Modeling of Algal - Bacterial Reactor

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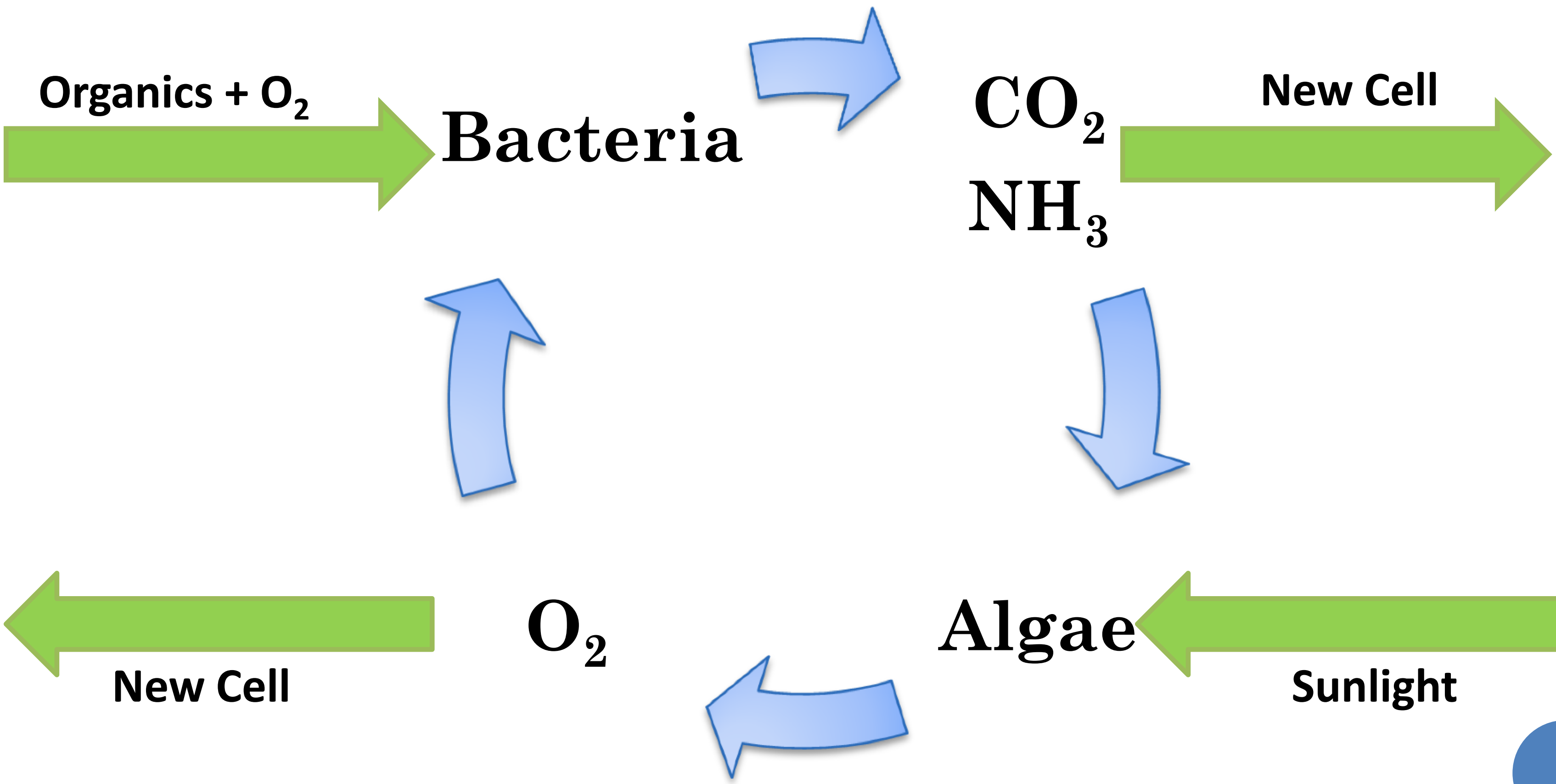
Symbiotic Relationship



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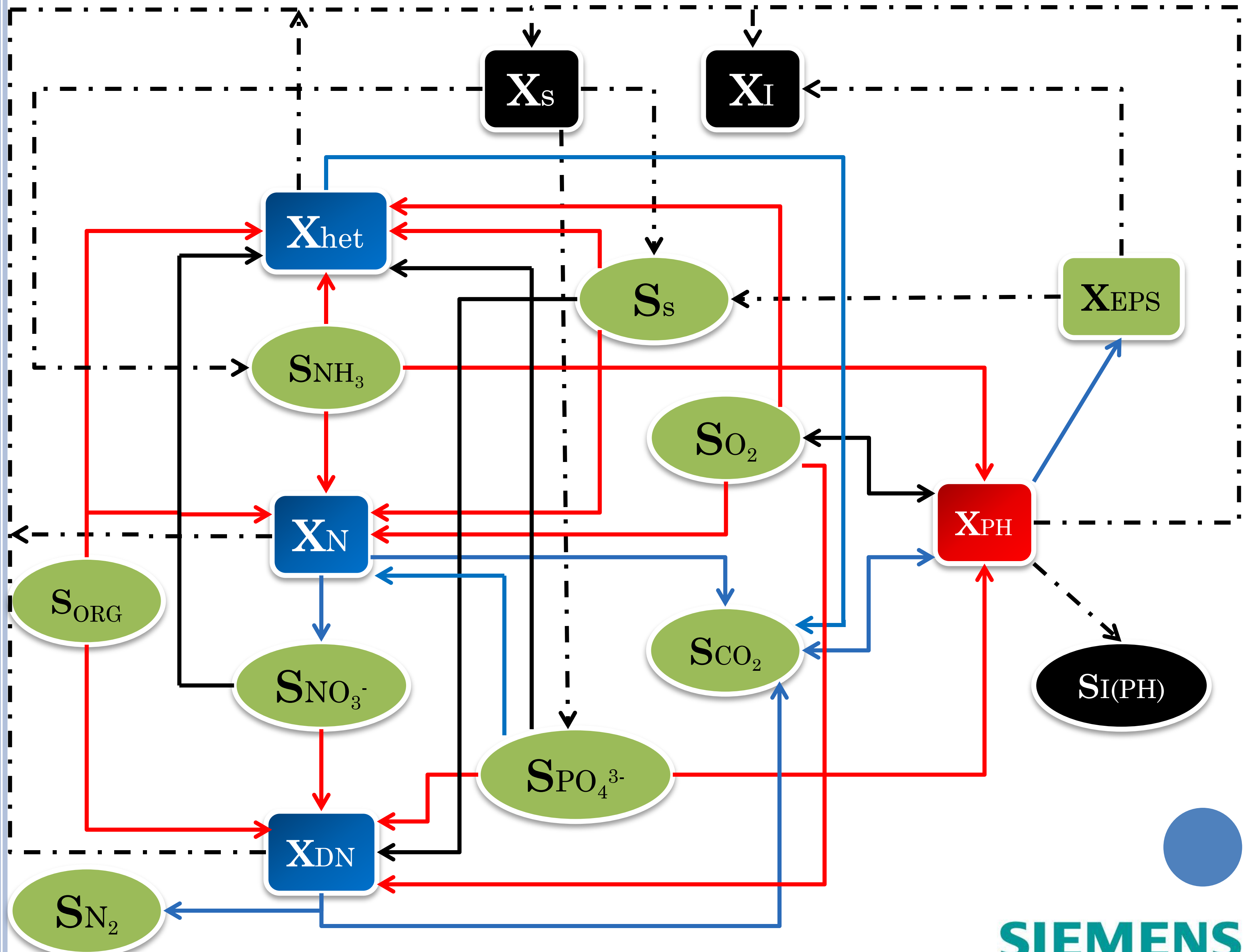
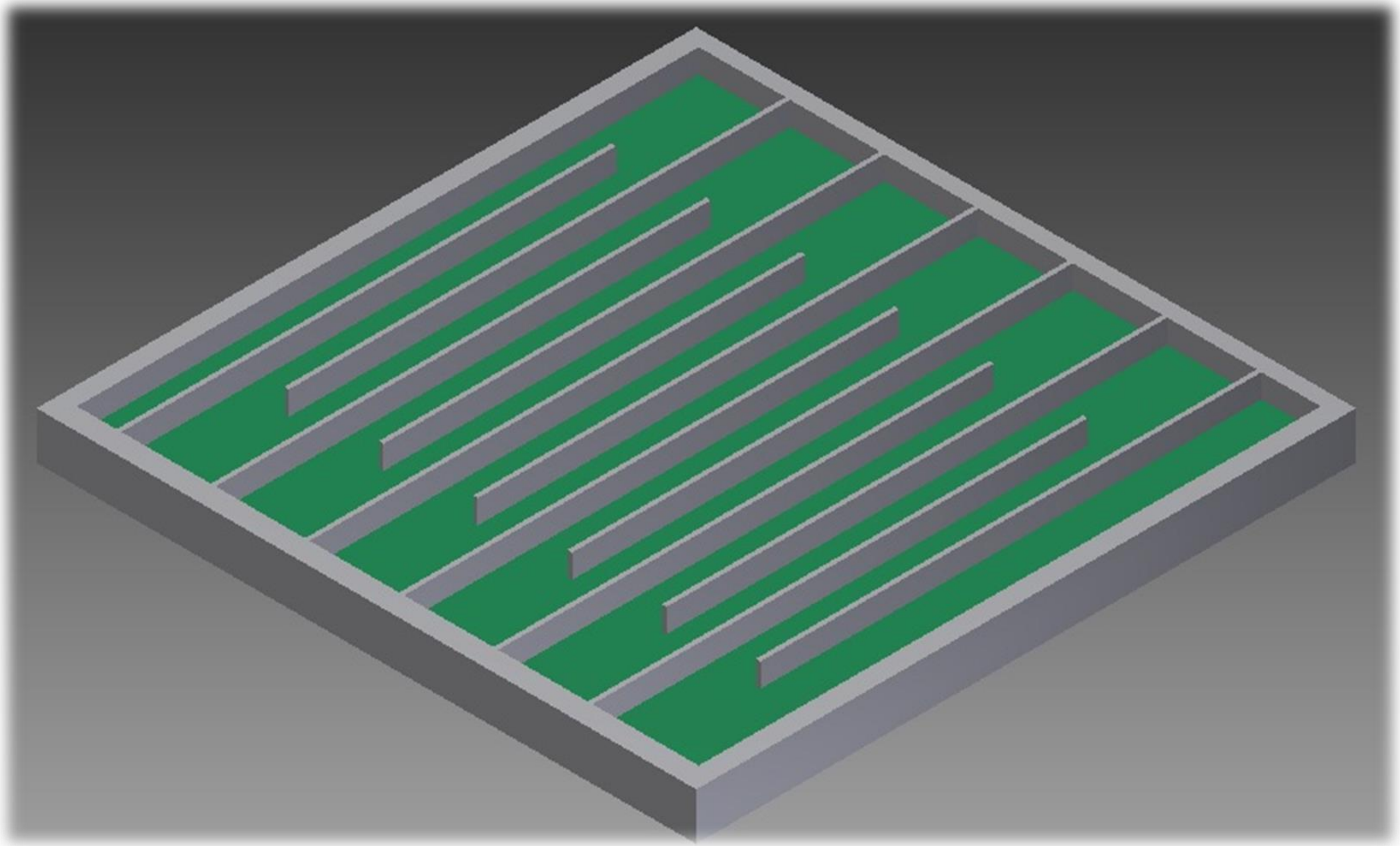


