Summer School 2012

Tecnologie sostenibili per la tutela dell'ambiente

Politecnico di Milano
25 Giugno 2012

MATHEMATICAL MODELLING OF MULTISPECIES BIOFILM FOR WASTEWATER TREATMENT

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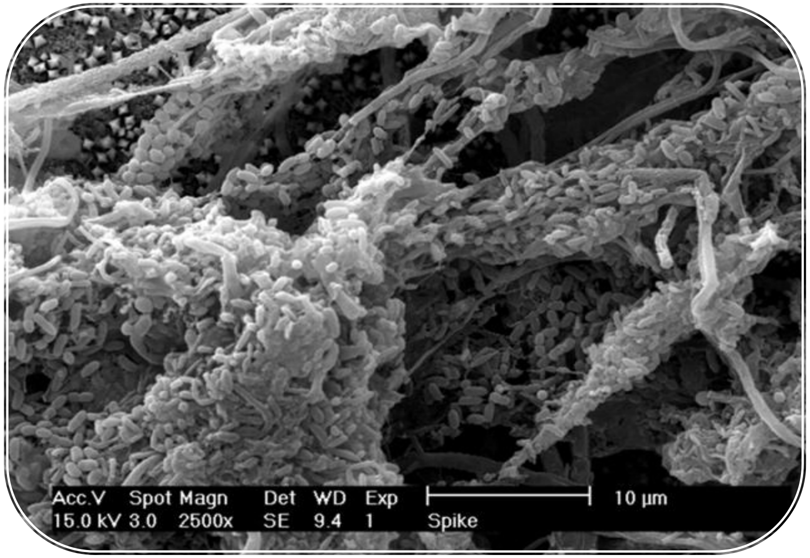
Biofilm definition



A biofilm is "a layer of prokaryotic and eukaryotic cells anchored to a substratum surface and embedded in an organic matrix of biological origin"

