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APPENDIX A

History of Beer

Beer is a one of oldest beverage in the world. The art of brewing is old as civilization. Between 10,000 and 15,000 years ago, some humans discontinued their nomadic hunting and gathering and settled down to farm. Grain was the first domesticated crop that started that farming process and the first raw material for the beer. Historians have traced the roots of brewing back to ancient African, Egyptian and Sumerian tribes, some 6,000 years ago. Written on clay tablets of ancient Mesopotamia, the making and drinking of beer are described in detail, sometimes listing a selection of different types (2)

There are some evidence has been found that the beer has been used in ancient Iraq (1). The Babylonians were used to export beer as far away as Egypt. When it was coming to Egypt, they have used beer not only as a drink but also as a medicine and prescribed for many illnesses. At this time, the raw material of beer was turning to Barley.

As the cultivation of barley spread north and west, brewing went with it. As time passed, the production of beer came under the watchful eye of the Roman Church. Christian abbeys, as centers of agriculture, knowledge and science, refined the methods of brewing. Initially in the making of beer for the brothers and for visiting pilgrims, later as a means of financing their communities. However, there was still very little known about the role of yeast in completing fermentation. Beer brewing played an important role in daily lives. Beer was clearly so desired that it led nomadic groups into village life. Beer was considered a valuable (potable) foodstuff and workers were often paid with jugs of beer (2).

The use of hops in beer was written in 822 by a “Carolingian Abbot”. Again in 1067 by “Abbess Hildegardof Bingen” has written about it. Flavoring beer with hops was known at least since the 9th century, but was only gradually adopted because of difficulties in establishing the right proportions of ingredients (1).

In 15th century England, an unhopped beer would have been known as ale, while the use of hops would make it a beer. Hopped beer was imported to England from the Netherlands as early as 1400 in Winchester, and hops were being planted on the island by 1428 (1).

It seems that different culture has used different kind of raw material for making beer (3)

a) Africa used millet, maize and cassava.

b) North America used persimmon although agave was used in Mexico.

c) South America used corn although sweet potatoes were used in Brazil.

d) Japan used rice to make *sake*.

e) China used wheat to make *samshu*.

f) Other Asian cultures used sorghum.

g) Russians used rye to make *quass* or *kvass*.

h) Egyptians used barley and may have cultivated it strictly for brewing as it made poor bread.

In 1420 Germen brewers developed lager method of brewing. While the England prefers top fermented Ale, in Germany bottom fermented Lager was the favorite. The production of lager, which requires a longer and colder fermentation process than ale, was well suited to Germany where the beer could be stored, even through the summer months, in ice-cold caves in the Alps.

In 1612 the first commercial brewery opened in New Amsterdam (NYC, Manhattan) after colonists advertised in London newspapers for experienced brewers. 1842 The first clear, golden-hued lager is produced in the town of Pilsen in Bohemia. 1850s, the modern era of brewing in the U.S. begins to take shape as German immigrants bring a love of lager and the technological expertise to make it to their new land. By the late 1800s, aided by the development of commercial refrigeration, automatic bottling and pasteurization, different kind of brands were come up.

In 1935 The American Can Company and “Kreuger Brewing” introduce the aluminum beer can for storing beer.

Today, the brewing industry is a huge global business, consisting of several multinational companies, and many thousands of smaller producers ranging from brewpubs to regional breweries. Advances in refrigeration, international and transcontinental shipping, marketing and commerce have resulted in an international marketplace, where the consumer has literally hundreds of choices between various styles of local, regional, national and foreign beers. More than 133 billion liters (35 billion gallons) are sold per year, producing total global revenues of $294.5 billion (£147.7 billion) in 2006 (1).

Beer history in Sri Lanka

Ceylon brewery (Lion) is the first brewery in Sri Lanka. It has established in Nuwara Eliya which is in up country side. The reason for the selection was cool climate and pure and clean water sources. The Ceylon brewery has established in 1881. Carlsberg acquires shareholding in Ceylon Brewery in 1996. The Ceylon brewery makes Lion Lager, Strong Beer and Carlsberg as brand.

APPENDIX B

MATLAB Code

parameters.m

```
%parameters

YXG=0.134;
YXM=0.268;
YXN=0.402;

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%temperature dependant parameters

miuG0=exp(35.77);
miuM0=exp(16.40);
miuN0=exp(10.59);

EmiuG=22.6e3;
EmiuM=11.3e3;
EmiuN=7.16e3;
%
KG0=exp(-121.3);
KM0=exp(-19.5);
KN0=exp(-26.78);

EKG=-68.6e3;
EKM=-14.4e3;
EKN=-19.9e3;
%
KdashG0=exp(23.33);
KdashM0=exp(55.61);

EKdashG=10.2e3;
EKdashM=26.3e3;

%
R=1.987; %cal/mol K
rho=1040; %kg/m3
Cp=4.016; %kJ/kg C
%

%
deltaHFG=-91.2;
deltaHFM=-226.3;
deltaHFN=-361.3;


%
```

```
%Ethanol parameters
%
YEG=1.92;
YEM=3.84;
YEN=5.76;
Kx = 365000;
X0=125;
%
%Nutrient parameters
YLX=0.0832;
YIX=0.0363;
YVX=0.0273;
KI=0.365;

KL0=exp(10.14);
KV0=exp(328);

EKL=5.95e3;
EKV=211.9e3;

toud=23.54;
R=1.987;
%Flavour parameters%%%%%%%%%%%%%

%Fusel alcohols

YIB=0.203;
YIA=0.557;
YMB=0.472;
YPE=0.235;

%Esters

YEA=0.000992;
YEC=0.000118;
YIAc=0.0269;

%Vicinal deketones

YVDK=0.000105;
KVDK0=exp(86.8);
EVDK=54.3e3;

%Acetaldehyde

YAAL=0.01;
KAAL0=exp(10.4);
EAAL=11.1e3;
```

beer.m

```
%Author Name :- Dilantha Warnasooriya
%programme   :- Beer model (growth, nutrient & flavour model)

%Test programme
%Function beer

function dxdt = beer(t,x,u)

%Naming status

%Growth model

G = x(1); %Glucose
M = x(2); %Maltose
N = x(3); %Maltotriose
X = x(4); %Biomass
E = x(5); %Ethanol
T = x(6); %Temperature

%--------------------------------------------------------------------

%Nutrient model

L = x(7); %Leucine
I = x(8); %Isoleucine
V = x(9); %Valine

%--------------------------------------------------------------------

%Flavor model%%%%%%%%%%%%%%%%%%%%%%%%%

%Fusel alcohols

IB = x(10); %Isobutyl alcohol
IA = x(11); %Isoamyl alcohol
MB = x(12); %2-methyl-1-butanol
P = x(13); %Propanol

%Esters

EA = x(14); %Ethyl acetate
EC = x(15); %Ethyl caproate
IAc = x(16); %Isoamyl acetate

%Vicinal diketones & Acetaldehyde

VDK = x(17); %Vicinal diketones
AAL = x(18); %Acetaldehyde

%-------------------------------------------------------------------
```

```
%Initial Inputs

parameters3;

%-------------------------------------------------------------------


%Growth Model

%Temperature dependency
%
miuG=miuG0*exp(-EmiuG/(R*(T+273.15)));
miuM=miuM0*exp(-EmiuM/(R*(T+273.15)));
miuN=miuN0*exp(-EmiuN/(R*(T+273.15)));

KG=KG0*exp(-EKG/(R*(T+273.15)));
KM=KM0*exp(-EKM/(R*(T+273.15)));
KN=KN0*exp(-EKN/(R*(T+273.15)));

KdashG=KdashG0*exp(-EKdashG/(R*(T+273.15)));
KdashM=KdashM0*exp(-EKdashM/(R*(T+273.15)));

%

miu1=miuG*G/(KG+G);
miu2=(miuM*M/(KM+M))*(KdashG/(KdashG+G));
miu3=(miuN*N/(KN+N))*(KdashG/(KdashG+G))*(KdashM/(KdashM+M));
miuX=(YXG*miu1+YXM*miu2+YXN*miu3)*Kx/(Kx+(X-X0)^2);

%

%Differential equations

dGdt = -miu1*X;
dMdt = -miu2*X;
dNdt = -miu3*X;
dXdt = miuX*X;
dEdt = (YEG*miu1+YEM*miu2+YEN*miu3)*X;

%temperature

dTdt=(1/(rho*Cp))*(-X*(deltaHFG*miu1+deltaHFM*miu2+deltaHFN*miu3));


%-------------------------------------------------------------------

%Nutrient model

D = 1-exp(-t/toud); %time delay

KL=KL0*exp(-EKL/(R*(T+273.15)));
KV=KV0*exp(-EKV/(R*(T+273.15)));

%Differential equations
```

```
dLdt = -YLX*dXdt*(L/(KL+L))*D;
dIdt = -YIX*dXdt*(I/(KI+I))*D;
dVdt = -YVX*dXdt*(V/(KV+V))*D;

%-------------------------------------------------------------------

%Flavor model

%Fusel alcohol%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

miuL = -(1/X)*dLdt;
miuI = -(1/X)*dIdt;
miuV = -(1/X)*dVdt;

%Differential equations

dIBdt = YIB*miuV*X;
dIAdt = YIA*miuL*X;
dMBdt = YMB*miuI*X;
dPdt = YPE*(miuV+miuI)*X;

%Esters%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

miuIA = (1/X)*dIAdt; %Assamption

%Differential equations

dEAdt = YEA*(miu1+miu2+miu3)*X;
dECdt = YEC*miuX*X;
dIAcdt = YIAc*miuIA*X;

%Vicinal diketones & Acetaldehyde Model%%%%%%%%%%%%%%%%%%%%

%Temperature dependency

KVDK=KVDK0*exp(-EVDK/(R*(T+273.15)));
KAAL=KAAL0*exp(-EAAL/(R*(T+273.15)));


%Differential equation

dVDKdt = YVDK*miuX*X - KVDK*VDK*X;
dAALdt = YAAL*(miu1+miu2+miu3)*X - KAAL*AAL*X;

%-------------------------------------------------------------------

%returen argument

dxdt=[dGdt;dMdt;dNdt;dXdt;dEdt;dTdt;dLdt;dIdt;dVdt;dIBdt;dIAdt;dMBdt
;dPdt;dEAdt;dECdt;dIAcdt;dVDKdt;dAALdt];
```