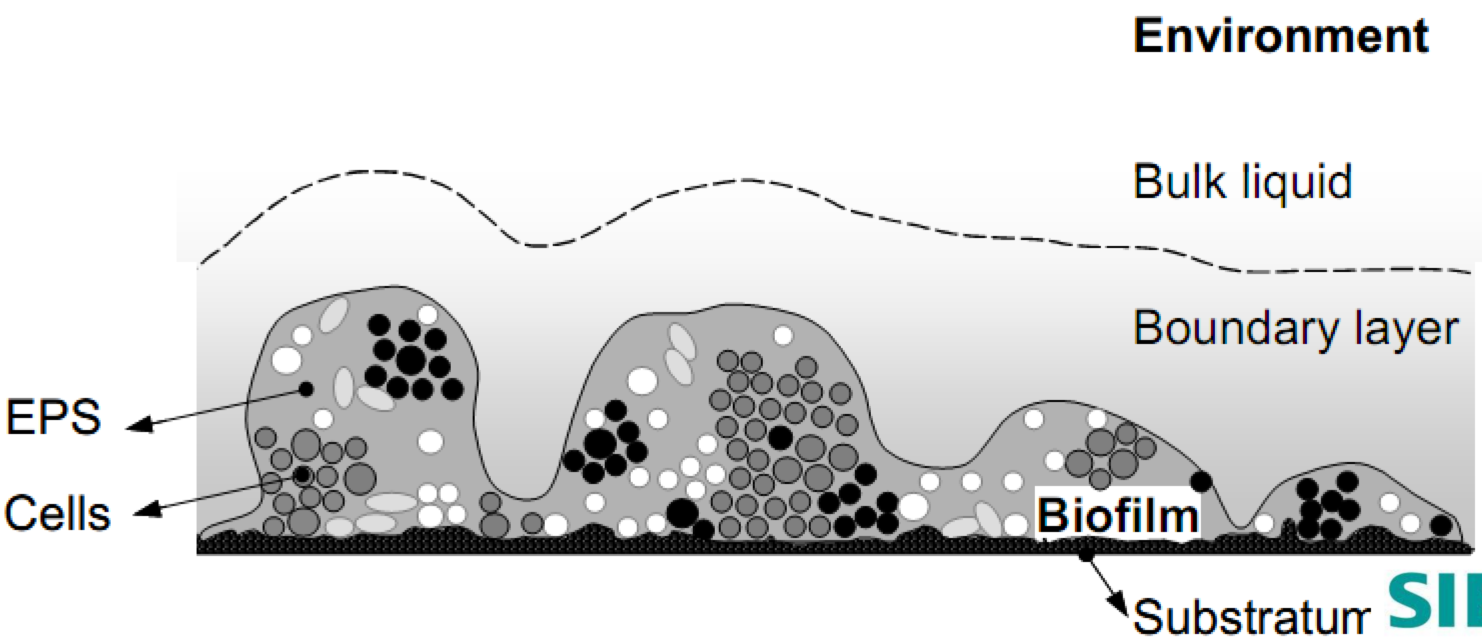
X_S
X_I
X_{het}
S_S
X_{EPS}
S_{NH_3}
S_{O_2}
X_{PH}
X_N
S_{ORG}
S_{CO_2}
$S_{NO_3^-}$
$S_{I(PH)}$
$S_{PO_4^{3-}}$
X_{DN}
S_{N_2}

PROBLEM STATEMENT



BIOFILM COMPARTMENT

- SUBSTRATUM
- BIOFILM
- BOUNDARY LAYER
- BULK LIQUID



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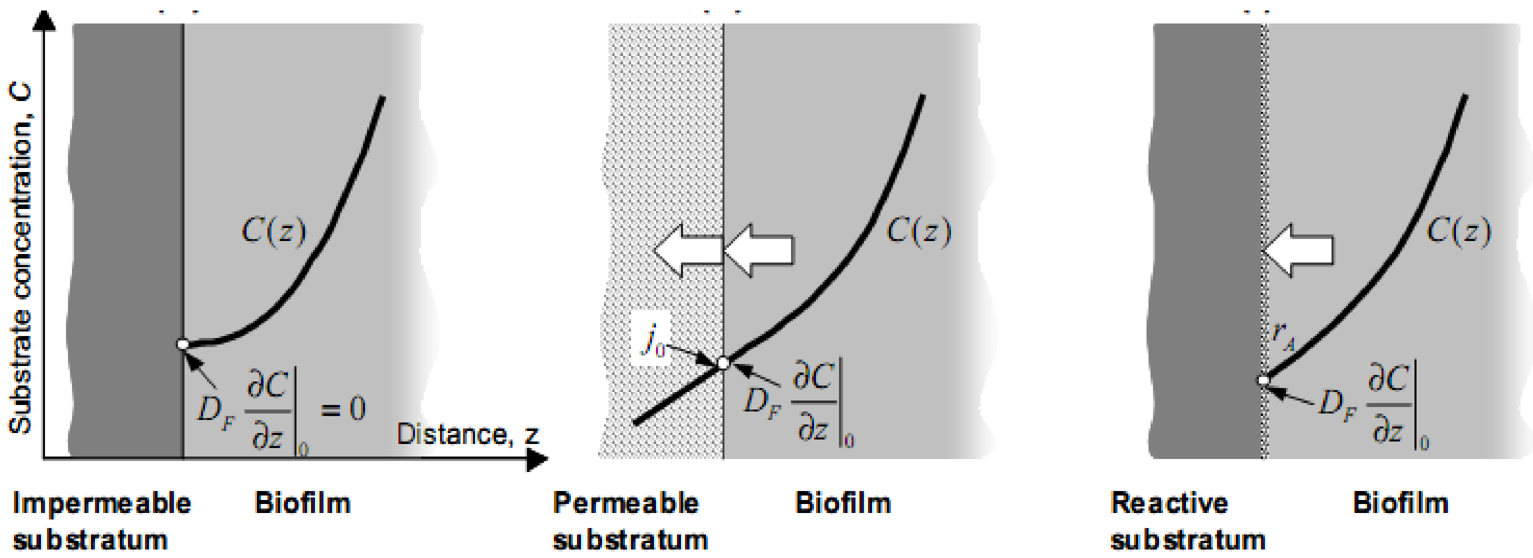
SUBSTRATUM

