Appendix A

Glossary

List of acronyms

BHI	Brain Heart Infusion
BioTeC	Bioprocess Technology and Control group
CFU	Colony Forming Unit
ESAB	*Escola Superior d'Agricultura de Barcelona*
FC	Flow Cytometer
FS	Forward Scattered light (flow cytometry)
IbM	Individual-based Modelling
IbMs	Individual-based Models
INDISIM	INDividual DIScrete SIMulation
MOSIMBIO	Modelling and Computer Simulation of Biological Systems group
MSE	Mean sum of Squared Errors
MSZ	Multisizer
NMTA	Nelder-Mead Threshold Accepting
PBC	Periodic Boundary Conditions
RBC	Red Blood Cells
SCT-UB	Scientific-Technical Services of the *Universitat de Barcelona*
SS	Side Scattered light (flow cytometry)

SSE	Sum of Squared Errors
TIP	Thermodynamics of Irreversible Processes
TA	Threshold Accepting
UB	*Universitat de Barcelona*
UPC	*Universitat Politècnica de Catalunya*

List of abbreviations

beg	beginning
bib	bibliography
ENV^-	pre-inoculation environment
ENV^+	present environment
exp	exponential phase
inf	inferior
max	maximum
min	minimum
ref	reference
s.u.	simulation units
sup	superior
X_0	initial value of *'X'*
X_f	final value of *'X'*

List of symbols

λ	lag parameter
μ	growth rate
$D(t)$	product distance
$D_{\overline{m}}(t)$	mean mass distance
$D_{pk}(t)$	mass distribution distance
m	bacterial individual mass
$\overline{m}(t)$	bacterial mean mass of a culture
m_d	individual bacterial mass at division
m_R	invidual mass to initiate reproduction cycle
$N(t)$	cell density
$p_{k_m}(t)$	instantaneous cell's biomass relative frequency
t_{FD}	time to the first division
t_G	generation time or doubling time
t_R	reproduction cycle duration
U	uptaken nutrient particles

Chapter 1

$\alpha(t)$	adjustment function
τ_i	individual adjustment period
b, c, T_{min}, T_{max}	parameters of Equation 1.4
$G(t)$	growing fraction population
g_1, g_2	mathematical attractors for defining lag parameter
k_n	constant for Equation 1.9
M	cell biomass
$NG(t)$	non-growing fraction population
$Q(t)$	physiological
s	excess biomass per cell
$s*$	total biomass per cell
s_{min}	minimum biomass per cell
t_{a_i}	individual adjustment period
t_{LAG_i}	individual lag time
t_{m_i}	individual generation time

Chapter 2

ρ	parameter to fix an interval of the growth curve
σ	standard deviation
(x, y)	coordinates of a spatial cell
B	increase in bacterial biomass
b	parameter of Equation 2.2
B_i	vector that describes a bacterium
c_s	concentration of substance s
d	mean distance between neighbouring cells
d_{max}	maximum movement radius
D_s	diffusion coefficient of a substance
E_{xy}	vector that describes a spatial cell
Enz	enzyme particles in a bacterial cell
I	maintenance constant
I_{gen}	index to control the extracellular enzyme particles synthesis
J_s	flux of a substance between neighbouring cells
m_1, m_2	individual bacterial masses after division
n_{enz}	enzyme particles synthesized by a bacterial cell
N_{mon}	number of monomers contained in a polymer
p_{mov}	probability for a bacteria to move
t_{enz}	time duration of extracellular enzyme particles
V_{enz}	enzyme synthesis rate per unit of mass and time step
Y	metabolic efficiency
Y_{enz}	energy cost of enzyme synthesis
Z_1, α, c, k, n	parameters of the uptake model

Chapter 3

$\overline{E}_k$	mean kinetic energy of the nutrient particles
r	radius of the accessible volume of nutrient particles around a bacterium
T	temperature

Chapter 4

Δm	biomass interval to define the classes of biomass
λ_{pseudo}	apparent lag or pseudolag of a culture
λ_{real}	real lag of a culture
μ_B	total biomass growth rate
μ_N	cell density growth rate
ρ	parameter to fix an interval of the growth curve
τ_B, t_B	parameters to distinguish the balanced growth
a	parameter of Equation 4.10
$B(t)$	total biomass of a culture
m_i	class of biomass
$p(m_i)$	biomass probability distribution of a bacterial culture
P_{EXP}	exponential phase
$P_{I(B)}$	initial phase in total biomass
$P_{I(N)}$	initial phase in cell density
$P_{T(B)}$	transition phase in total biomass
$P_{T(N)}$	transition phase in cell density
R	mean of duplications per hour of an individual cell
t_1, t_2	temporal limits of transition phase in cell density
t_e, N_e	coordinates of an exponential point of the growth curve
Z, γ, β	parameters of Equation 4.4

Chapter 5

d	equivalent diameter
$D_{\overline{d}}(t)$	mean diameter distance
$D_{pk_d}(t)$	diameter distribution distance
$D_d(t)$	product distance
fs	forward scatter channels
N	number of channels
$p_{km}(t)$	instantaneous cell's diameter relative frequency
R	mean of duplications per hour of an individual cell
ss	side scatter channels

Chapter 6

Γ, α, β	parameters to fix the thresholds (NMTA)
γ, ρ, χ, σ	coefficients of NMTA geometric operations
ξ	random simplex shift probability (NMTA)
ρ	radius of the trust region (NEWUOA)
$\hat{\rho}$	re-scaled radius of the trust region (NEWUOA)
τ_r	threshold value for round r (NMTA)
A, B, C	parameters of a Weibull distribution
$C_{exp}(t)$	experimentally measured cell concentration
$C_{sim}(t)$	simulation output of cell concentration
$f(m; A, B)$	Weibull distribution
$F(\overrightarrow{x})$	objective function (NEWUOA)
g	number of generations per hour
m	number of interpolation points (NEWUOA)
n	total number of data points
n_{pi}	number of points to be tested for each parameter (grid search)
n_R	number of stepping rounds (NMTA)
$n_{S,r}$	number of simplex steps in round r (NMTA)
p_i	parameters to be estimated
$\hat{p}_i$	re-scaled parameters to be estimated (NEWUOA)
$Q(\overrightarrow{x})$	quadratic model (NEWUOA)
R_1, R_2, R_3	number of evaluations of the objective function at each simplex vertex (NMTA)
t_s	time step
u_{max}	mean maximum uptake rate
V_d	bacterial volume at division
$\overrightarrow{x}$	vector with a combination of parameters to be estimated (NEWUOA)
Y	yield