Oligosaccharide Production

Some enzyme catalyzed reactions are very complex. For this reason their rigorous modeling leads to complex kinetic equations with a large number of constants.

Such models are unwieldy and are usually not suitable for practical purposes. One approach to simplify them is to neglect formation of enzyme substrate complexes altogether and to deal only with overall reactions of the react ants to products.

An example of such a reaction is the enzymatic lactose hydrolysis, a complex process involving a multitude of sequential reactions leading to higher saccharide (oligosaccharides) intermediates. The mechanistic model is rather complex even when only trisaccharides are considered (Eq. 1a-c).

Oligosaccharide Production: System

$$La + E \rightleftharpoons La\,E \longrightarrow Ga + Gl + E \qquad (1.a)$$

$$Ga\,E + La \rightleftharpoons E + Tr \qquad (1.b)$$

$$Ga\,E + H_2O \longrightarrow E + Ga \qquad (1.c)$$

Neglecting the enzyme complexes, however, gives a simplified model (Eq. 2a-b) requiring only three constants:

$$La \xrightarrow{K_I} Ga + Gl \qquad (2.a)$$

$$La + Ga \underset{K_2}{\overset{K_1}{\rightleftharpoons}} Tr \qquad (2.b)$$

Oligosaccharide Production: Mass Balance

The simplified batch reactor model from Eq.2 is equivalent to the Michaelis-Menten product inhibition model:

Lactose
$$\frac{dLa}{dt} = -K_I \cdot La - K_1 \cdot La \cdot G + K_2 \cdot Tr \tag{3}$$

Galactose
$$\frac{dGa}{dt} = K_I \cdot La - K_1 \cdot La \cdot G + K_2 \cdot Tr \tag{4}$$

Trisaccaride
$$\frac{dTr}{dt} = K_1 \cdot La \cdot G - K_2 \cdot Tr \tag{5}$$

with initial conditions: $La_0 = 150\ mmol/m^3$ $\quad Ga_0 = 0$ $\quad Tr_0 = 0$

Range of kinetic constants:

$K_I = 0.02 - 0.06\ \min^{-1}$

$K_1 = 0.02 - 0.1\ L/mmol \cdot \min$ $\quad K_2 = 1 - 50\ \min^{-1}$

Oligosaccharide Production: Program

As first step in solving the problem with MATLAB is to write the function file. This file will be saved in the folder bin and the name of the file will later be required for processing in the Command Window of MATLAB

```
function dy = oligo_func(t,y,KI,K1,K2)
dy = zeros(4,1);          % Column vector
% LA = y(1);                % Lactose Concentration
% GA = y(2);                % Galactose Concentration
% TR = y(3);                % Trisacharid Concnetration
% GL = y(4);                % Glucose Concnetration

dy(1)  = -KI*y(1) - K1*y(1)*y(2) + K2*y(3);
dy(2)  = -K1*y(1)*y(2) + KI*y(1) + K2*y(3);
dy(3)  = -K2*y(3) + K1*y(1)*y(2);
dy(4)  = KI*y(1);
```

Oligosaccharide Production: Program

In this section the ODEs with initial condition values are solved and plotted in diagram.

