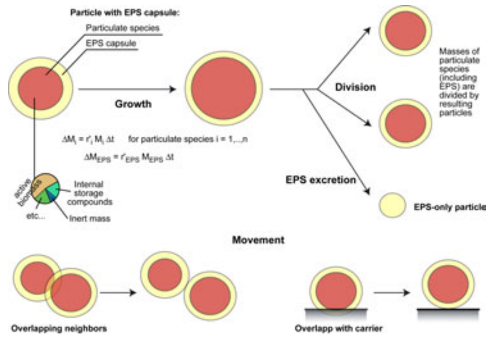
Schematic representation of processes involved in biofilm formation

The spatial heterogeneity of bacterial biofilms has an important impact in overall biofilm behavior and, consequently, in the several human activities where biofilms are involved, from biotechnology applications to health related issues. Properties such as thickness, density and surface shape of the biofilm have special relevance in the operation of biofilm reactors by affecting their performance (mass transfer and conversion). Biofilm dynamics is vital to understand biofilm processes and to enable designing biofilm systems according to the requirements of a specific application. However, biofilm dynamics can be complex to assess due to the intricate collection of processes involved.

A numerical framework for describing the dynamics of bacterial biofilms structure and composition in 2D or 3D is explained here. The model allows the description of multi-species biofilms with arbitrary solute species (e.g. carbon sources, dissolved oxygen, soluble metabolites) as well as arbitrary number of bacteria types constituted fixed species (e.g. active biomass, inert biomass, EPS). For each biofilm system to analyze, a set of mass balance equations is used to define relations between involved species. Diffusion-reaction equations are solved numerically to compute concentration fields for solute species and local conversion rates for particulate species. Spreading of the biomass is modeled using and individual-based approach in which hard spherical compartments consume nutrients, grow, divide producing new individuals of the same species, and push each other as they grow. The effect of biomass detachment on overall dynamics of the system is implemented using a moving front approach simulated by the level set method. This modeling concept constitutes a bottom-up approach were overall behavior of the community is derived from the actions and interactions occurring at the scale of the unicellular organisms that constitute it.

The structure/activity relationship in biofilms





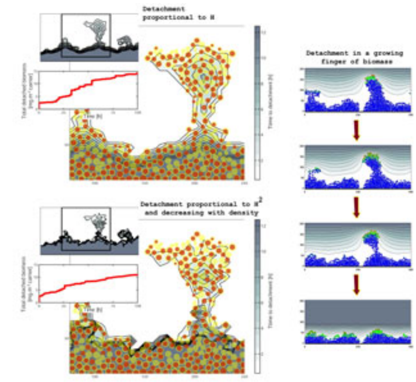
The behavior of agents used for Individual Based Modeling of biomass spreading

IbM is a bottom-up approach were large-scale dynamics is derived from the behavior of multiple agents acting independently [3]. The agents are spherical entities that react to local environmental conditions according to a simple set of rules that mimic the processes carried out by a bacterial cell: growth by intake of nutrients, production and excretion of metabolites such as **extracellular polymeric substances (EPS)** [4] and division, resulting in the creation of an offspring agent. Movement of an agent occurs if pushed by a neighboring agent or at the proximity of the solid surface.

Framework for implementation of biofilm models

A package using concepts from previous models [1-4] that provides a generalized framework for the implementation of biofilm models:

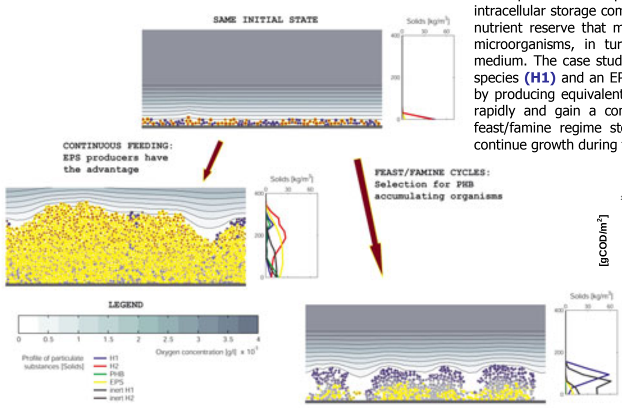
- **Multidimensional structure modeling (integrated methods for 2D/3D)**
- **Biomass spreading using Individual Based Modeling (IbM)**
- **Structured biomass allowing any number of particulate species**
- **Specific functions for modeling EPS formation**
- **Any number of solute species and reactions**
- **Detachment forces**



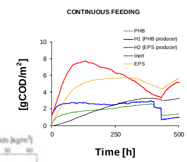
Modeling the effect of detachment forces on the structure

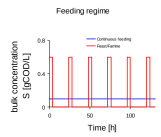
Detachment forces are modeled using a detachment speed function. The actual rate of detachment is derived from applying the detachment speed to the biofilm structure. By removing the biomass not connected to the carrier (floating biomass) at any given iteration also sloughing is included: A large cluster of biomass may detach when its attachment base is eroded. Shrinking of the biofilm (reduction of volume) as a consequence of biomass losses via specific model mechanisms such as cell lysis or EPS decay is also implemented.

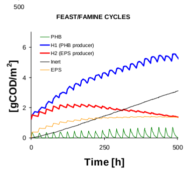
Case study selection for PHB accumulating organisms using feast/famine cycles



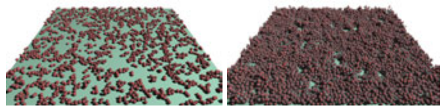
In the presence of surplus source of carbon and energy microorganisms may produce intracellular storage compounds such as polyhydroxybutyrate (PHB). PHB constitutes a nutrient reserve that may be used when external substrate becomes limited. Some microorganisms, in turn, excrete large amounts of polysaccharides (EPS) to the medium. The case study demonstrates the competition between a PHB accumulating species **(H1)** and an EPS producer **(H2)**. With constant feeding, H1 and H2 start out by producing equivalent quantities of polymers. However EPS-producers spread more rapidly and gain a competitive edge due to the oxygen gradient present. In the feast/famine regime storage of PHB during feast periods allows H1 organisms to continue growth during the famine period.



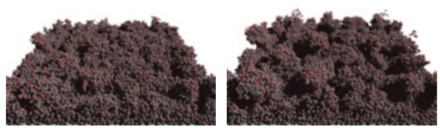




Integrated 2D/3D methods using the same code



Simulations may be performed in both 2D and 3D using the same framework. Example simulation: Rough biofilm obtained for a biofilm of single species EPS producers with growth limited by oxygen. Detachment forces also present.



References

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