beersct.m

```
%Script for beer

tspan=[0 200];

%Initial concentrations

%u=[G;M;N;X;E;T;L;I;V;IB;IA;MB;P;EA;EC;IAC;VDK;AAL]

u=[70;220;40;125;0;10;1.3;0.6;2.1;0;0;0;0;0;0;0;0;0];

[t,x]=ode15s(@beer,tspan,u);

%Growth Model

figure('Name','Growth Model','NumberTitle','off')

subplot(321);
plot(t,x(:,1));
title('Glucose concentration [mol/m3]');
xlabel('Time (hours)');
ylabel('G (mol/m3)');
grid on
%
subplot(322);
plot(t,x(:,2));
title('Maltose concentration [mol/m3]');
xlabel('Time (hours)');
ylabel('M (mol/m3)');
grid on
%
subplot(323);
plot(t,x(:,3));
title('Moltotriose concentration [mol/m3]');
xlabel('Time (hours)');
ylabel('N (mol/m3)');
grid on
%
subplot(324);
plot(t,x(:,4));
title('Biomass concentration [mol/m3]');
xlabel('Time (hours)');
ylabel('X (mol/m3)');
grid on
%
subplot(325);
plot(t,x(:,5));
title('Ethanol Concentration [mol/m3]');
xlabel('Time (hours)');
ylabel('E (mol/m3)');
grid on
%
subplot(326);
plot(t,x(:,6));
title('Temperature [C]');
```

```
xlabel('Time (hours)');
ylabel('T (C)');
grid on
%
%Nutrient model

figure('Name','Nutrient Model','NumberTitle','off')

subplot(221);
plot(t,x(:,7));
title('Leucine concentration [mol/m3]');
xlabel('Time (hours)');
ylabel('L (mol/m3)');
grid on
%
subplot(222);
plot(t,x(:,8));
title('Isoleucine concentration [mol/m3]');
xlabel('Time (hours)');
ylabel('I (mol/m3)');
grid on
%
subplot(223);
plot(t,x(:,9));
title('Valine concentration [mol/m3]');
xlabel('Time (hours)');
ylabel('V (mol/m3)');
grid on

%Fusel alcohol formation

figure('Name','Fusel Alcohol Formation Model','NumberTitle','off')

subplot(221);
plot(t,x(:,10));
title('Isobutyl Alcohol concentration [mol/m3]');
xlabel('Time (hours)');
ylabel('IB (mol/m3)');
grid on
%
subplot(222);
plot(t,x(:,11));
title('Isoamyl Alcohol concentration [mol/m3]');
xlabel('Time (hours)');
ylabel('IA (mol/m3)');
grid on
%
subplot(223);
plot(t,x(:,12));
title('2-Methyl-1-Butanal concentration [mol/m3]');
xlabel('Time (hours)');
ylabel('MB (mol/m3)');
grid on
%
subplot(224);
plot(t,x(:,13));
title('Propanol concentration [mol/m3]');
```

```
xlabel('Time (hours)');
ylabel('P (mol/m3)');
grid on

%Esters formation

figure('Name','Esters Formation Model','NumberTitle','off')

subplot(221);
plot(t,x(:,14));
title('Ethyl acitate concentration [mol/m3]');
xlabel('Time (hours)');
ylabel('EA (mol/m3)');
grid on
%
subplot(222);
plot(t,x(:,15));
title('Ethyl caproate concentration [mol/m3]');
xlabel('Time (hours)');
ylabel('EC (mol/m3)');
grid on
%
subplot(223);
plot(t,x(:,16));
title('Isoamyl acetate concentration [mol/m3]');
xlabel('Time (hours)');
ylabel('IAc (mol/m3)');
grid on

%Vicinal diketones & Acetaldehyde formation

figure('Name','Vicinal diketones & Acetaldehyde Formation
Model','NumberTitle','off')

subplot(211);
plot(t,x(:,17));
title('Vicinal diketones concentration [mol/m3]');
xlabel('Time (hours)');
ylabel('VDK (mol/m3)');
grid on
%
subplot(212);
plot(t,x(:,18));
title('Acetaldehyde concentration [mol/m3]');
xlabel('Time (hours)');
ylabel('AAL (mol/m3)');
grid on

figure ('Name','Temperature profile')

plot(t,x(:,6));
title('Industrial Temperature Profile 1 ');
xlabel('Time (hours)');
ylabel('Temperature (C)');
grid on
```

APPENDIX C

Developing Dynamic Model on MATLAB Simulink

1. Growth Model

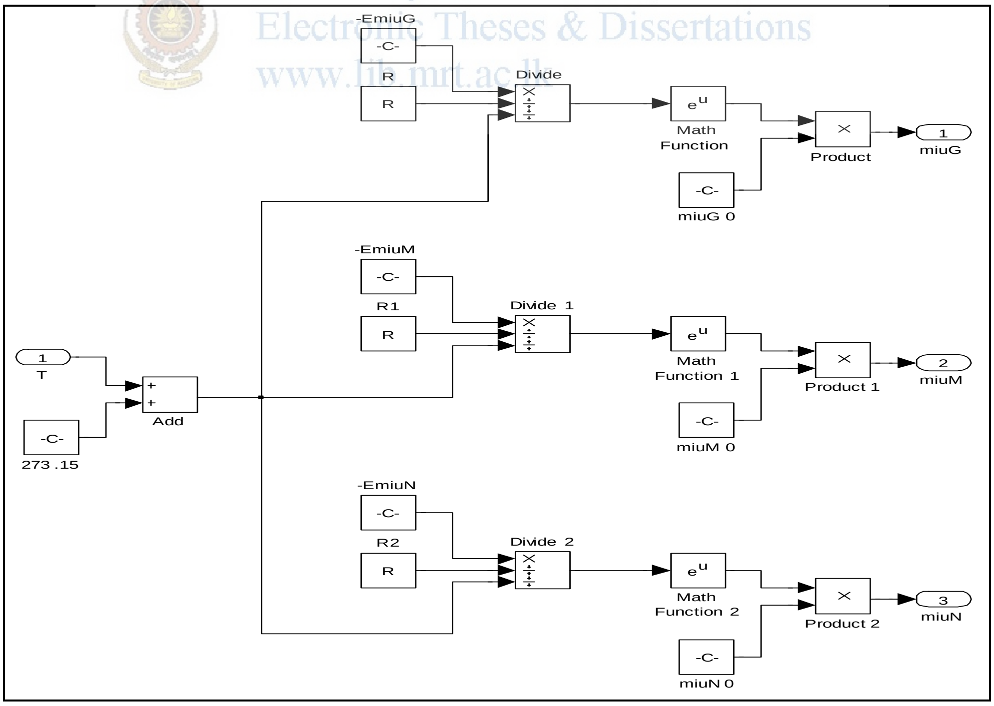
Temperature Driven System

$$\mu_i = \mu_{i0} exp\left(-\frac{E_{\mu i}}{RT}\right), \quad i = G, M, N \qquad (1)$$