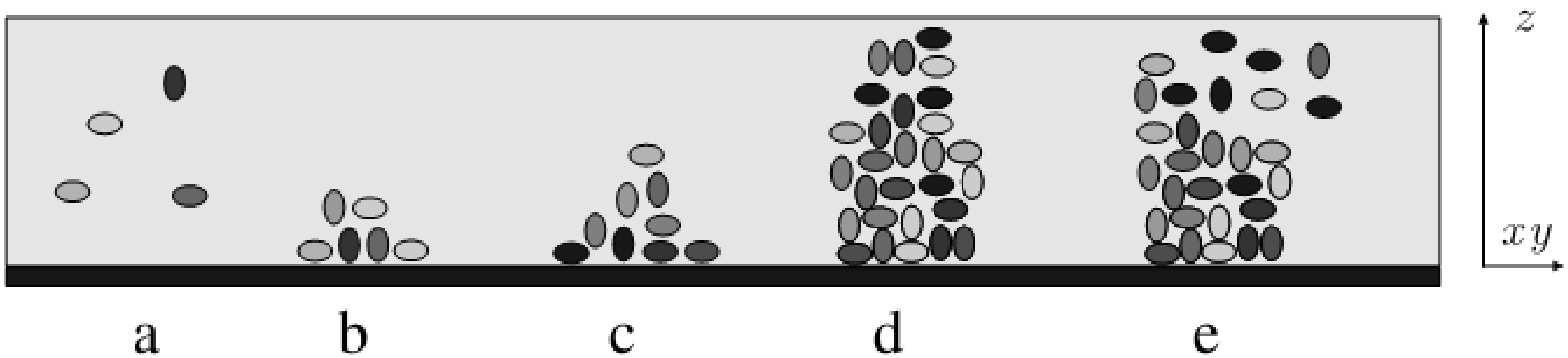
Cells → EPS → Surface

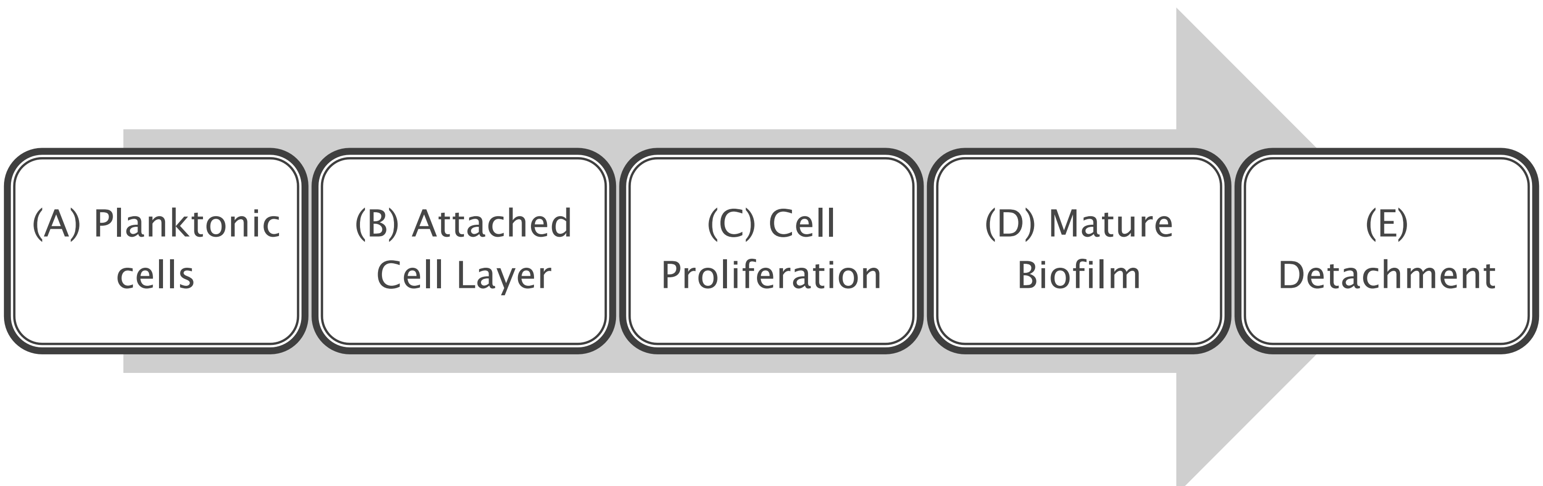
- Bacteria in biofilms are protected from washout
- Physical structure allowing for distinct biological niches
- Microbial activity can modify the internal environment
- Variety of microbial groups contributing to the conversion of different organic and inorganic substrates
- Resistance to antimicrobial agents

APPLICATIONS

- Removing contaminants from soil or ground water
- Crucial for cycling nutrients in the Earth's biosphere
- Wastewater treatment (since 19^{th})

Biofilm definition



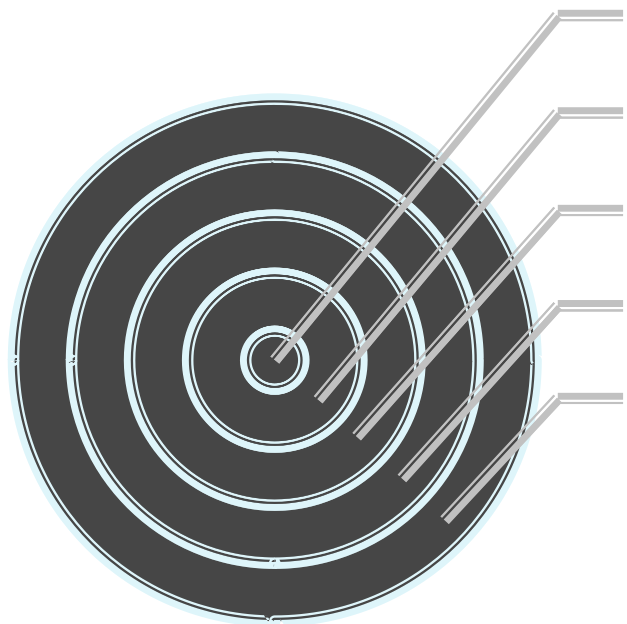


WHY MODELLING?