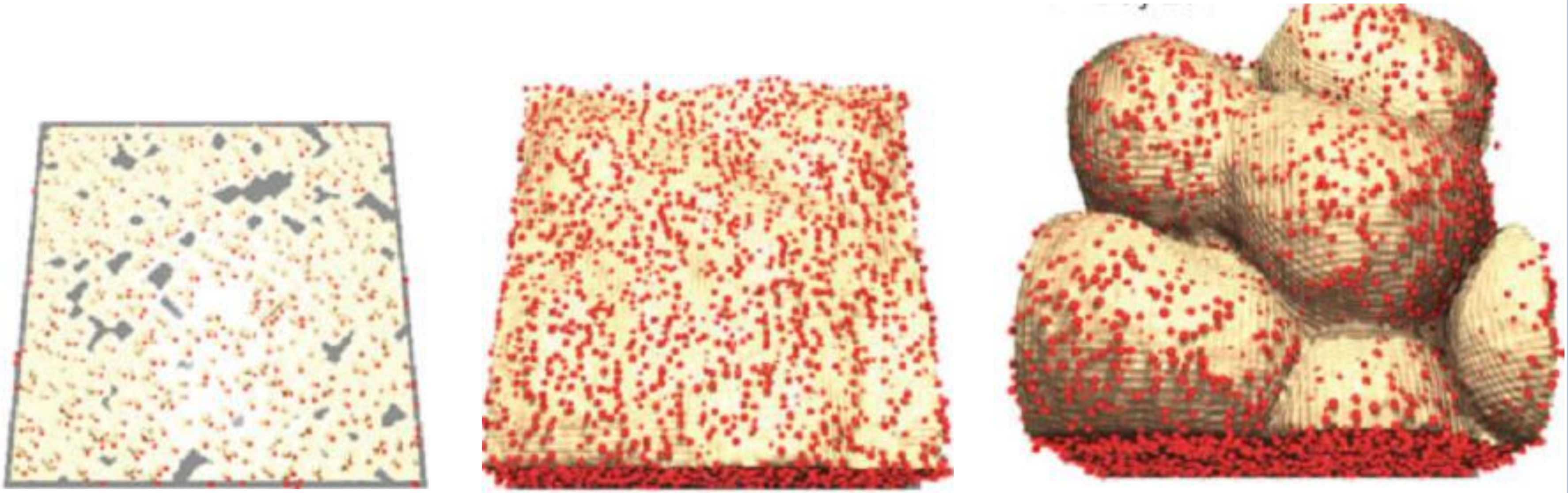
The solid surface on which the biofilm grows is called ***substratum****.*



Note: *In our case the substratum is neither impermeable nor Reactive*

Biofilm

It can be defined as thin layer of microorganism adhering to the surface of the structure (substratum), which may be organic or inorganic together with the polymer that they secrete.



DAY 0 **DAY 11** **DAY 26**

Irregular Biofilm surface development in the oxygen limitation condition
Heterotrophic bacteria represented by red spheres and EPS by light-yellow surface

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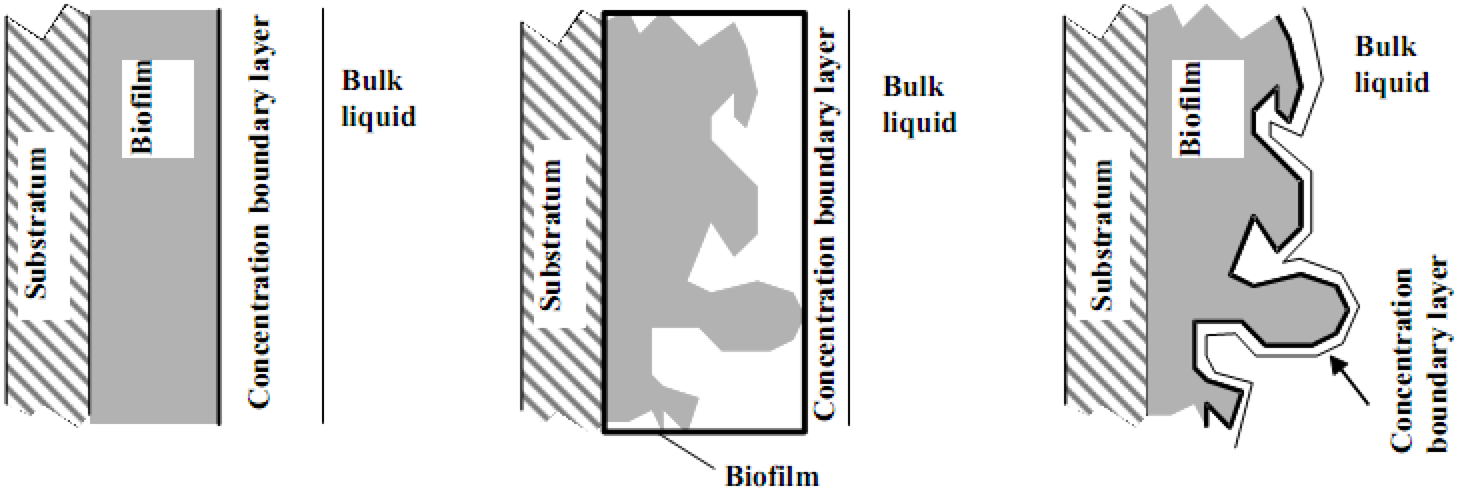
Boundary Layer

The solute concentration at the biofilm surface and in a completely mixed bulk liquid are often significantly different. So to accommodate this concentration gradient MTBL is assumed in which all resistance to mass transfer are taken.



It can be parallel to substratum or biofilm depending on the modeling needs and assumption but the later one is more complex if biofilm has a irregular shape.

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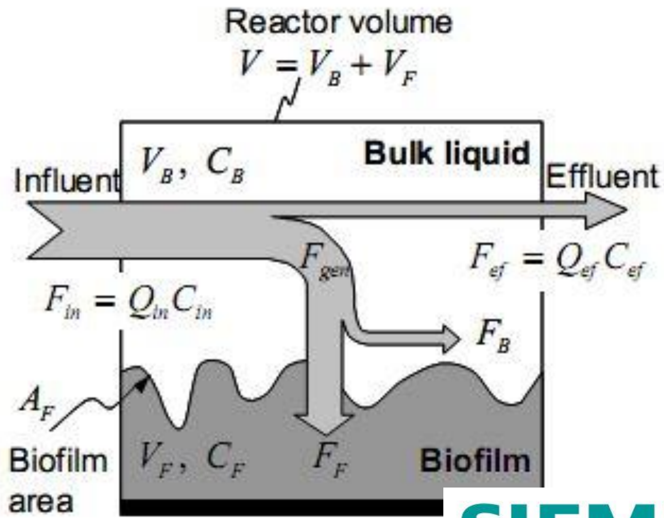
Bulk Liquid

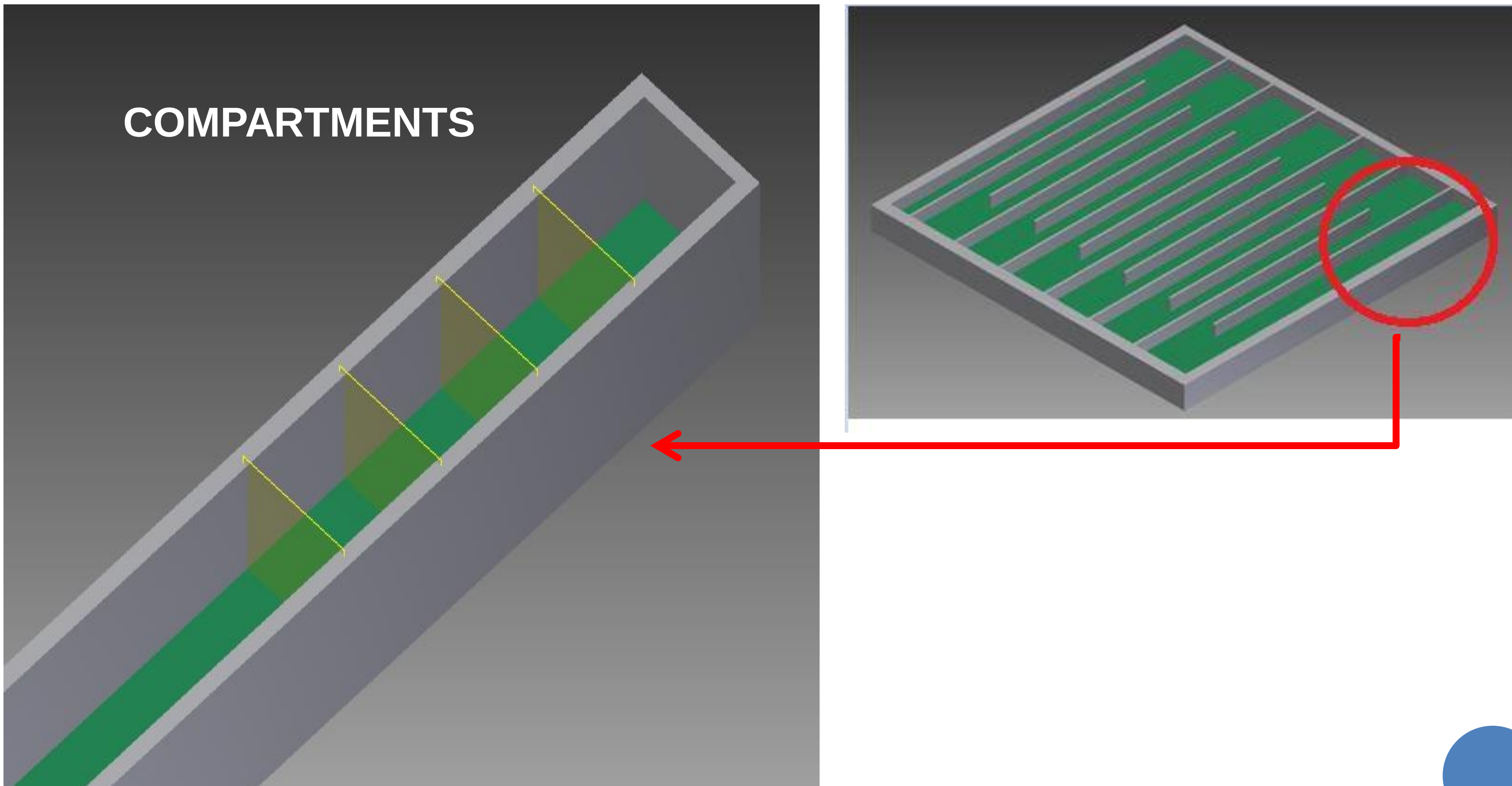
Boundary condition for biofilm with varying concentration because of substrate removal
Two ways to handle.