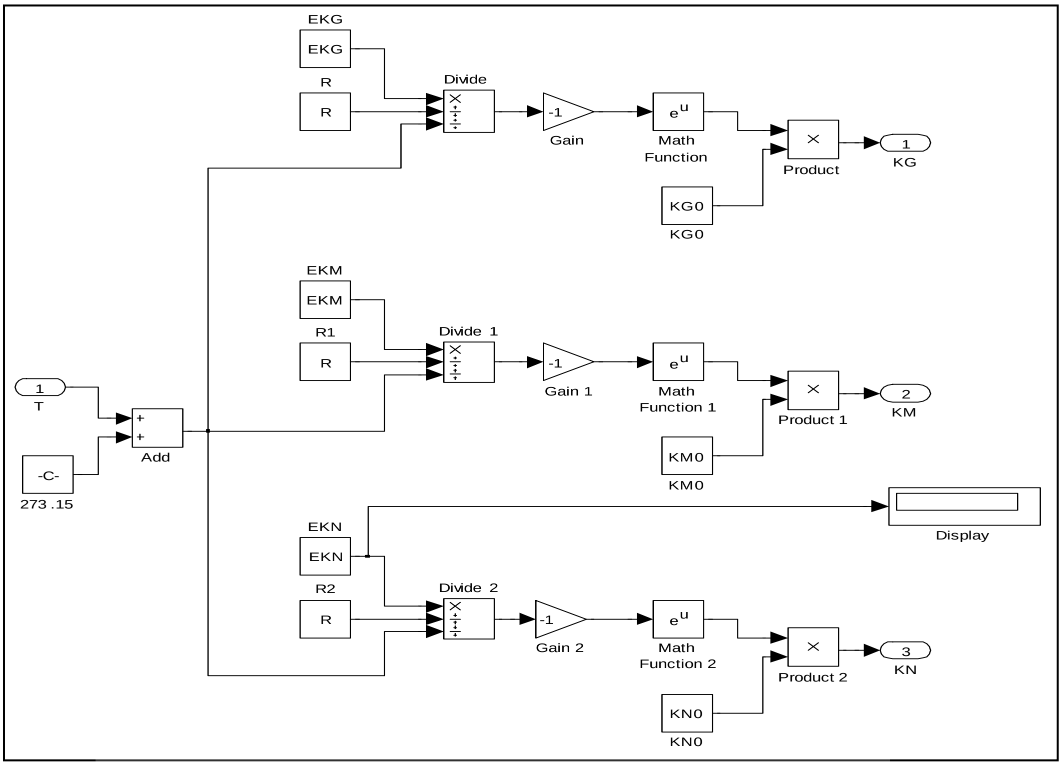
$$K_i = K_{i0} exp\left(-\frac{E_{Ki}}{RT}\right), \quad i = G, M, N \qquad (2)$$

$$K'_i = K'_{i0} exp\left(-\frac{E'_{Ki}}{RT}\right), \quad i = G, M \qquad (3)$$

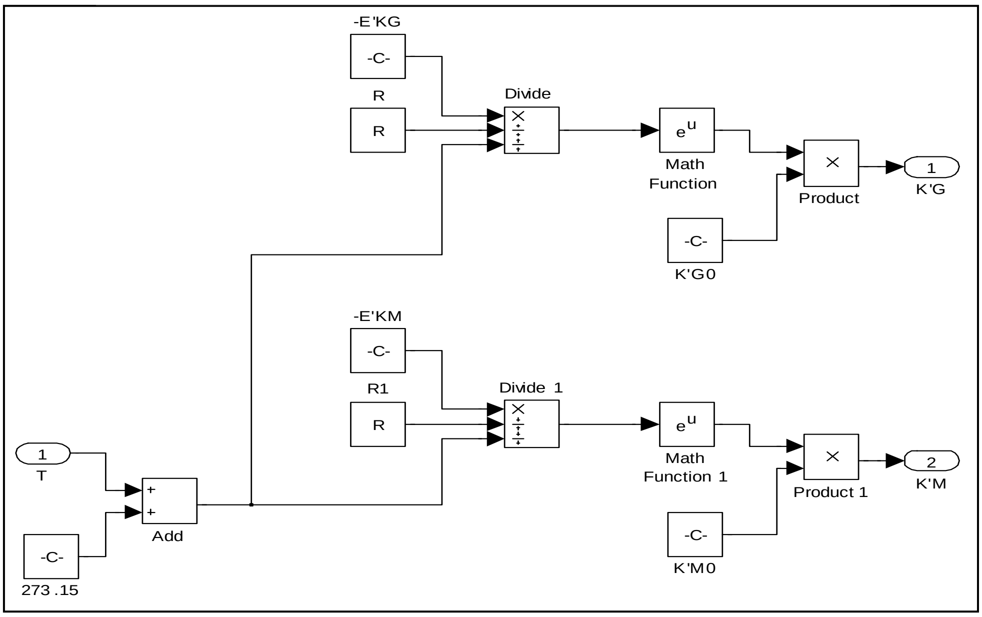
Simulink Model – Equation (1)



Equation (2)



Equation (3)

