General note: the test % text in green" are comments and additional notes/explanations.

```
Function Regulatory model

Tic %start of time calculation (how look took the ode solver to solve)
clear all
clc
% Recalculate the x's every iteration, as described by the formulas.
Carab = x(1);          % mol/dm3 concentration arabinose inside
CmRNAAraC = x(2);      % mol/dm3 concentration of AraC-mRNA
CPAraC = x(3);         % mol/dm3 concentration of AraC-protein
CmRNAmfp5 = x(4);      % mol/dm3 concentration of mfp5-mRNA
CPmfp5 = x(5);         % mol/dm3 concentration of mfp5 in ctyoplasm
CPmfp5_peri = x(6);    % mol/dm3 concentration of mfp5 in periplasm
CPmfp5_o_m_inact=x(7);% mol/dm3 concentration of inactive mfp5-protein
                        in outer membrane
CPmfp5_o_m_act = x(8);% mol/dm3 concentration of active mfp5-protein
                        in outer membrane

% initial (guess) values of the x's
ini = [0 0 0 0 0 0 0 0];
% start=0, 1000 steps of 1)
tini=0; tend=1000; dt=1;
%define options for the ode-solver
opt = odeset('RelTol',1e-10, 'AbsTol',1e-10);
%Define the ode solver, calling the formulars, start, steps and
options.
[t x] = ode45(@Reg_modeldt, tini:dt:tend , ini , opt);

% Defining the graphs including the results
t;x;
figure(1)
subplot( 3,3,1)
hold
off
plot( t(:,1), x(:,1), 'LineWidth', 2 )title('Carab' );ylabel
('mol/dm3' )xlabel( 't' );grid onbox onsubplot( 3,3,2)hold off
plot( t(:,1), x(:,2), 'LineWidth', 2 )title( 'CmRNAAraC'
);ylabel( 'mol/dm3' )xlabel( 't' );grid onbox onsubplot( 3,3,3)
hold off
plot( t(:,1), x(:,3), 'LineWidth', 2 )title( 'CPAraC' );ylabel(
'mol/dm3' )xlabel( 't' );grid onbox onsubplot( 3,3,4)hold off
plot( t(:,1), x(:,4), 'LineWidth', 2 )title( 'CmRNAmfp5'
);ylabel( 'mol/dm3' )xlabel( 't' );grid onbox onsubplot( 3,3,5)
hold off
plot( t(:,1), x(:,5), 'LineWidth', 2 )title( 'CPmfp5' );ylabel(
'mol/dm3' )xlabel( 't' );grid onbox onsubplot( 3,3,6)hold off
plot( t(:,1), x(:,6), 'LineWidth', 2 )title( 'CPmfp5_peri '
);ylabel( 'mol/dm3' )xlabel( 't' );grid onbox onsubplot( 3,3,7)
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hold off
plot( t(:,1), x(:,7), 'LineWidth', 2 )title( 'CPmfp5_o_m_inact'
;ylabel( 'mol/dm3' )xlabel( 't' );grid onbox onsubplot( 3,3,8)
hold off
toc % End of time calculation (how took the odesolver to solve
it)
end
function
dx = Reg_modeldt( t , x )
Carab = x(1);        % mol/dm3 concentration arabinose inside
CmRNAAraC = x(2);    % mol/dm3 concentration of AraC-mRNA
CPAraC = x(3);       % mol/dm3 concentration of AraC-protein
CmRNAmfp5 = x(4);    % mol/dm3 concentration of mfp5-mRNA
CPmfp5 = x(5);       % mol/dm3 concentration of mfp5 in ctyoplasm
CPmfp5_peri = x(6); % mol/dm3 concentration of mfp5 in periplasm
CPmfp5_o_m_inact=x(7);    % mol/dm3 concentration of inactive
                            mfp5-protein in outer membrane
CPmfp5_o_m_act = x(8);    % mol/dm3 concentration of active mfp5-