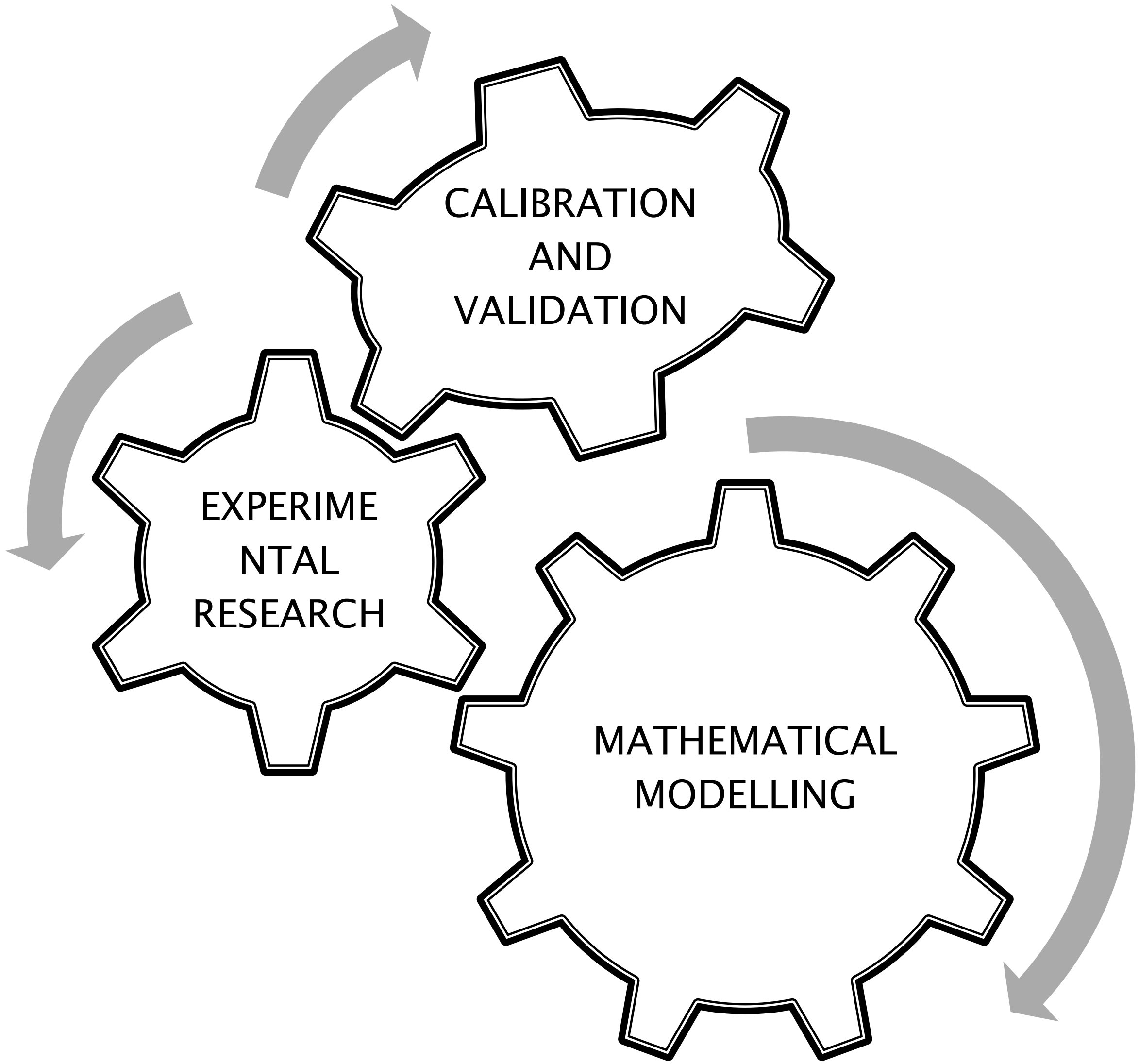
(1) MODELS ARE THE BASIC TOOLS FOR ENGINEERING

