Function Regulatory model

Tic %start of time calculation (how look took the ode solver to solve)
clear all
c1c
% 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_model dt, 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 on;box on;subplot( 3,3,2)
hold off
plot( t(:,1), x(:,2), 'LineWidth', 2 )title('CmRNAAraC');ylabel ('mol/dm3');xlabel('t');grid on;box on;
subplot( 3,3,3)
hold off
plot( t(:,1), x(:,3), 'LineWidth', 2 )title('CPAraC');ylabel ('mol/dm3');xlabel('t');grid on;box on;
subplot( 3,3,4)
hold off
plot( t(:,1), x(:,4), 'LineWidth', 2 )title('CmRNAmfp5');ylabel ('mol/dm3');xlabel('t');grid on;box on;
subplot( 3,3,5)
hold off
plot( t(:,1), x(:,5), 'LineWidth', 2 )title('CPmfp5');ylabel ('mol/dm3');xlabel('t');grid on;box on;
subplot( 3,3,6)
hold off
plot( t(:,1), x(:,6), 'LineWidth', 2 )title('CPmfp5_peri');ylabel ('mol/dm3');xlabel('t');grid on;box on;
subplot( 3,3,7)
hold off
plot( t(:,1), x(:,7), 'LineWidth', 2 )title( 'CPmfp5_o_m_inact' );ylabel( 'mol/dm3' );xlabel( 't' );grid on box on subplot( 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(outter+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;
% dm^2 surface of the inner side of periplasm membrane
Amop = 4*pi*((R-xmo)*10^-5)^2;
% dm^2 surface of outer membrane on periplasm side.

% Diffusion
Da = 1*10^-12; % Diffusion coefficient of arabinose. Obtained from Alon (2009), 1000 um^2/s diffusion constant for arabinose in membrane
Di = 1*10^-10; % Diffusion coefficient of mfp5-protein from cytoplasm to periplasm
Dout = 1*10^-10; % Diffusion coefficient of mfp5-protein from periplasm to outer membrane
mol/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/dm^3/s, Hill equation, rate of change of Arac-mrna
% dCmRNAAraC = dBetamRNAAraC - AlphaMAraC * CmRNAAraC; % mol/dm^3/s, dx(2), rate of change of AraC-mRNA
% dCPAraC = parac*BetamRNAAraC/AlphaMAraC - AlphaPAr%CaraC; %
\text{mol/dm}^3/\text{s}, \text{dx(3)}, \text{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; %
\text{nmol/l/s}, \text{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; % \text{mol/l}, activation coefficient K

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

% rate of change
% \text{mol/dm}^3/\text{s} increase of internal arabinose concentration per
\text{time iteration}
vCarab = Ja * Acell / Vcell;
% \text{mol/dm}^3/s, rate of change of Arac-mrna
dCmRNAAraC = BetamRNAAraC - AlphaMAraC * CmRNAAraC;
% \text{mol/dm}^3/s, Production rate Arac-protein
dCPAraC = pAraC*BetamRNAAraC/AlphaMAraC - AlphaPAr%CaraC;
% \text{mol/l/s}, production rate of mfp5-mRNA
dCmRNAmfp5 = BetamRNAmfp5 - AlphaMmfp5 * CmRNAmfp5;
% \text{mol/l/s}, production rate of mfp5-protein
dCPmfp5 = pmfp5*BetamRNAmfp5/AlphaMmfp5 - AlphaPmfp5*Cpmfp5;
% \text{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;
% mol/l/s, production rate of activated mfp5-proteins
\[ dCPmfp5\_o\_m\_act = Jout \times Amop / V_{membrane}; \]

% Change
\[ \text{dx}(1) = v_{Carab}; \quad \text{dx}(2) = dC_{mRNAAraC}; \quad \text{dx}(3) = dCP_{AraC}; \quad \text{dx}(4) = dC_{mRNAmfp5}; \quad \text{dx}(5) = dCP_{mfp5}; \quad \text{dx}(6) = dCPmfp5\_peri; \quad \text{dx}(7) = dCPmfp5\_o\_m\_inact; \quad \text{dx}(8) = dCPmfp5\_o\_m\_act; \]
\[ \text{dx} = \text{dx}'; \]
\text{end}