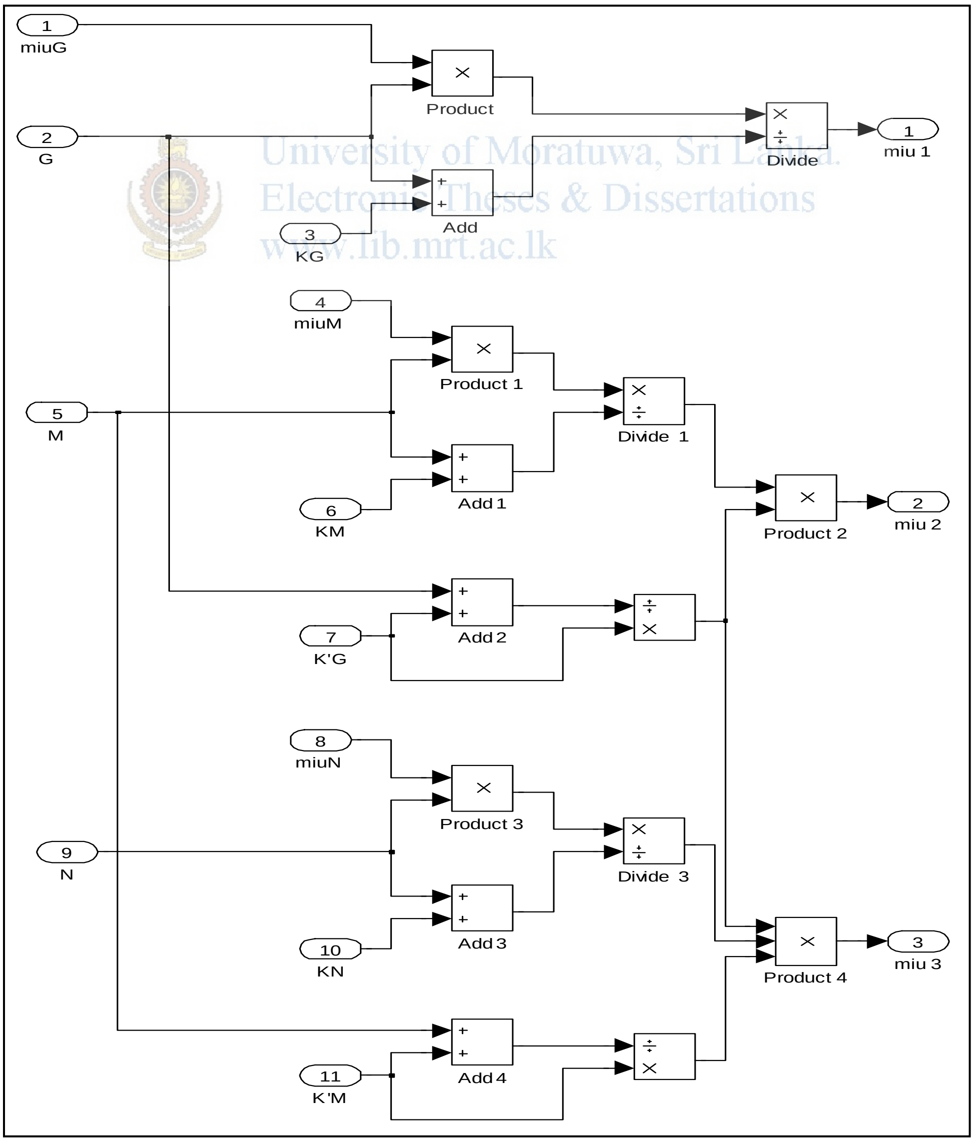


Modeling Specific Growth Rates

$$\mu_1 = \frac{\mu_G G}{K_G + G} \tag{4}$$

$$\mu_2 = \frac{\mu_M M}{K_M + M} \frac{K'_G}{K'_G + G} \tag{5}$$

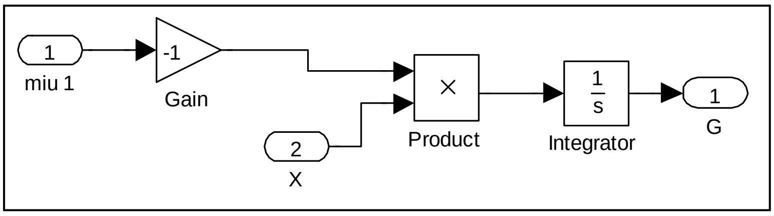
$$\mu_3 = \frac{\mu_N N}{K_N + N} \frac{K'_G}{K'_G + G} \frac{K'_M}{K'_M + M} \tag{6}$$



Sugar Consumption Model

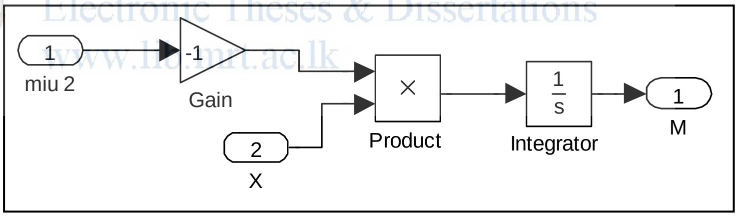
- Glucose

$$\frac{dG}{dt} = -\mu_1 X$$



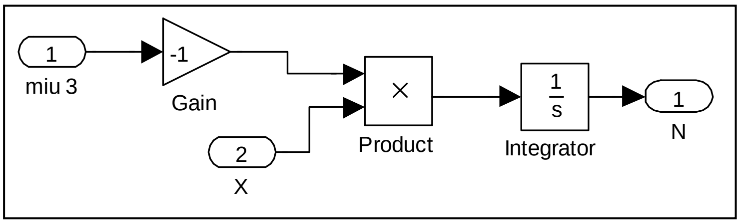
- Maltose

$$\frac{dM}{dt} = -\mu_2 X$$



- Maltotriose

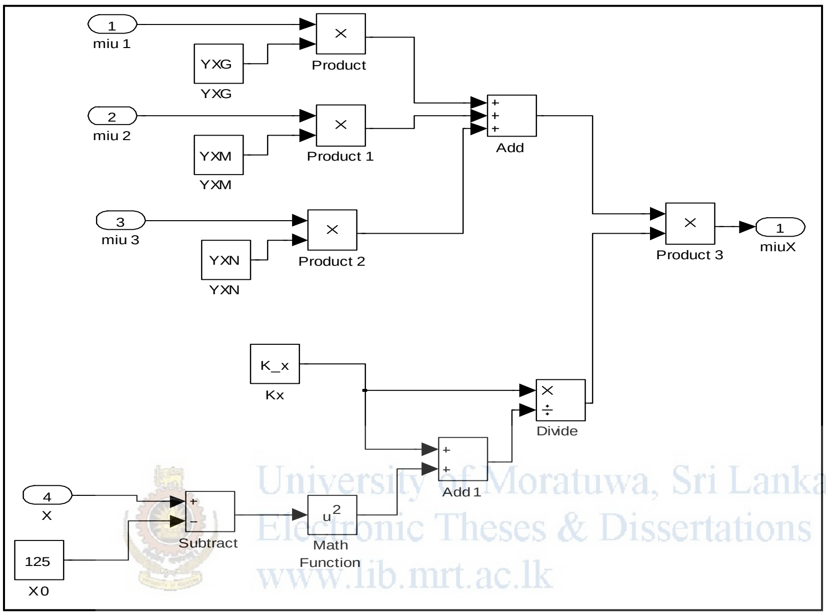
$$\frac{dN}{dt} = -\mu_3 X$$

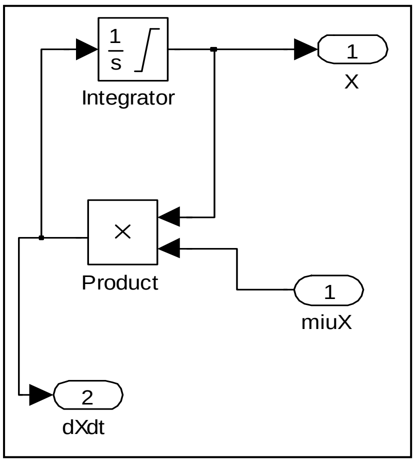


Biomass Growth Rate

$$\mu_X = (Y_{XG}\mu_1 + Y_{XM}\mu_2 + Y_{XN}\mu_3)\frac{K_X}{K_X + (X - X_0)^2}$$