(2) MODELS HELPS US ACHIEVE A BETTER UNDERSTANDING OF THE PROCESS

GOALS FOR BIOFILM MODELLING



- UNDERSTAND FUNDAMENTAL MECHANISMS
- LINK DIFFERENT TYPES OF MECHANISMS
- PRE-MODEL EXPERIMENTAL DESIGN
- CREATE NOVEL PROCESS DESIGNS
- IMPROVE THE PERFORMANCE OF A PROCESS



Objectives research plan

Literature Review

FIRST GENERATION MODELS (1970s)

- Harris and Hansford 1976
- Harremoes 1976
- LaMotta 1976
- Williamson and McCarty 1976
- Rittmann and McCarty

SECOND GENERATION MODELS (1980s)

- Kissel et al. 1984
- Wanner and Gujer 1984,1986
- Rittmann and Manem 1992

THIRD GENERATION MODELS (since 1990s)

- Picioreanu et al. 1998,2001,2004
- Noguera et al. 1999
- Kreft et al. 1998,2001
- Eberl et al. 2001
- Pizarro et al. 2001
- Xavier et al. 2005

TIME →

CONTINUUM MODELS

- do not take directly into account small-scale details of an individual microrganism;
- generate deterministic solutions ;
- biofilm density, porosity and surface shape are to be specified as model input;
- difficult to derive and handle numerically

DISCRETE–DIFFERENTIAL MODELS

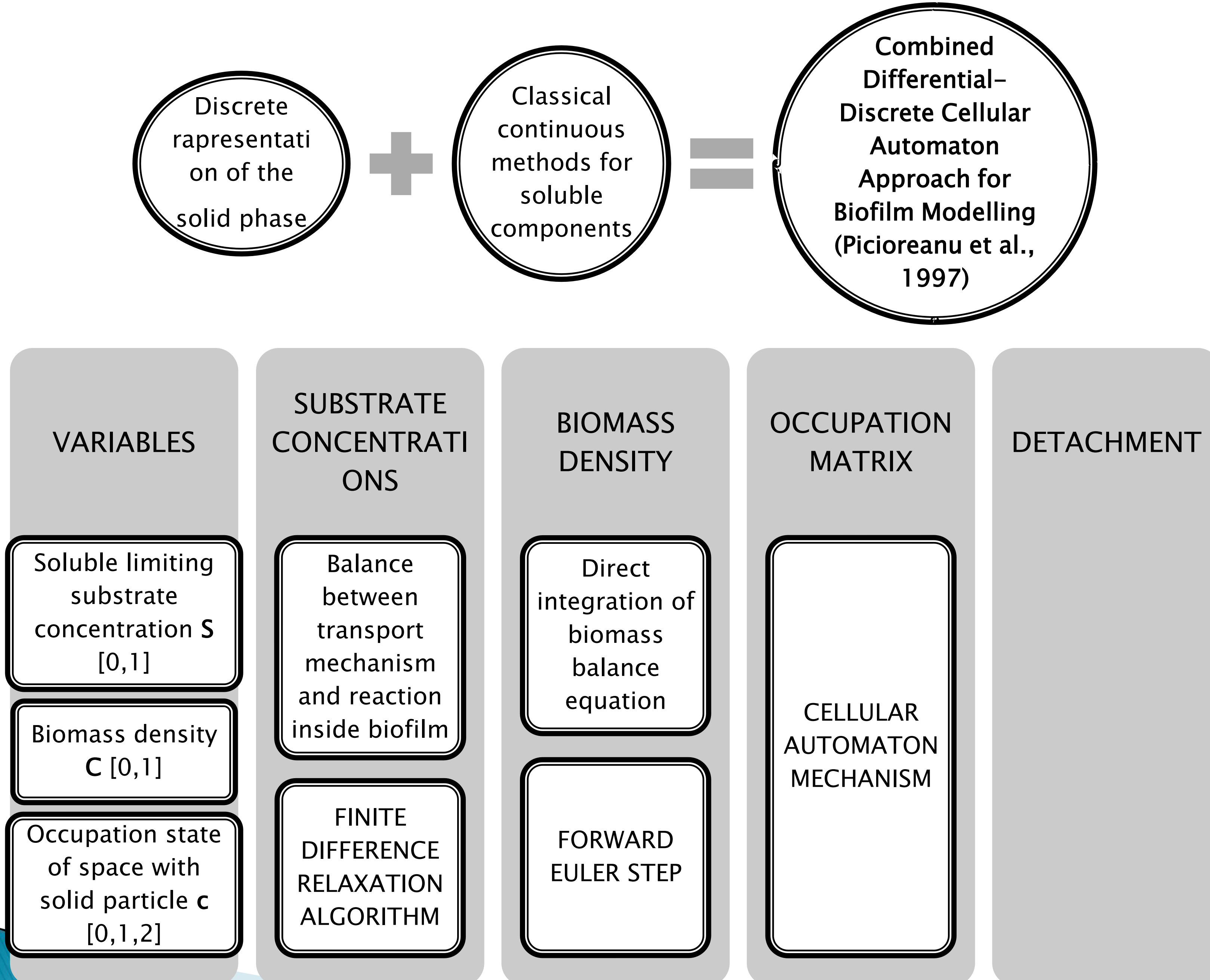
- represent typical structural heterogeneity of biofilm;
- elements of randomness;
- use of abstract mathematical parameters