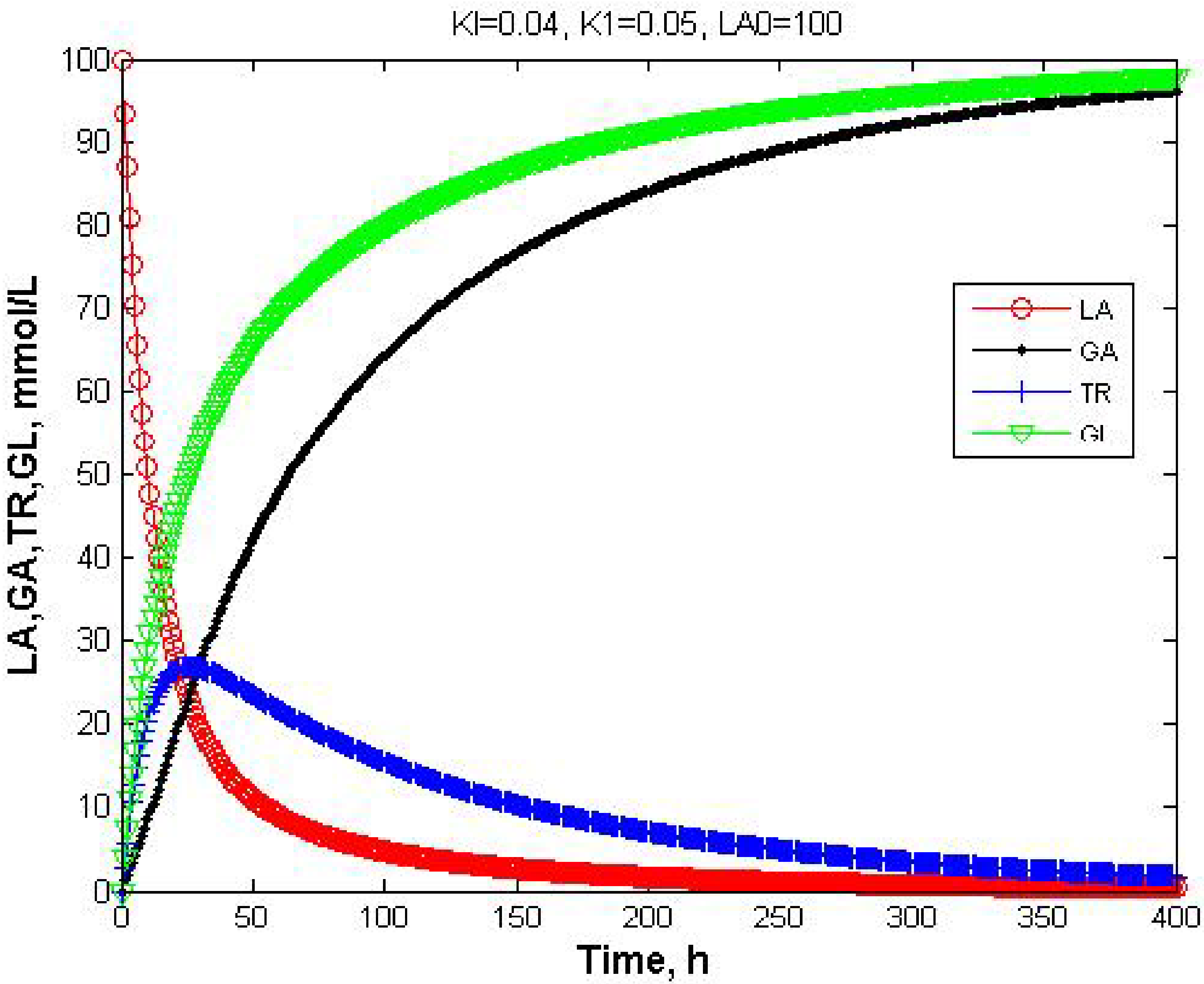
```
KI = 0.04;  K1 = 0.05;  K2 = 1;          % Reaction Rate Constants
Tint = 1;  Tfin = 400;                   % Initial and Final Temperature
LA0 = 100;                               % Initial Lactose Concentration
GA0 = 0;                                 % Initial Galactose Concentration
TR0 = 0;                                 % Initial Trisaccharid Concentration
GL0 = 0;                                 % Initial Glucose Concentration
Cinit = [LA0 GA0 TR0 GL0];               % Initial concentration
Tspan = linspace(0,Tfin,Tfin/Tint);      % Time span
[T C] = ode45(@(t,y) oligo_func(t,y,KI,K1,K2),Tspan,Cinit); % Solve ODE
plot(T,C(:,1),'-ro',T,C(:,2),'-k.',T,C(:,3),'-b+',T,C(:,4),'-gv')
title('KI=0.04, K1=0.05, LA0=100')
% C(:,1):LA
% C(:,2):GA
% C(:,3):TR
% C(:,4):GL
h = legend('LA','GA','TR','GL',0);
set(h,'fontsize',8);
xlabel('Time, h','fontsize',12,'fontweight','b');
ylabel('LA,GA,TR,GL, mmol/L','fontsize',12,'fontweight','b');
```