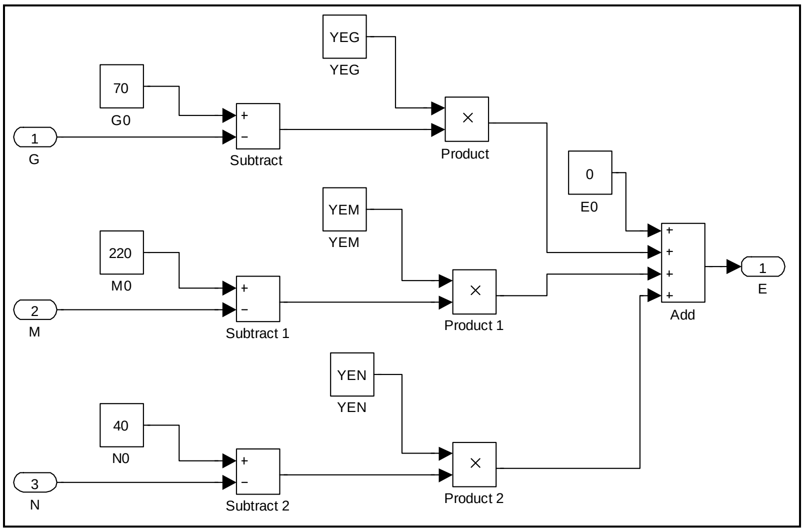
$$\frac{dX}{dt} = \mu_X X$$





Ethanol Production

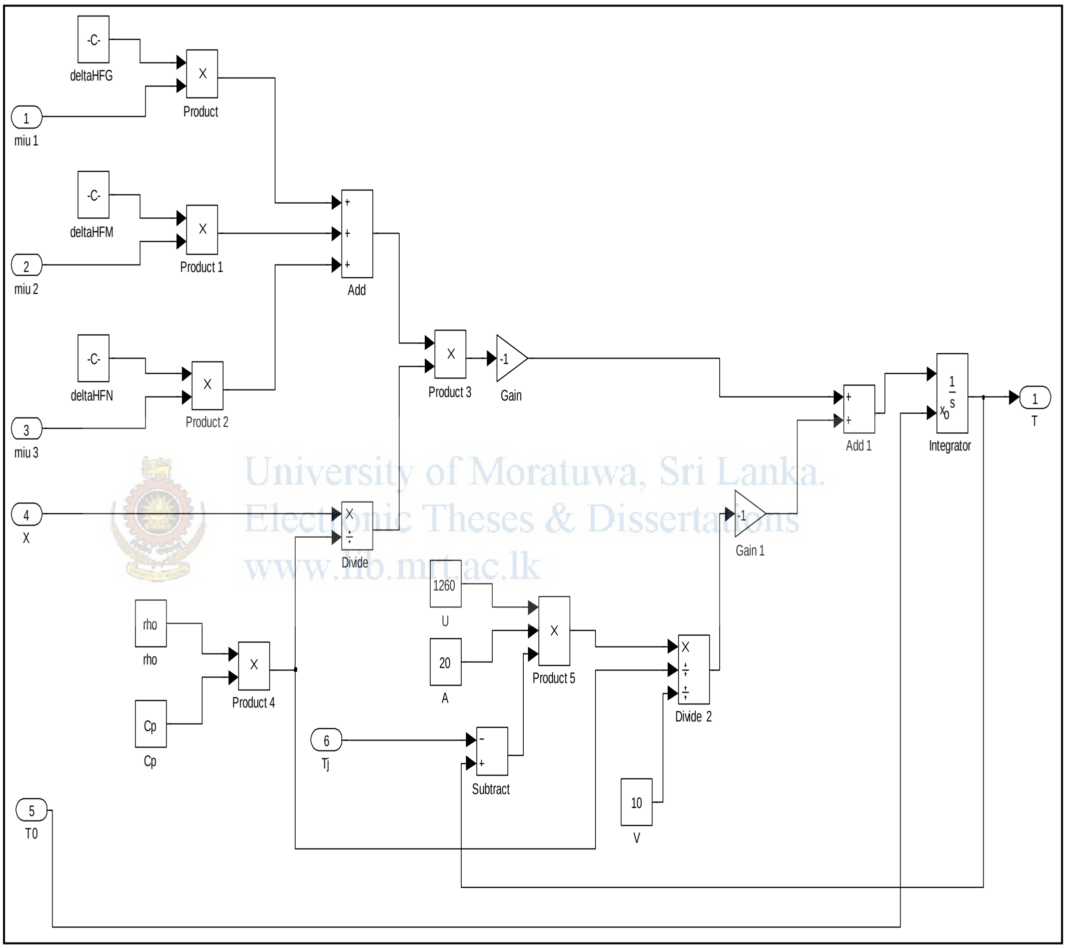
$$E = E_0 + Y_{EG}(G_0 - G) + Y_{EM}(M_0 - M) + Y_{EN}(E_0 - E)$$



Temperature Model

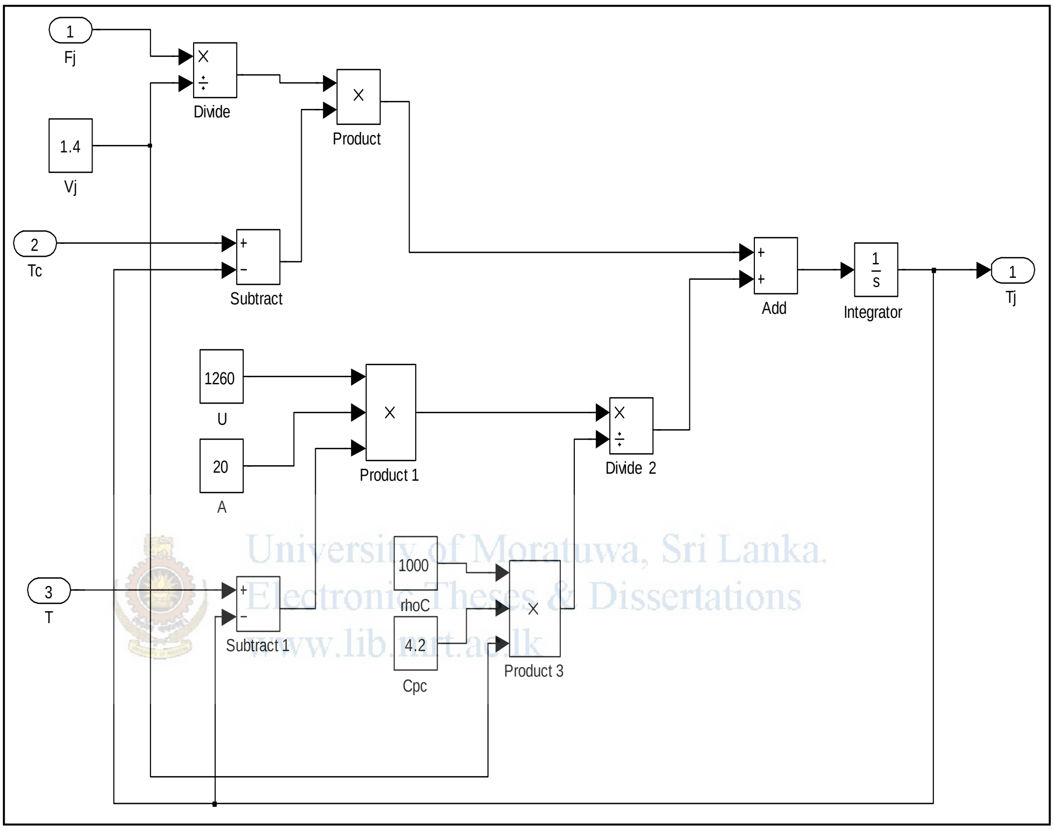
For the reactor

$$\frac{dT}{dt} = -\frac{X}{\rho Cp}(\Delta H_1\mu_1 + \Delta H_2\mu_2 + \Delta H_3\mu_3) - \frac{UA(T-T_J)}{\rho CpV}$$

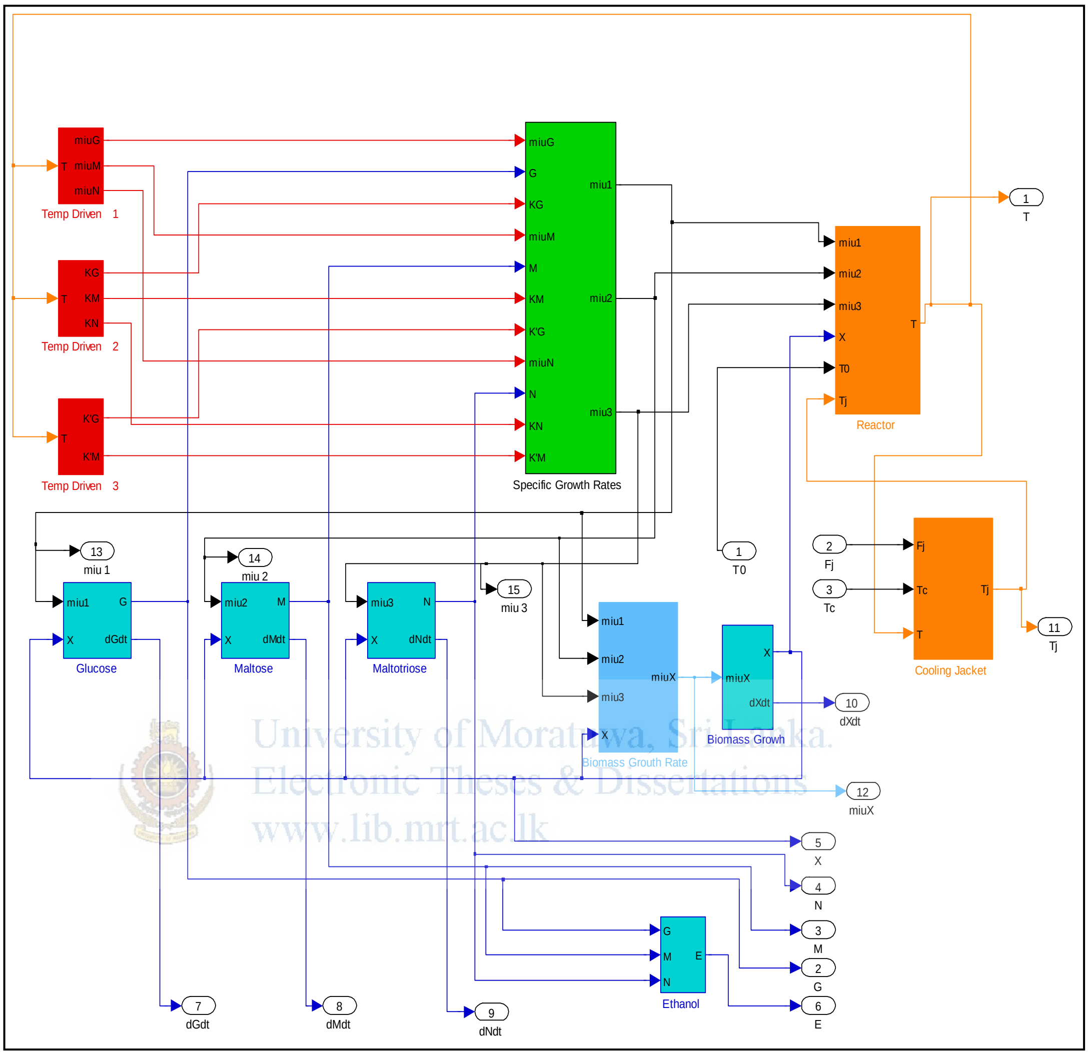


For the Cooling jacket

$$\frac{dT_J}{dt} = \frac{F_C}{V_J}(T_C - T_J) + \frac{UA(T-T_J)}{\rho_C Cp_C V_J}$$