MASS TRANSPORT FROM THE BULK LIQUID (DIFFUSION) → BIODEGRADATION WITHIN THE BIOFILM → BIOFILM GROWTH AND DECAY → ATTACHMENT AND DETACHMENT

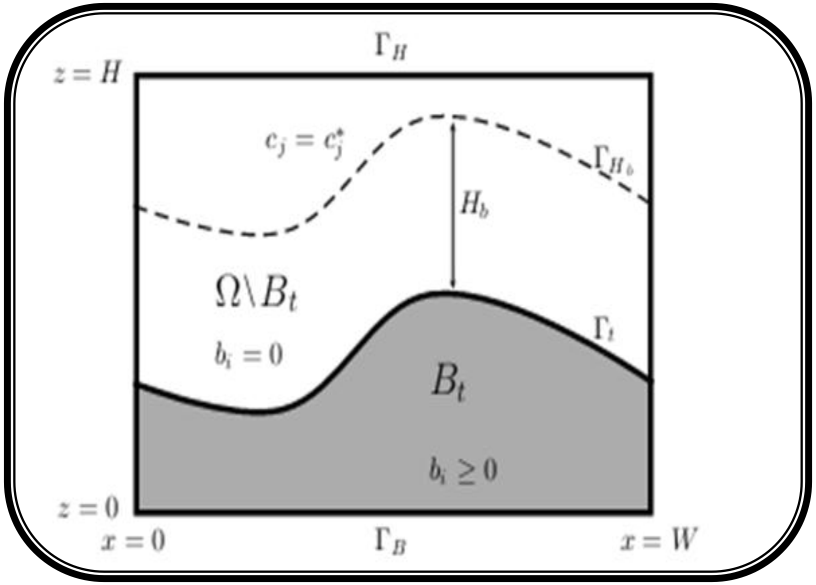
INVESTIGATOR

Wanner and Gujer 1986

# OF SUBSTRATES	REACTOR MODEL	EXTERNAL MASS TRANSFER	KINETIC EXPRESSION	BIOFILM GROWTH AND LOSS	BIOFILM THICKNESS	GEOMETRY OF MODEL EQ.	SOLUTION OF MODEL EQUATIONS
Multiple	*Not Considered*	*Not Considered*	*Double Monod*	*Considered*	*Variable with time*	*Planer*	*Numerical*