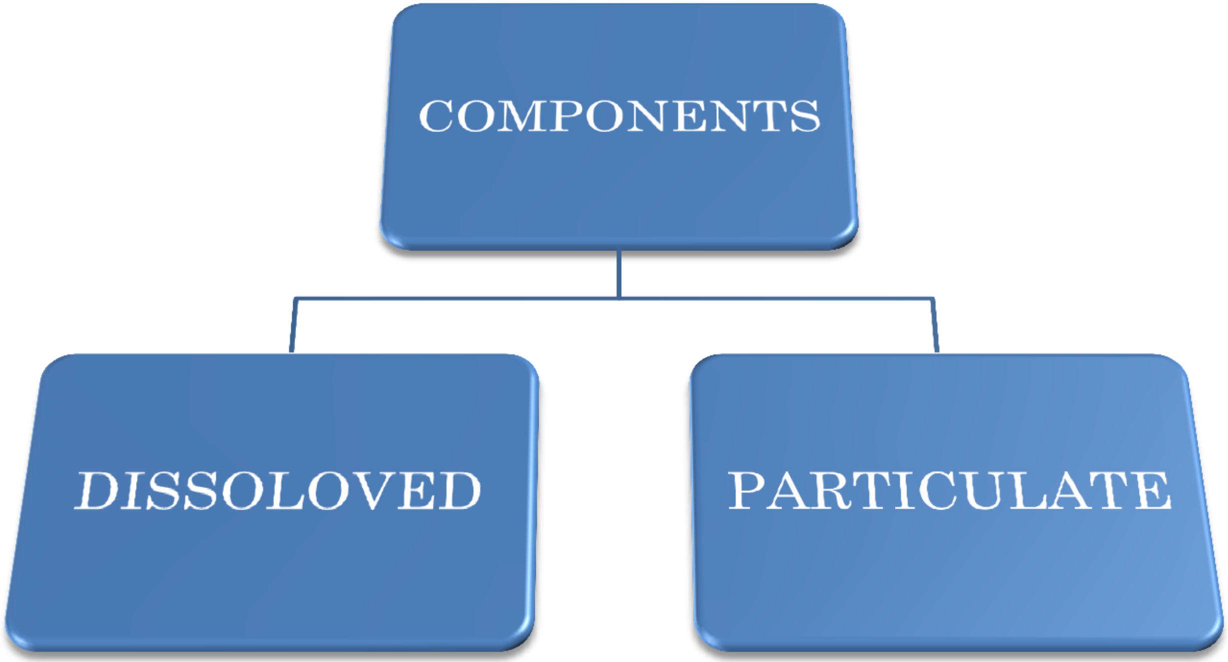
1.Entire domain as one and use ***NS equation*** *and* ***CONTINUITY equation*** *to solve them.*

2.Break the domain to ***various compartments/sub domain*** *to apply constant bulk concentration assumption*



ASSUMPTION




COMPONENTS
DISSOLOVED
PARTICULATE

Dissolved Components

Dissolved Component includes SUBSTRATES, METABOLIC INTERMEDIATES and Various PRODUCTS of MICROBIAL CONVERSION PROCESS.

ASSUMPTION:- *for one microbial metabolic activity within the biofilm, growth rate is controlled by one growth limiting substrate. As long as the concentrations of other dissolved component do not become the rate limiting at any location within biofilm, they do not need to be considered rate limiting step.*

If the above assumption can't be guaranteed then multiple substrate should be solved Simultaneously increasing modeling complexity and computing demands.

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Which is Rate Limiting ?

$$r_g = \mu_{\max,H} \frac{S_S}{K_S + S_S} \frac{S_{O2}}{K_{O2} + S_{O2}} X_H$$

$$r_S = \frac{1}{Y_H} r_g$$

$$r_{O2} = \frac{(1 - Y_H)}{Y_H} r_g$$

r_{g} : *heterotrophic growth rate*
r_s : *growth rate of substrate*
r_{O2} : *growth rate of oxygen*

Coefficient of oxygen and substrate utilization

$$\nu_{S,O2} = \frac{r_S}{r_{O2}} = \frac{1}{(1 - Y_H)}$$

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Ratio of substrate penetration and utilization

$$\gamma_{S,O2} = \frac{1}{\nu_{S,O2}} \frac{D_S}{D_{O2}} \frac{S_{LF,S}}{S_{LF,O2}}$$

(D_s,D_{O2}): Diffusion rates
($S_{LF,S}$,$S_{LF,O2}$): Substrate concentration at the surface of biofilm

If,

$\gamma_{S,O2} >> 1$	Oxygen is potentially limiting inside of the biofilm, but organic substrate is fully penetrating the biofilm.
$\gamma_{S,O2} \approx 1$	Not clear whether oxygen or organic substrate is limiting inside of the biofilm. A multi-substrate model should be used to evaluate the biofilm.
$\gamma_{S,O2} << 1$	Organic substrate is potentially limiting inside of the biofilm, but oxygen is fully penetrating the biofilm.

Particulate Components

Particulate Components include active microbial cells, dead or inert cells, EPS and any other organic or inorganic particles embedded in the biofilm solid matrix.

We have taken microbial cells and dead cells in our model.

The concentration of particulate components or total amount of biofilm change over time, to make model a dynamic system. This is done to predict how biofilm grows with time ?

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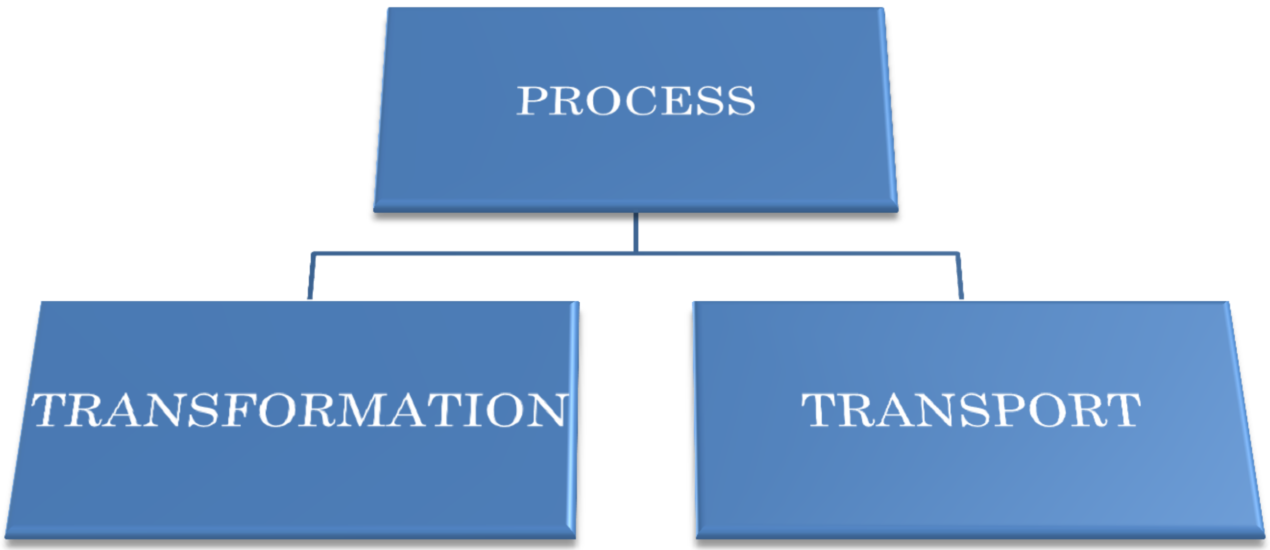