                            protein in outer membrane
cCsout = 55*10^-5;   % mol/dm3 concentration arabinose outside
                       based on ref

% Membrane parameters with use of bionumbers.org (see ref also)
x = 0.0225;     % (+/-) 20nm = 0.02 um thickness of total
membrane(outer+periplasm+inner)
R = 0.64;       % um radius of the obviously sphere-shaped cells,
normal 1.1 um^3, since spherical boll : 4/3*pi*r^3
xmo = 0.0080;   % um thickness of outer membrane varying from 8
to 15 um (see ref)
xmi = 0.004;    % um thickness of inner membrane (see ref)
xperi = 0.0105;% um thickness of periplasm, see ref

% Volume Calculations
Vcell = 4/3*pi*((R-x) *10^-5)^3;
% dm3 volume of the cell assume it's a sphere, only take into
account the cytoplasm
Vperi = 4/3*pi*((R-xmo)*10^-5)^3 - 4/3*pi*((R-x+xmi)*10^-5)^3;
% dm3 volume of periplasm
Vmembrane = 4/3*pi*(R*10^-5)^3 - 4/3*pi*((R-xmo)*10^-5)^3;
% Vmo = Vcell - 4*pi*((R-xmo)*10^-6)^3/3; % m3 volume of the
outer membrane (volume of the cell - volume cell w/o outer
membrane)

% Surface Calculations
Acell = 4*pi*(R*10^-5)^2;
% dm2 surface of the cell (outside the cell)
Amip = 4*pi*((R-x+xmi)*10^-5)^2;
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% dm2 sufrace of the inner side of periplasm membrane
Amop = 4*pi*((R-xmo)*10^-5)^2;
% dm2 surface of outer membrane on periplasm side.

% Diffusion
Da = 1*10^-12; % Diffusioncoefficient of arabinose. Obtained
from Alon (2009), 1000 um^2/s diffusion constant for arabinose
in membrane
Di = 1*10^-10; % Diffusioncoefficient of mfp5-protein from
cytoplasm to periplasm
Dout = 1*10^-10; % Diffusioncoefficient of mfp5-protein from
periplasm to outer membranemol/dt diffusion constant for Mp
through periplasm

% Flux Calculations(by use of Fick's law)
Ja = -Da * (Carab - cCsout)/(x*10^-5); % diffusion of arabinose
of entire membrane
Ji = -Di * ((CPmfp5_peri*Vperi - CPmfp5*Vcell)/Vperi)/(xmi*10^-
5); % diffusion of mfp5-protein from cytoplasm to periplasm
Jout = -Dout * ((CPmfp5_o_m_inact*Vmembrane -
CPmfp5_peri*Vperi)/Vmembrane)/(xmo*10^-5); % diffusion of mfp5-
protein from cytoplasm to periplasm

% AraC protein production
pAraC = 10 ; % average amount of copies of protein per strand of
mRNA before degradation
NrhcAraC = 25 ; % Number of copies of AraC gene present due to
high copy number plasmid
nPolyAraC = 1 ; % Number of active RNA-polymerases present on 1
gene of AraC
Rtrans = 80 ; % nt/s, Speed of RNA-polymerase
BetaMrnamaxAraC = Rtrans/756 * NrhcAraC * nPolyAraC * 10^-9;
% nmol/l/s, maximum production of AraC-mRNA
n = 1 ; % number of arabinose molecules required to activate
ThalfMAraC = 4 * 60 ; % s , halftime Arac-mRNA
ThalfPAraC = 2 * 60 ; % s , halftime Arac-protein
AlphaMAraC = log(2) / ThalfMAraC ; % 1/s , degradation rate
Arac-mRNA
AlphaPAraC = log(2) / ThalfPAraC ; % 1/s , degradation rate
Arac-protein
KAraC = cCsout/1000 ; % mol/l , activation coefficient K