Literature Review



A Multidimensional Multispecies Continuum Model for Heterogeneous Biofilm Development (Klapper et al., 2007)

EQUATIONS:
CONSERVATION OF MASS

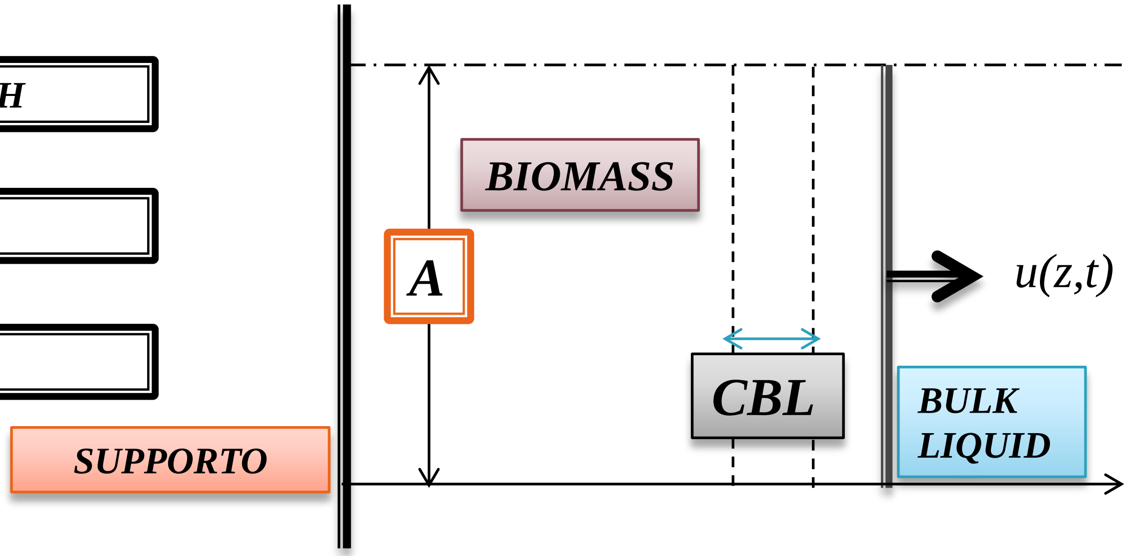
Transport by diffusion is several orders of magnitude faster than changes due to growth and advection . So it will be considered quasi steady state for substrate balance.

Transport of biomass is governed by an advective process

1) Continuum models' simulations are based upon accepted numerical methods with an existing error analysis
2) Concentrations of biomass may be described by one or more density fields, that obey to some sort of conservation law (mass or momentum)
3) Generation of determinsitic solutions…possibility of analytical study
4) Applied to a planar biofilm system, the model reduces to a one-dimensional model equivalent to W.-G.