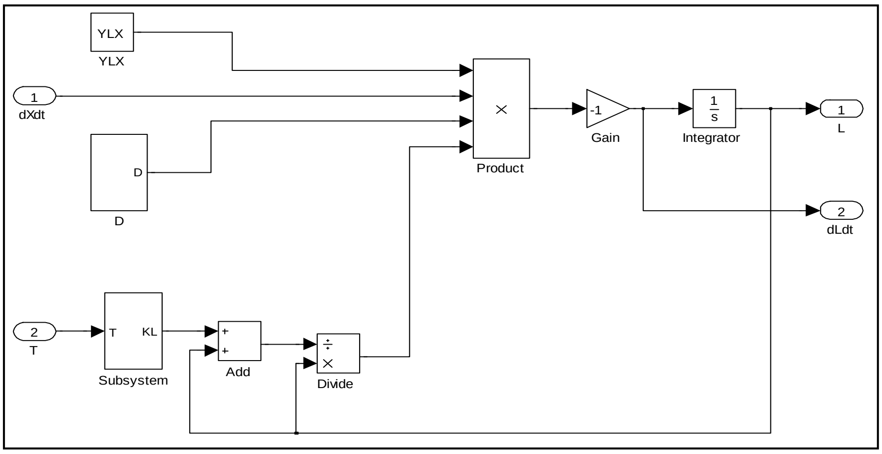
The Complete Growth System



Nutrient Model

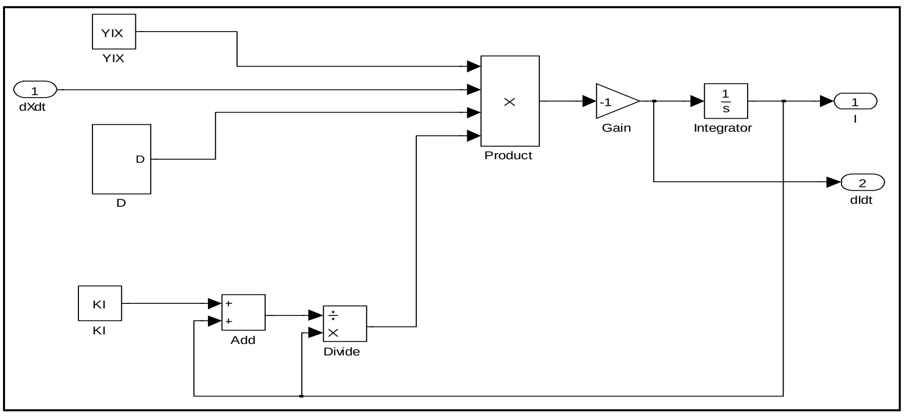
4. Leucine (L)

$$\frac{dL}{dt} = -Y_{LX}\frac{dX}{dt}\frac{L}{(K_L + L)}D$$



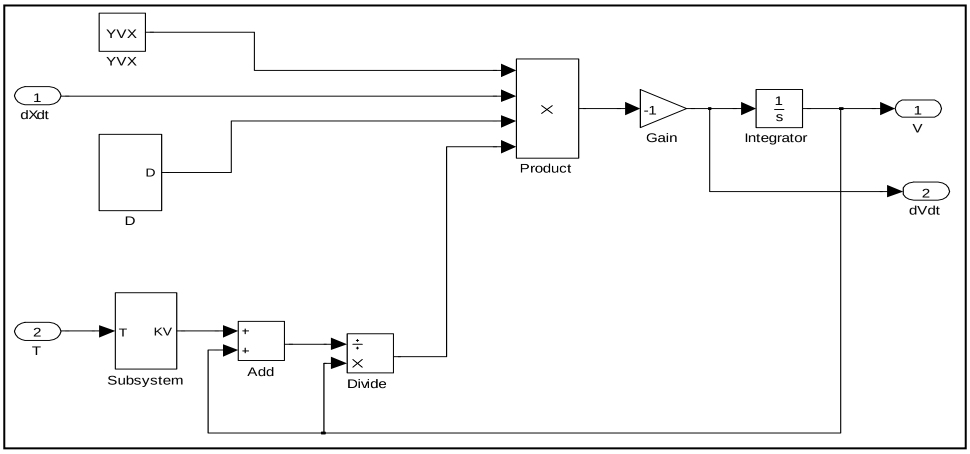
2.Isoleucine (I)