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TRANSFORMATION

Typical rate laws found in biofilm models:

MONOD equation for one limiting substrate

$$\mu = \mu_{\max} \frac{S}{K_S + S}$$

μ: specific growth rate (T^{-1})
μ_{max}: maximum specific growth rate (T-1)
S: Concentration of rate limiting substrate (ML^{-3})
K_s: Concentration giving one half the maximum rate (ML^{-3})

$$r_X = \mu X$$

r_x = volumetric production rate (T^{-1})
X = Concentration of microbial species ($ML^{-3}T^{-1}$)

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Inactivation Rate

$$r_{in} = -b\,X$$

r_{in} = inactivation state ($ML^{-3}\,T^{-1}$)
b = first order inactivation rate constant (T^{-1})

Substrate Utilization

$$r_S = -\frac{1}{Y} r_X$$

Y= yield coefficient (M_x/M_s)
r_s= rate of substrate use ($ML^{-3}\,T^{-1}$)

$$r_H = \mu_{\max,H} \frac{S_S}{K_S + S_S} X_H - b_H X_H$$

$$r_S = -\frac{1}{Y_H} \mu_{\max,H} \frac{S_S}{K_S + S_S} X_H$$

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TRANSPORT

$$j_z = u_z C - D\frac{\partial C}{\partial z} - D_T\frac{\partial C}{\partial z} - \zeta DC\frac{F}{RT}\frac{\partial \Phi}{\partial z}$$

j_z: mass flux of the component ($ML^{-2}T^{-1}$)
U_z: advective velocity (LT^{-1})
D: coefficient of molecular diffusion (L^2T^{-1})
D_T: coefficient of turbulent dispersion (L^2T^{-1})
ζ: ion charge (eN^{-1})
F: Faraday Constant (Ite^{-1})
ϕ: Electric Potential ($L^2MT^{-3}I^{-1}$)
Θ: Temperature (T)
R: Universal gas constant ($L^2MT^{-2}\Theta^{-1}N^{-1}$)

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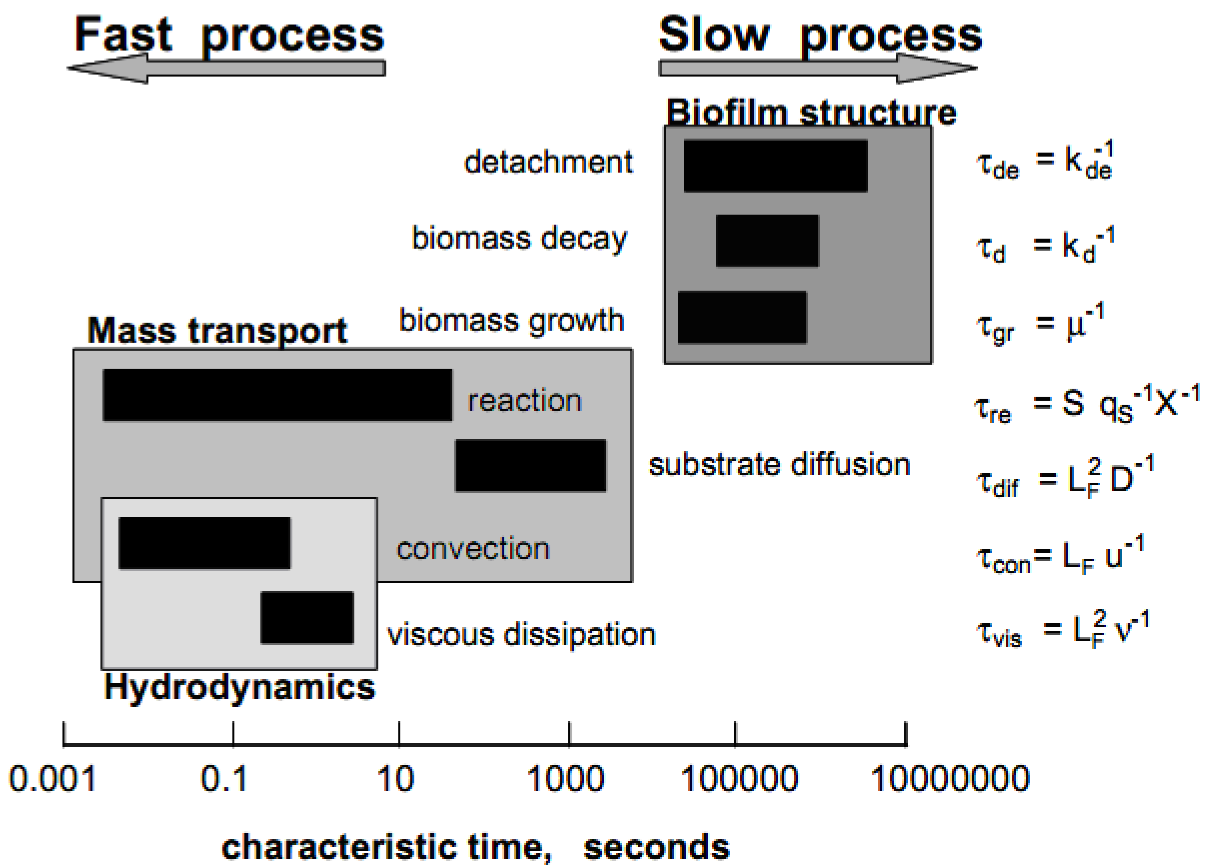
Time Scale Analysis



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Mass Balance Equation

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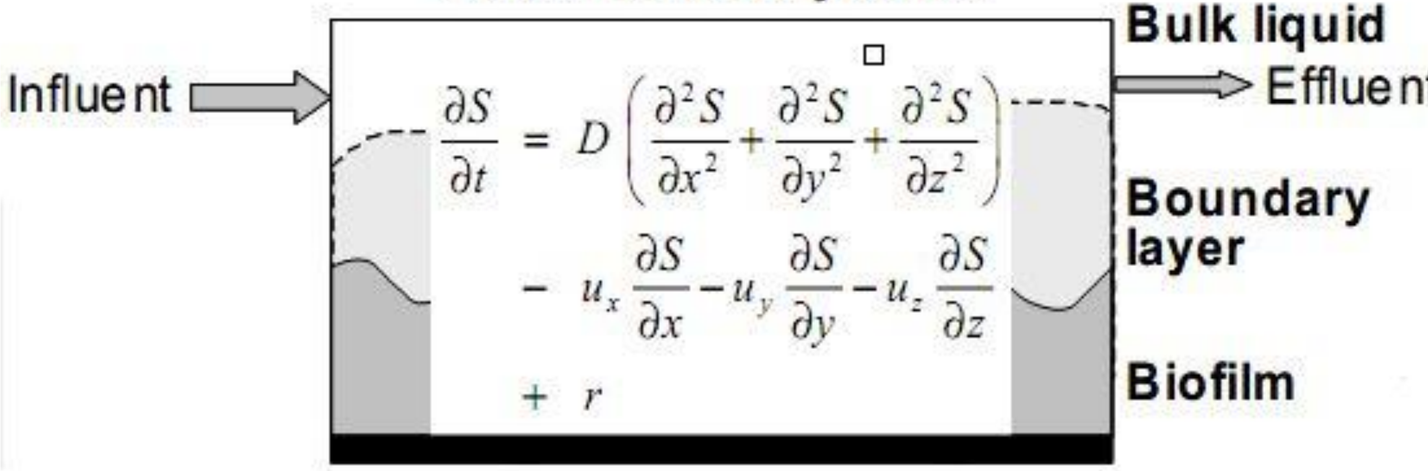
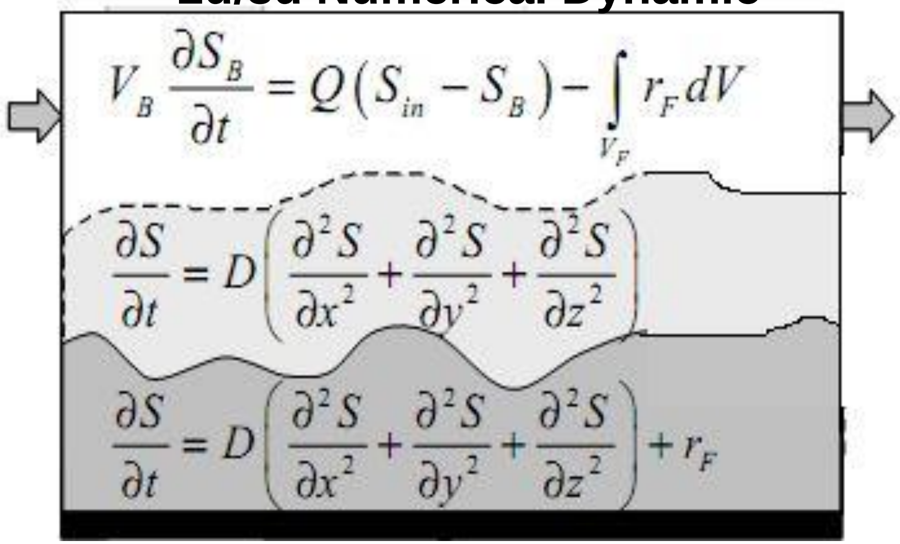
General model
3d numerical dynamic