Oligosaccharide Production: Nomenclature

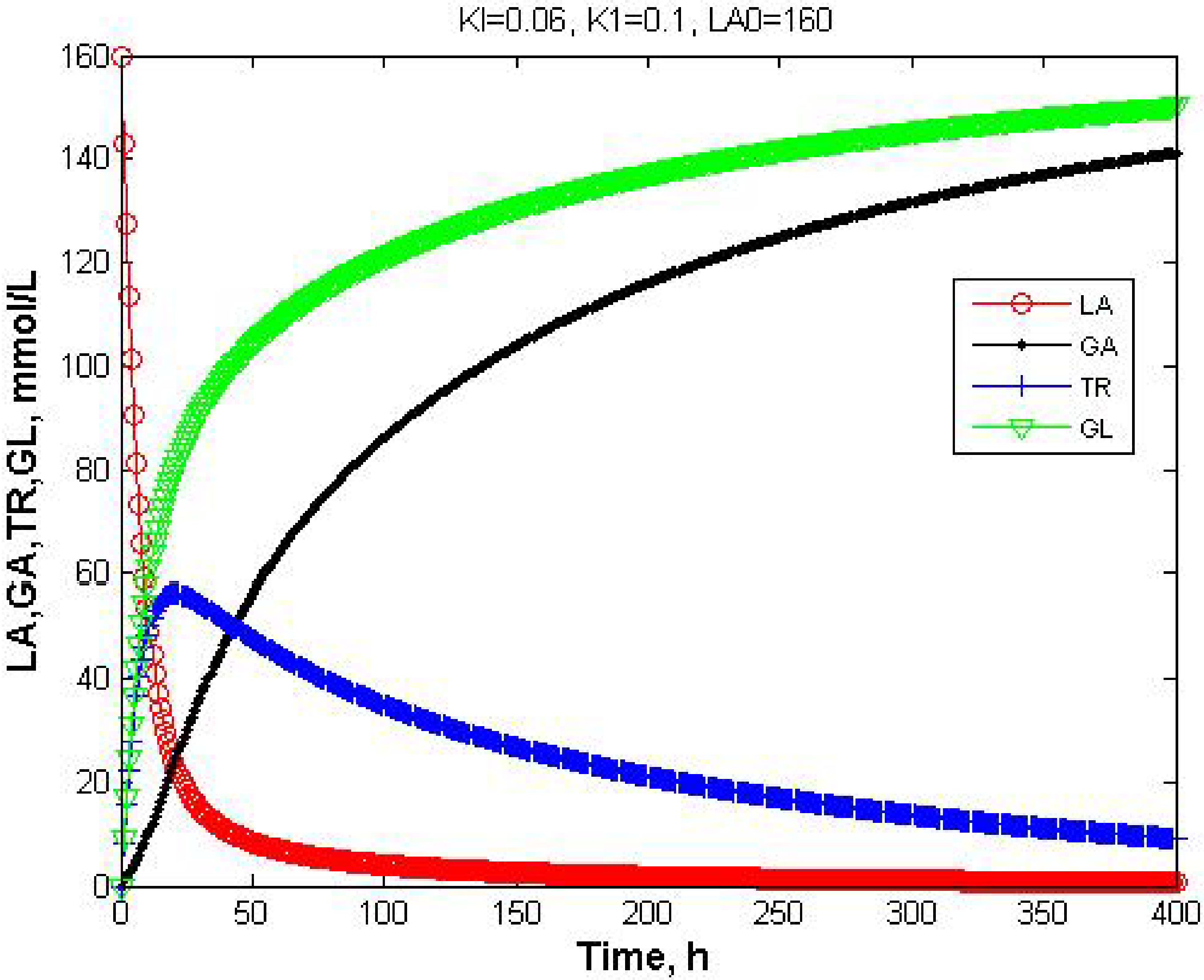
Symbol	Description	Unit
Ga	Galactose concentration	mmol/L
Gl	Glucose concentration	mmol/L
K_l	Reaction rate constant La → Ga + Gl	1/min
K_1	Reaction rate constant La + Ga → Tr	L/(mmol min)
K_2	Reaction rate constant Tr → La + Ga	1/min
La	Lactose concentration	mmol/L
Tr	Trisaccharide concentration	mmol/L

Index	Description
0	Refers to initial concentration

Oligosaccharide Production: Results



Oligosaccharide Production: Results



Oligosaccharide Production: Results