Developed Mathematical Model

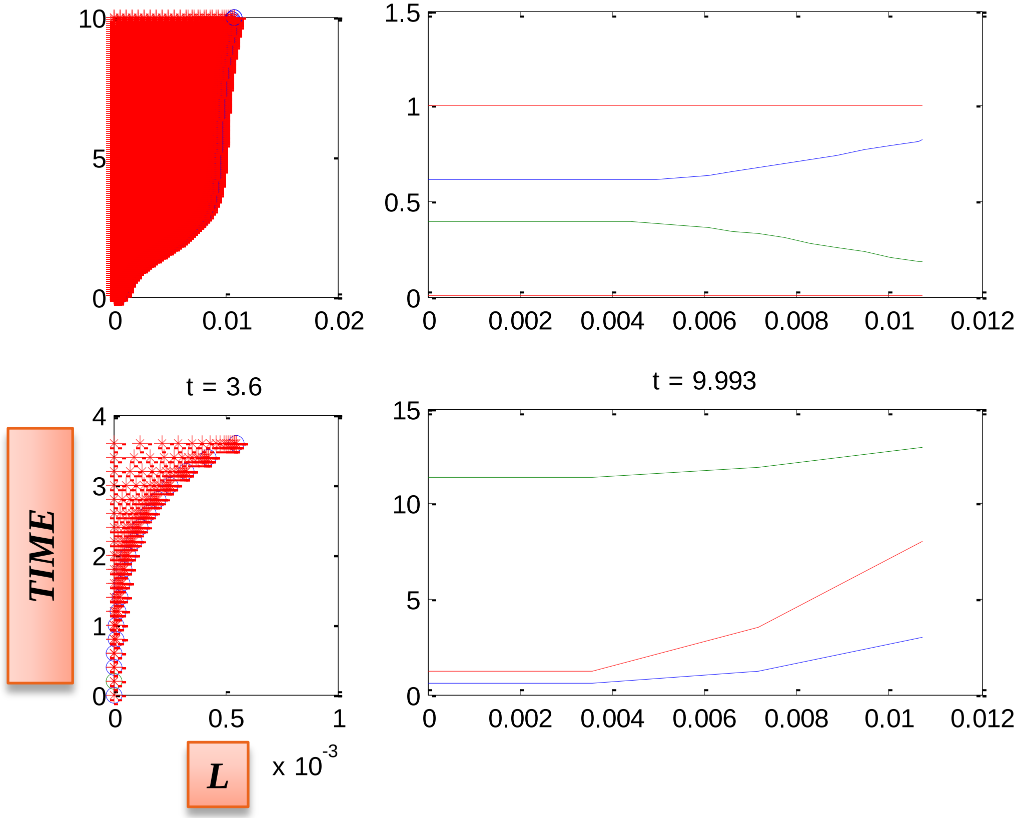
- *CONTINUUM APPROACH*
- *ONE-DIMENSION (1D)*
- *L(0)=0*



1 **GROWTH OF BIOMASS** ⟺ 2 **SUBSTRATE DIFFUSION**

***n* PARTIAL DIFFERENTIAL HYPERBOLIC EQUATIONS** ⟺ ***m* PARTIAL DIFFERENTIAL PARABOLIC EQUATIONS**

METHOD OF CHARACTERISTICS



$$\frac{\partial}{\partial t} X_i(z,t) + u(z,t)\frac{\partial}{\partial z} X_i(z,t) = \rho_i r_{M,i}(z,t,\mathbf{X},\mathbf{S}) - X_i(z,t)\frac{\partial}{\partial z}u(z,t),\ \ 0 < z \leq L(t),\ \ t > 0,$$

$$\frac{\partial}{\partial z}u(z,t) = \sum_{i=1}^{n} r_{M,i}(z,t,\mathbf{X},\mathbf{S}),\ \ 0 < z < L(t),\ \ t > 0,\ \ i = 1, \ldots n,$$

$$\dot{L}(t) = u(L(t),t) + \sigma,\ \ t > 0,$$

$$\frac{\partial}{\partial t} S_j(z,t) - \frac{\partial}{\partial z}\left(D_j \frac{\partial}{\partial z} S_j(z,t)\right) = r_{S,j}(z,t,\mathbf{X},\mathbf{S}),\ \ 0 < z < L(t),\ \ t > 0,\ \ j = 1, \ldots m.$$

a) Improving developed model in terms of time calculation
b) Develop a 2D model
c) Set-up a lab-scale reactor
…

Future actvities

THANKS FOR THE ATTENTION