2d/3d Numerical Dynamic



S: denotes the concentration of substrates

1d Numerical Dynamic

$$V_B \frac{\partial S_B}{\partial t} = Q(S_{in} - S_B) - j_F A_F$$

$$j_F = \int_0^{L_F} r_F dz = D \frac{dS}{dz}\Big|_{L_F} = k_c (S_B - S_F)$$

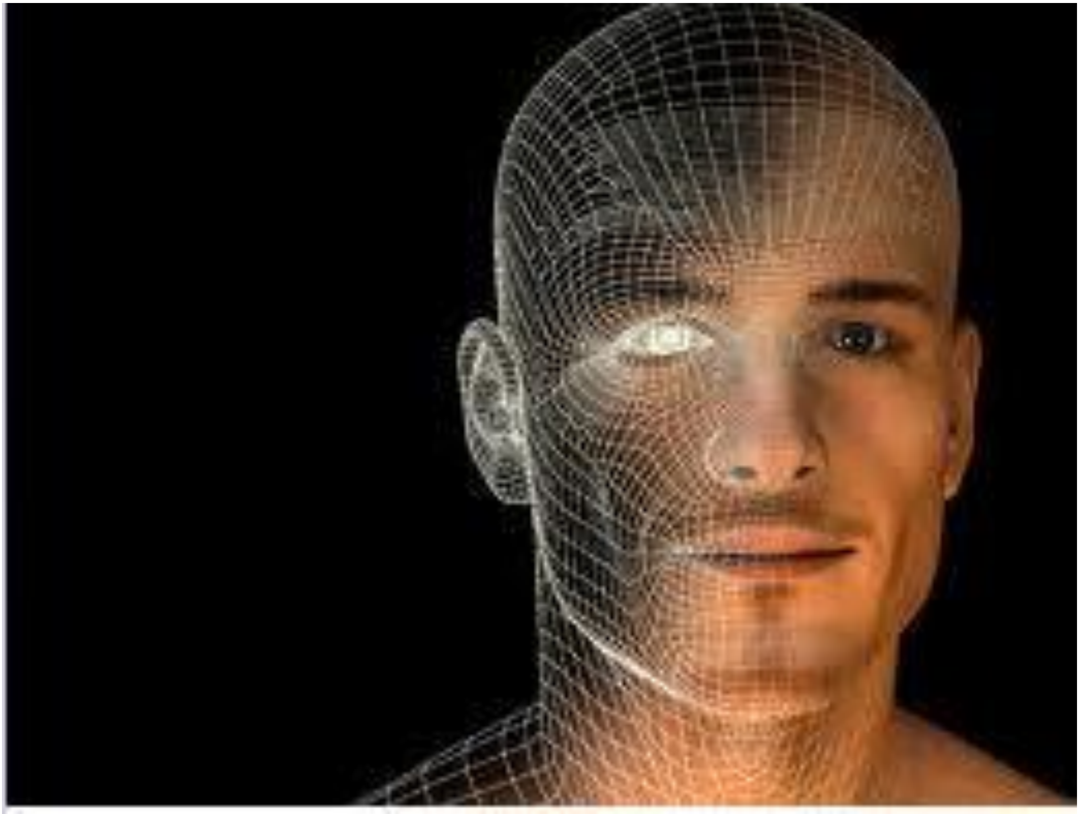
$$\frac{\partial S}{\partial t} = D \frac{\partial^2 S}{\partial z^2} + r_F \Rightarrow \begin{cases} S(z)\ and\ j_F \\ numerical \end{cases}$$

1d Numerical Steady State

$$Q(S_{in} - S_B) = A_F j_F$$

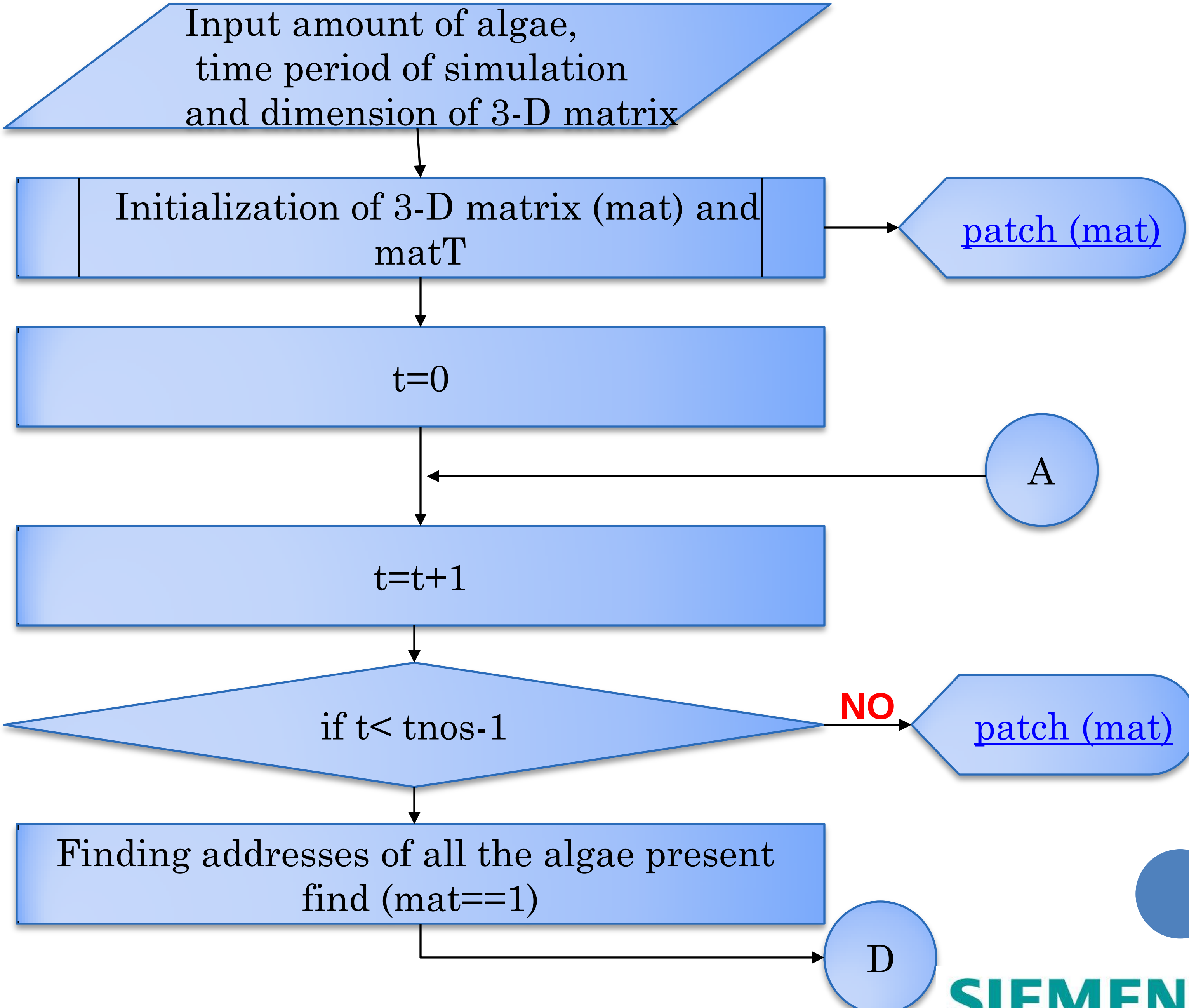
$$j_F = \int_0^{L_F} r_F dz = D \frac{dS}{dz}\Big|_{L_F} = k_c (S_B - S_F)$$

$$D \frac{d^2 S}{dz^2} + r_F = 0 \Rightarrow \begin{cases} S(z)\ and\ j_F \\ numerical \end{cases}$$