$$\frac{dI}{dt} = -Y_{IX}\frac{dX}{dt}\frac{I}{(K_I + I)}D$$

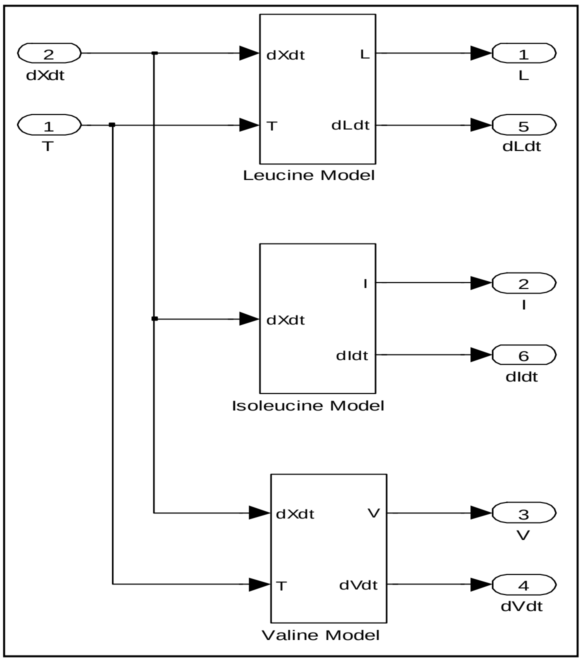


3. Valine (V)

$$\frac{dV}{dt} = -Y_{VX}\frac{dX}{dt}\frac{V}{(K_V + V)}D$$



Complete Nutrient System



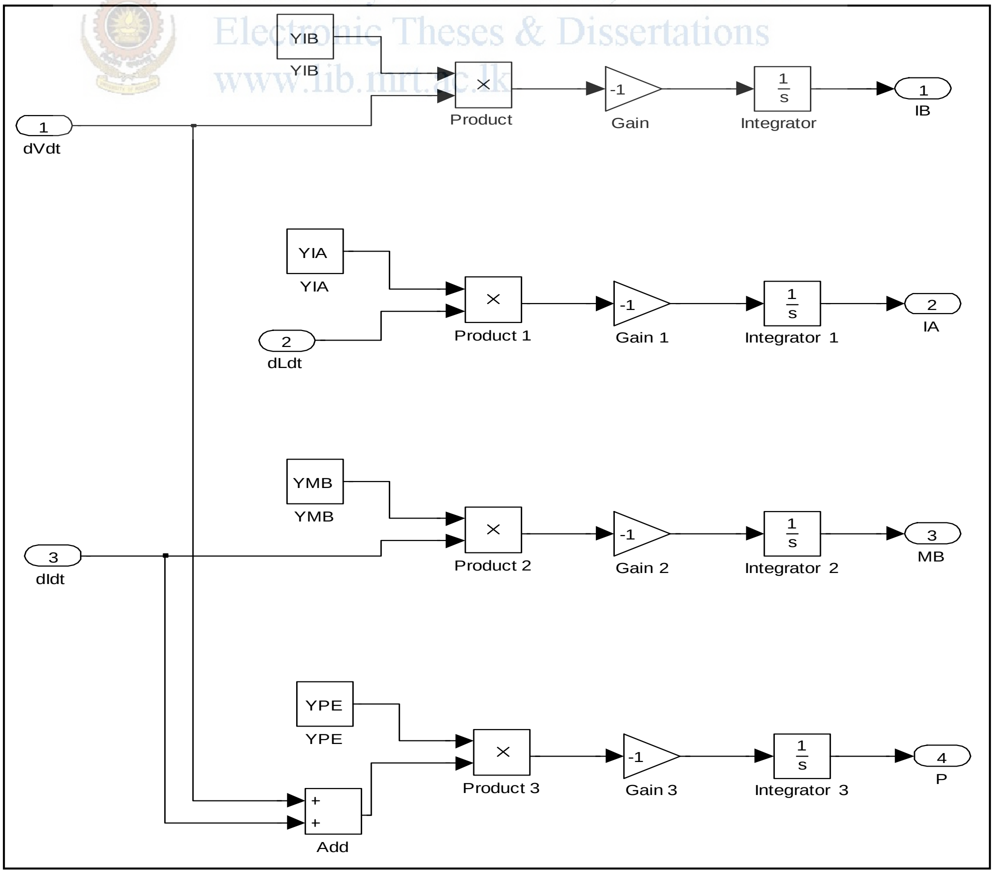
Fusel Alcohol Model

$$\frac{dIB}{dt} = Y_{IB}\mu_V X \qquad \mu_V = -\frac{1}{X}\frac{dV}{dt}$$

$$\frac{dIA}{dt} = Y_{IA}\mu_L X \qquad \mu_L = -\frac{1}{X}\frac{dL}{dt}$$

$$\frac{dMB}{dt} = Y_{MB}\mu_I X \qquad \mu_I = -\frac{1}{X}\frac{dI}{dt}$$

$$\frac{dP}{dt} = Y_{PE}(\mu_V + \mu_I)X$$



Ester Model

1. Ethyl acetate (EA)

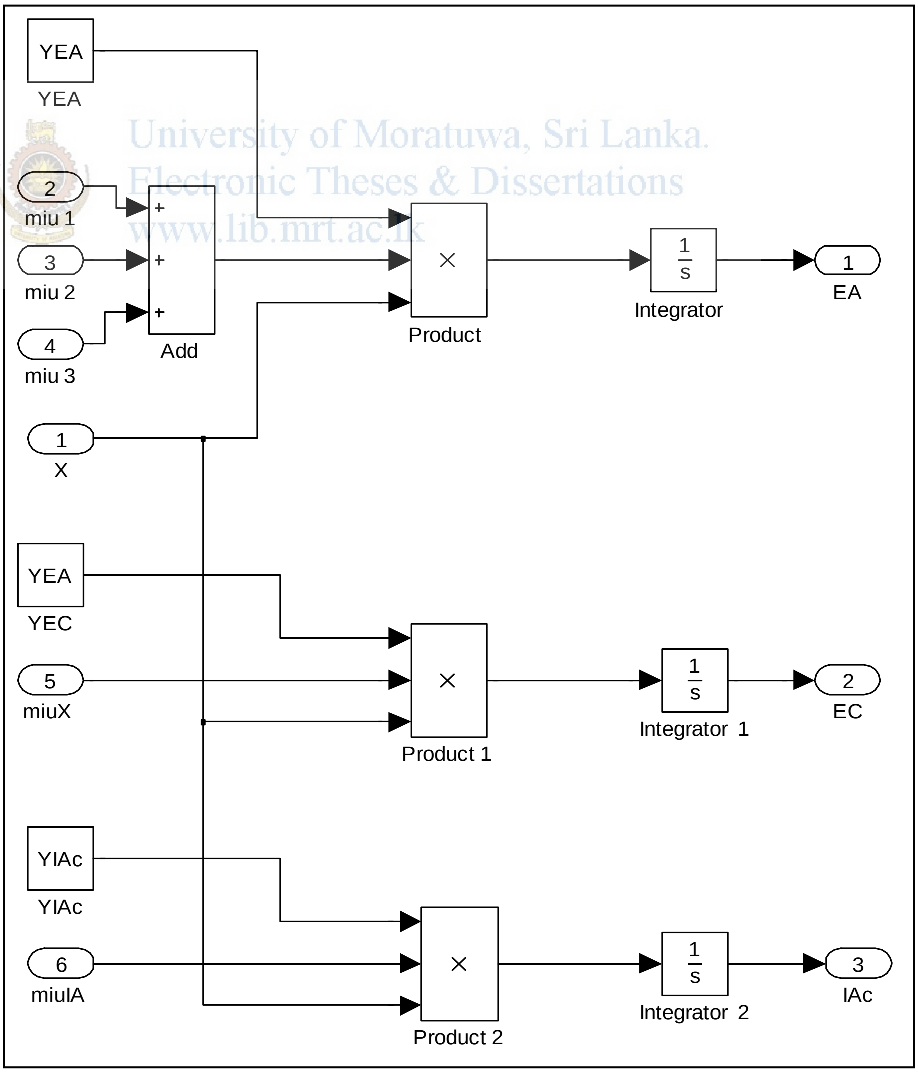
$$\frac{dEA}{dt} = Y_{EA}(\mu_1 + \mu_2 + \mu_3)X$$

2. Ethyl caproate (EC)

$$\frac{dEC}{dt} = Y_{EC}\mu_X X$$

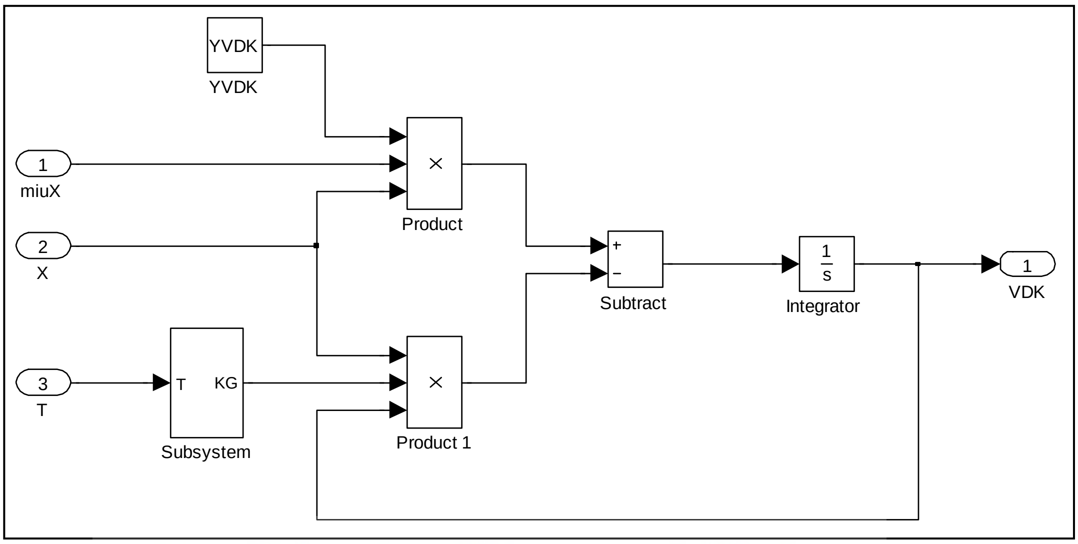
3. Isoamyl acetate. (IAc)