% Formules
BetamRNAAraC = BetaMrnamaxAraC * Carab^n / (KAraC^n + Carab^n);
% mol/dm3/s , Hill equation, rate of change of Arac-mrna
% dCmRNAAraC = dBetamRNAAraC - AlphaMAraC * CmRNAAraC; %
mol/dm3/s , dx(2), rate of change of AraC-mRNA
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% dCPAraC = parac*BetamRNAAraC/AlphaMAraC - AlphaPAraC*CAraC; %
mol/dm3/s , dx(3), Production rate Arac-protein


% Mfp5 protein production
pmfp5 = 10 ; % average amount of copies of protein per strand of
mRNA before degradation
Nrhcmfp5 = 25; % Number of copies of mfp5 gene present due to
high copy number plasmid
nPolymfp5 = 1 ; % Number of active RNA-polymerases present on 1
gene of mfp5
Rtrans = 80 ; % nt/s, Speed of RNA-polymerase
BetaMrnamaxmfp5 = Rtrans/3400 * Nrhcmfp5 * nPolymfp5 * 10^-9; %
nmol/l/s, maximum production of mfp5-mRNA
n = 1 ; % number of AraC molecules required to activate
ThalfMmfp5 = 4 * 60 ; % s , halftime mfp5-mRNA
ThalfPmfp5 = 2 * 60 ; % s , halftime mfp5-protein
AlphaMmfp5 = log(2) / ThalfMmfp5 ; % 1/s , degradation rate
mfp5-mRNA
AlphaPmfp5 = log(2) / ThalfPmfp5 ; % 1/s , degradation rate
mfp5-protein
KMfp5 = cCsout/1000 ; % mol/l , activation coefficient K

% Formules
BetamRNAmfp5 = BetaMrnamaxmfp5 * CPAraC^n / (KMfp5^n +
CPAraC^n); % mol/l/s , rate of change of Arac-protein
% dCmRNAmfp5 = BetamRNAmfp5 - AlphaMmfp5 * CmRNAmfp5; % mol/l/s
, production rate of mfp5-mRNA
% dCPmfp5 = pmfp5*dBetamRNAmfp5/AlphaMmfp5 - AlphaPmfp5*Cmfp5; %
mol/l/s , Production rate of mfp5-protein

% rate of change
% mol/dm3/s increase of internal arabinose concentration per
time iteration
vCarab = Ja * Acell / Vcell;
% mol/dm3/s , rate of change of Arac-mrna
dCmRNAAraC = BetamRNAAraC - AlphaMAraC * CmRNAAraC;
% mol/dm3/s , Production rate Arac-protein
dCPAraC = pAraC*BetamRNAAraC/AlphaMAraC - AlphaPAraC*CPAraC;
% mol/l/s , production rate of mfp5-mRNA
dCmRNAmfp5 = BetamRNAmfp5 - AlphaMmfp5 * CmRNAmfp5;
% mol/l/s , production rate of mfp5-protein
dCPmfp5 = pmfp5*BetamRNAmfp5/AlphaMmfp5 - AlphaPmfp5*CPmfp5;
% mol/l/s , production rate of mfp5-protein in periplas,
dCPmfp5_peri= Ji * Amip / Vperi;
% diffusion rather than reaction
dCPmfp5_o_m_inact = Jout * Amop / Vmembrane;
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% mol/l/s , production rate of activated mfp5-proteins
dCPmfp5_o_m_act = Jout * Amop / Vmembrane ;


% Change
dx(1) = vCarab;           % Csi
dx(2) = dCmRNAAraC;       % dmRNA of AraC-mRNA
dx(3) = dCPAraC;          % dCPAraC of AraC-protein
dx(4) = dCmRNAmfp5;       % dmRNA of mfp5-mRNA
dx(5) = dCPmfp5;          % dCPmfp5 of mfp5-protein
dx(6) = dCPmfp5_peri;     % dCPmfp5_peri of mfp5 in periplasm
dx(7) = dCPmfp5_o_m_inact;     % dCPmfp5_o_m_inact of inactive
                                 protein in outer membrane
dx(8) = dCPmfp5_o_m_act;       % dCPmfp5_o_m
dx = dx';
end
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