Modeling

ALGAE 14 days



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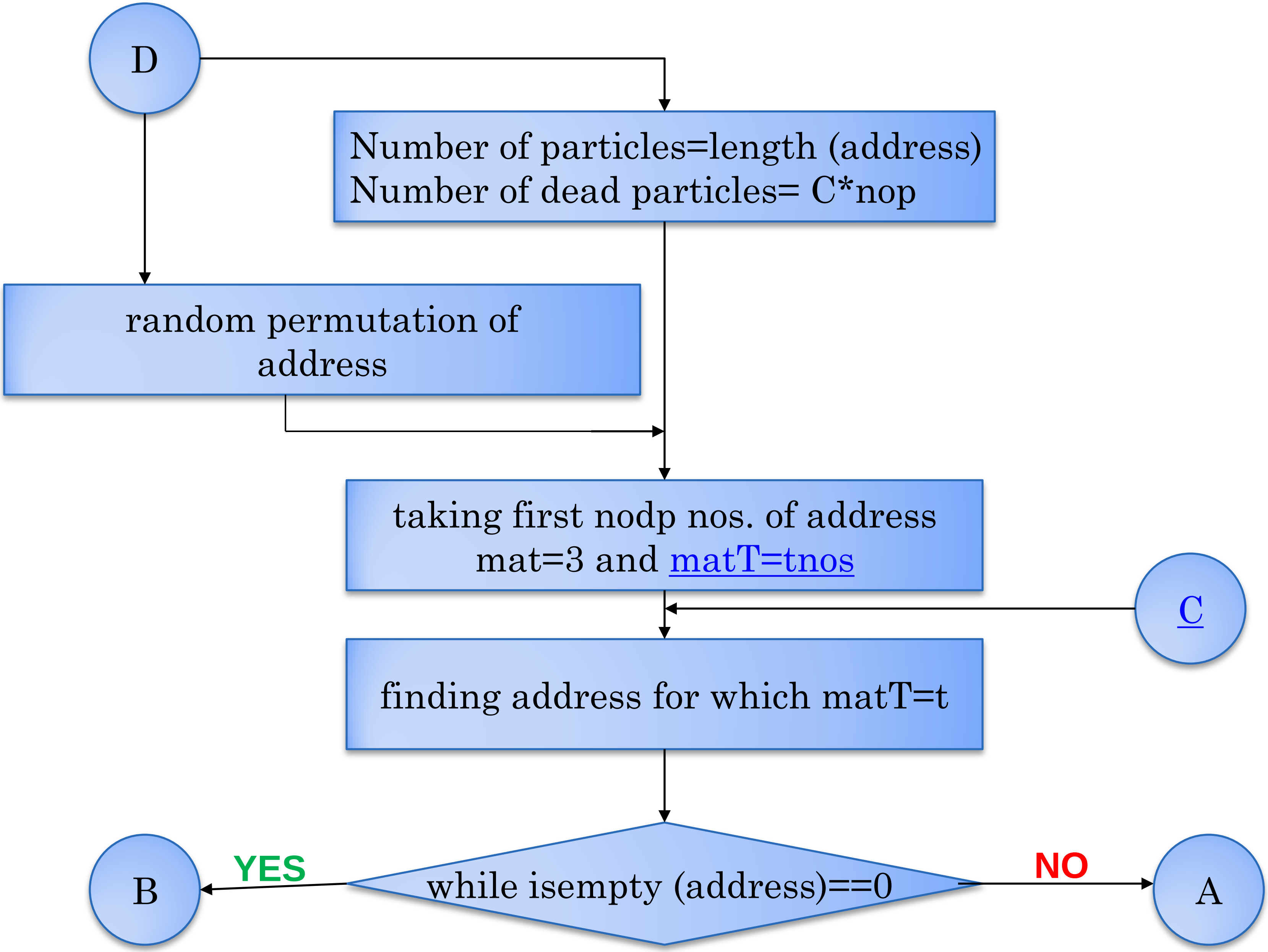
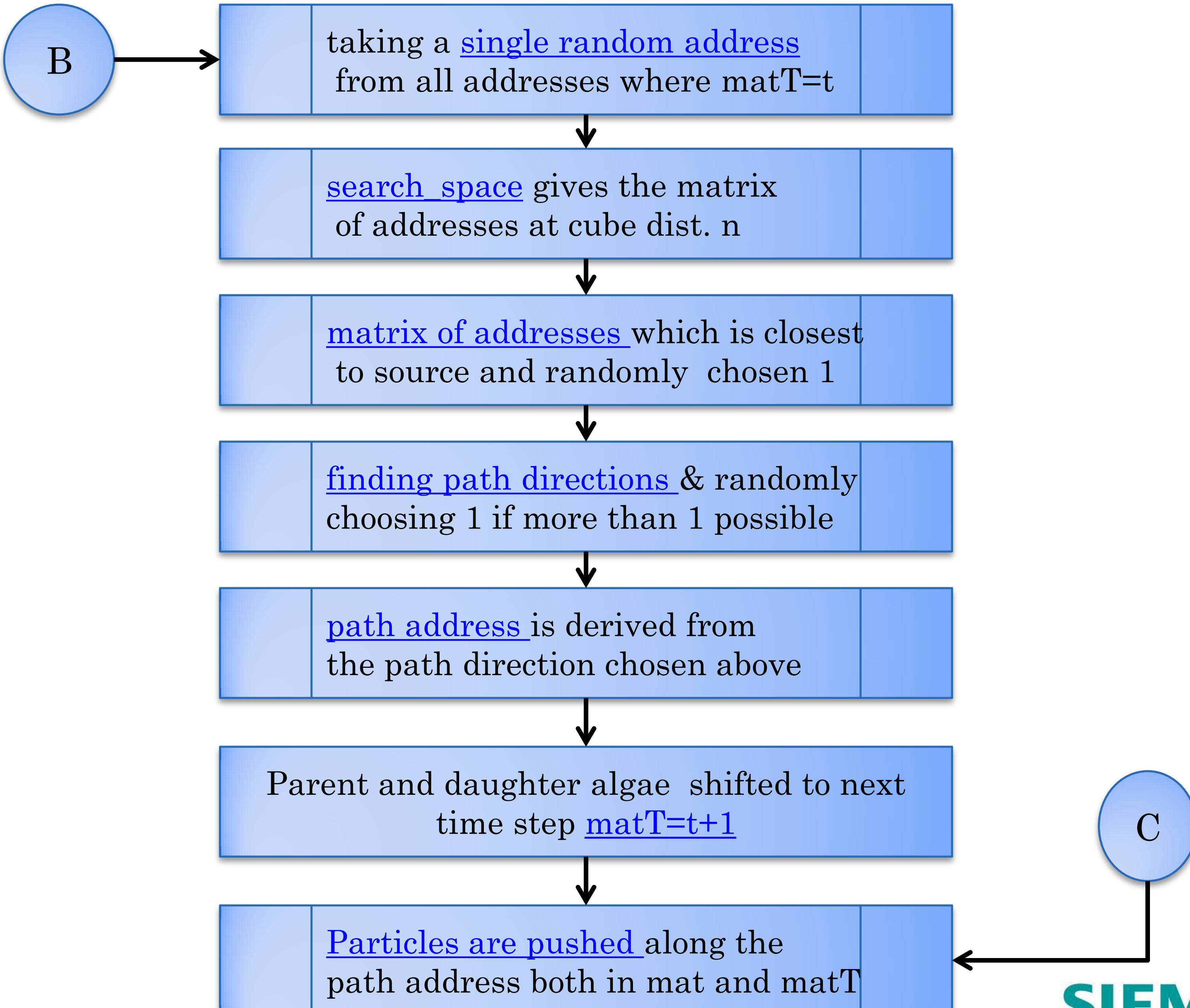

D
Number of particles=length (address)
Number of dead particles= C*nop
random permutation of address
taking first nodp nos. of address
mat=3 and matT=tnos
C
finding address for which matT=t
B
YES
while isempty (address)==0
NO
A


B
taking a single random address from all addresses where matT=t
search_space gives the matrix of addresses at cube dist. n
matrix of addresses which is closest to source and randomly chosen 1
finding path directions & randomly choosing 1 if more than 1 possible
path address is derived from the path direction chosen above
Parent and daughter algae shifted to next time step matT=t+1
Particles are pushed along the path address both in mat and matT
C

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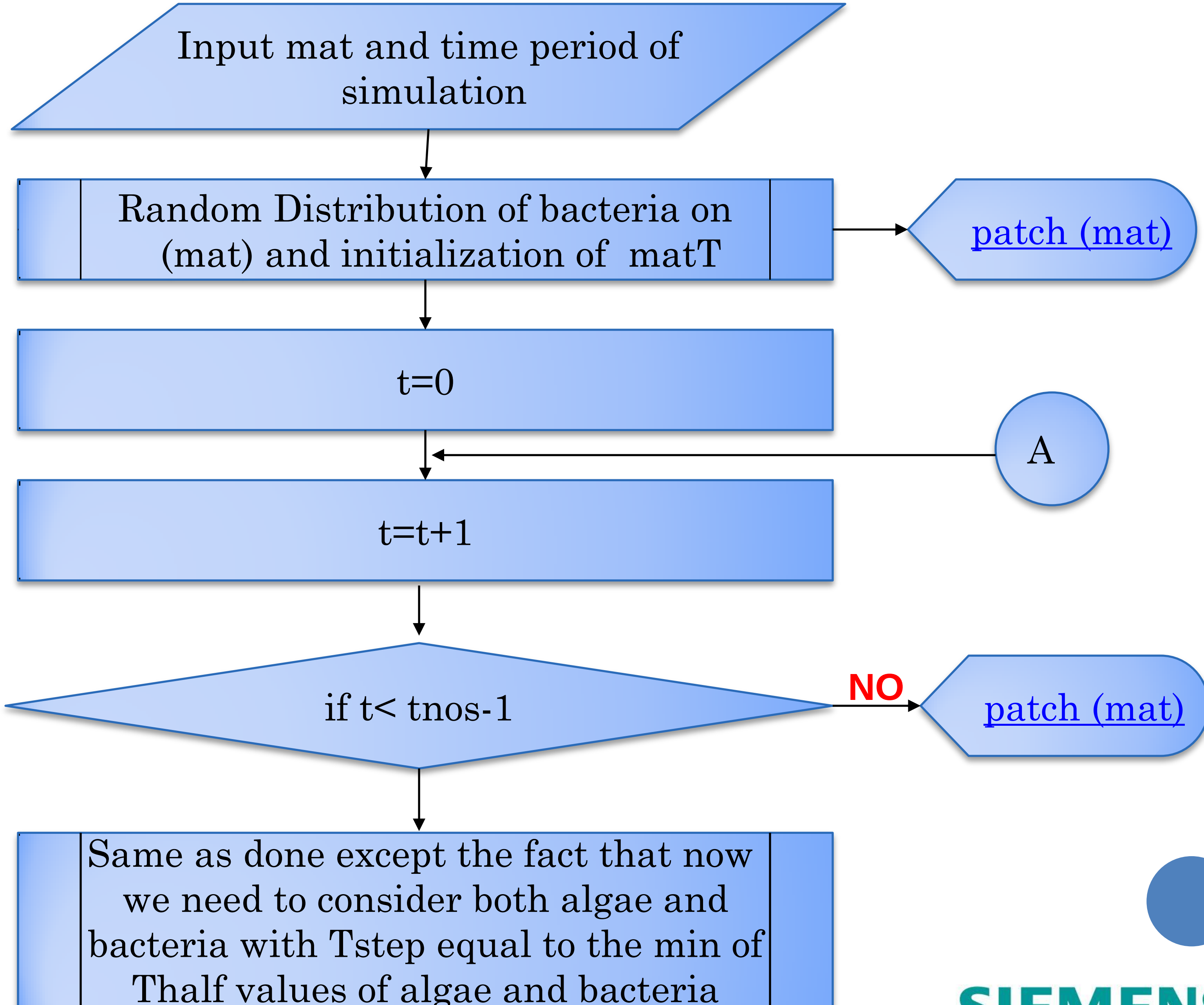
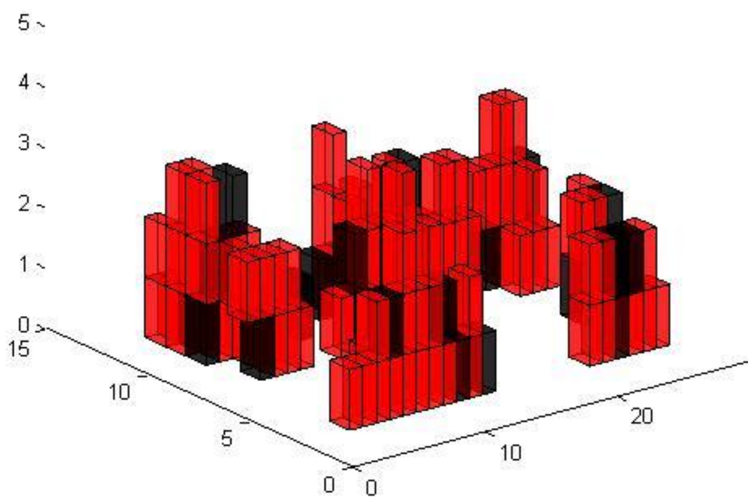
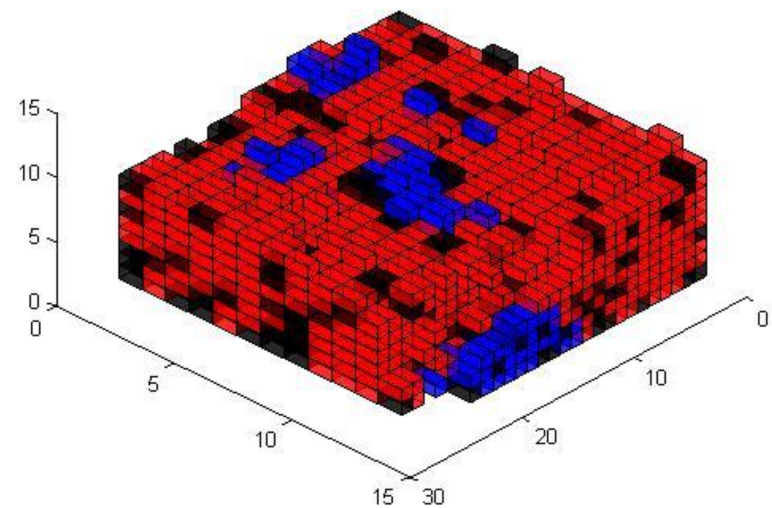
ALGAE plus Bacteria next 7 days



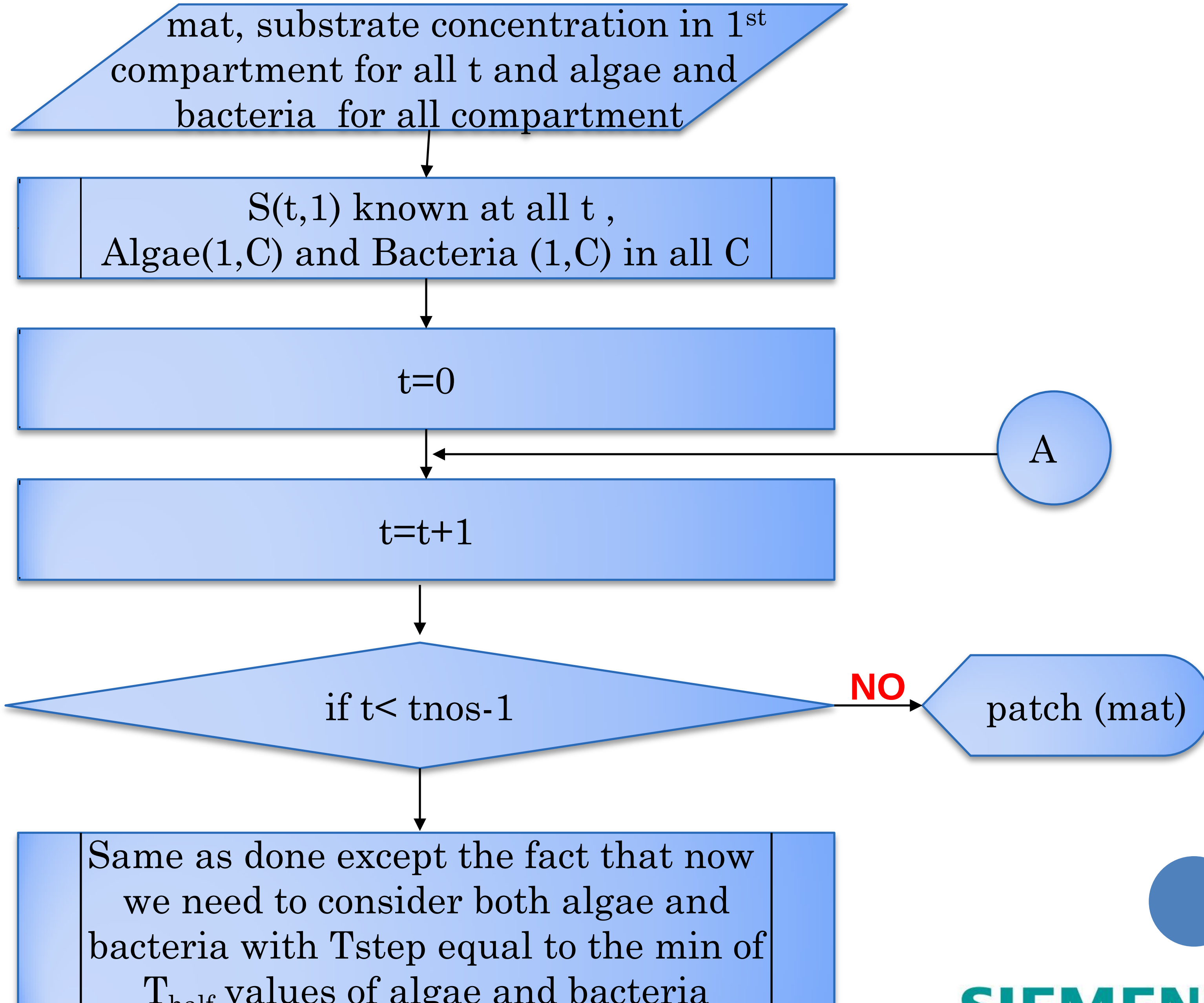
Results at different time





At the end of 6 days **At the end of 16 days**

Continuous Mode




Thank you!