$$\frac{dIAc}{dt} = Y_{IAc}\mu_{IA} X$$



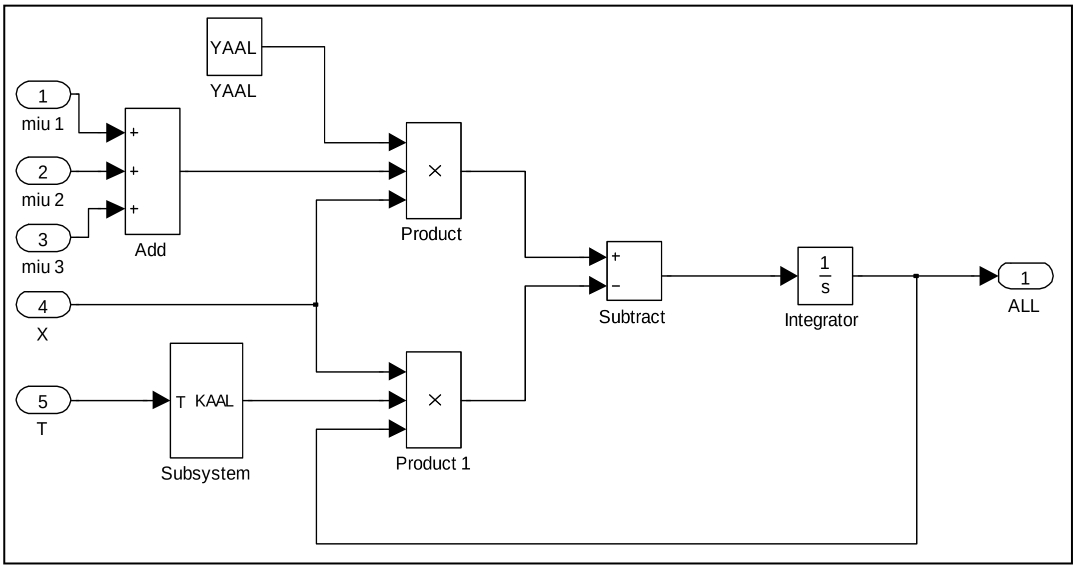
Vicinal Diketones Model (VDKs)

$$\frac{d(VDK)}{dt} = Y_{VDK}\mu_X X - K_{VDK}(VDK)\ X$$

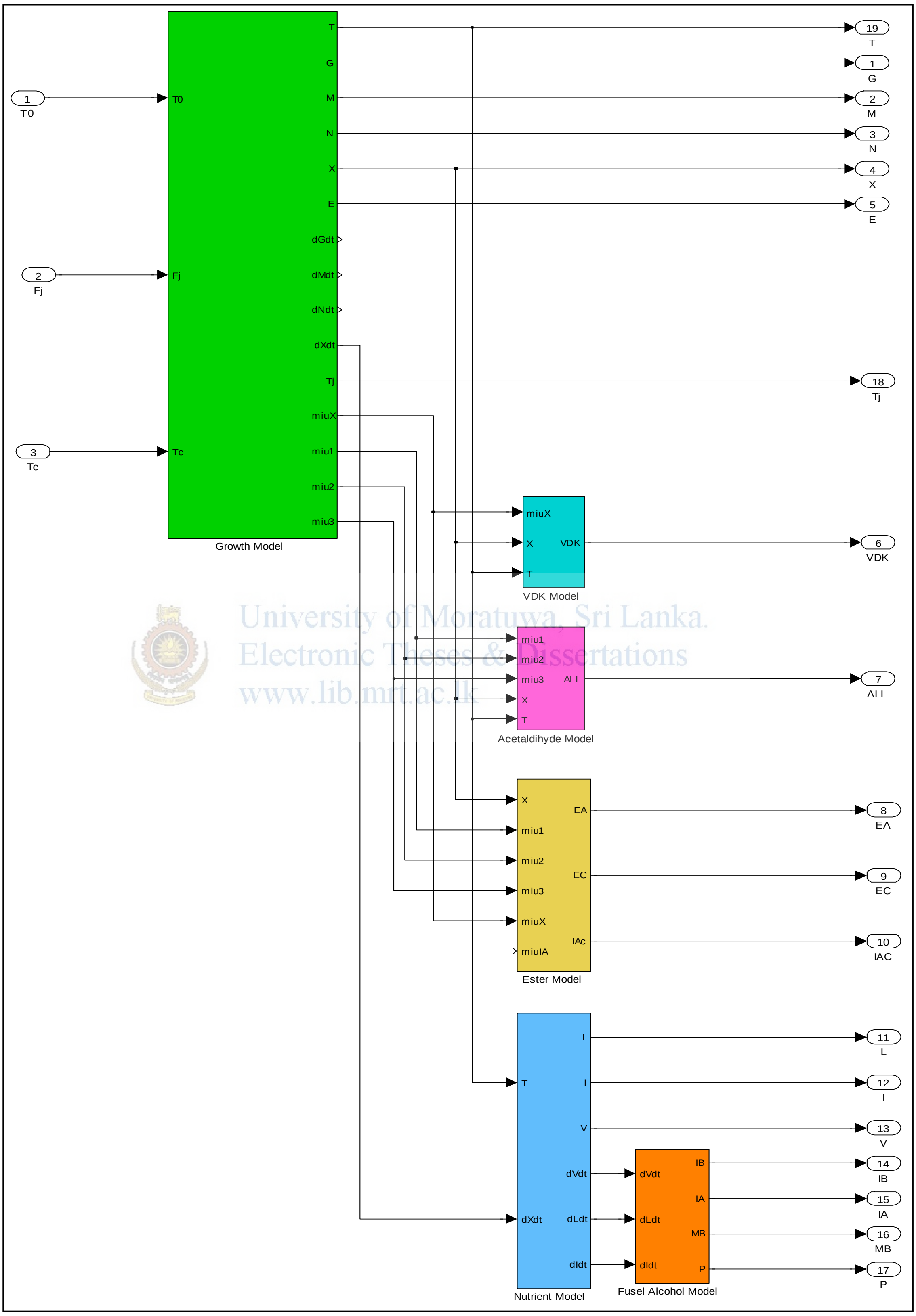


Acetaldehyde Model (AAL)

$$\frac{d(AAl)}{dt} = Y_{AAl}(\mu_1 + \mu_2 + \mu_3)X - K_{AAl}(AAl)X$$



Fermentation System



APPENDIX D

Modelica code

FermReact.mo

```
//Modelica code for Beer Flavour Model

model FermReact

//parameters

parameter Real YXG=0.134;

parameter Real YXM=0.268;

parameter Real YXN=0.402;

//-----------------------------------

//temparature dependant parameters

parameter Real miuG0=exp(35.77);

parameter Real miuM0=exp(16.40);

parameter Real miuN0=exp(10.59);


parameter Real EmiuG=22.6e3;

parameter Real EmiuM=11.3e3;

parameter Real EmiuN=7.16e3;

//

parameter Real KG0=exp(-121.3);

parameter Real KM0=exp(-19.5);

parameter Real KN0=exp(-26.78);

parameter Real EKG=-68.6e3;

parameter Real EKM=-14.4e3;

parameter Real EKN=-19.9e3;

//

parameter Real KdashG0=exp(23.33);

parameter Real KdashM0=exp(55.61);
```

```
parameter Real EKdashG=10.2e3;
parameter Real EKdashM=26.3e3;
//
parameter Real R=1.987;
parameter Real rho=1040;
parameter Real Cp=4.016;
//
parameter Real deltaHFG=-91.2;
parameter Real deltaHFM=-226.3;
parameter Real deltaHFN=-361.3;

//Ethanol parameters
parameter Real YEG=1.92;
parameter Real YEM=3.84;
parameter Real YEN=5.76;
parameter Real Kx = 365000;
parameter Real X0=125;

//Nutrient parameters
parameter Real YLX=0.0832;
parameter Real YIX=0.0363;
parameter Real YVX=0.0273;
parameter Real KI=0.365;

parameter Real KL0=exp(10.14);
parameter Real KV0=exp(328);

parameter Real EKL=5.95e3;
parameter Real EKV=211.9e3;

parameter Real toud=23.54;
```

```
//Flavour parameters
//Fusel alcohols
parameter Real YIB=0.203;
parameter Real YIA=0.557;
parameter Real YMB=0.472;
parameter Real YPE=0.235;

//Esters
parameter Real YEA=0.000992;
parameter Real YEC=0.000118;
parameter Real YIAc=0.0269;

//Vicinal deketones
parameter Real YVDK=0.000105;
parameter Real KVDK0=exp(86.8);
parameter Real EVDK=54.3e3;

//Acetaldehyde
parameter Real YAAL=0.01;
parameter Real KAAL0=exp(10.4);
parameter Real EAAL=11.1e3;

//Naming status---------------------------

//growth model
Real G(start = 70);
Real M(start = 220);
Real N(start = 40);
Real X(start = 125);
Real E(start = 0);
Real T(start = 8);
```

```
//Neutriamt model
Real L(start = 1.3);
Real I(start = 0.6);
Real V(start = 2.1);

//Fusel alcohol model
Real IB(start = 0);
Real IA(start = 0);
Real MB(start = 0);
Real P(start = 0);

//Ester model
Real EA(start = 0);
Real EC(start = 0);
Real IAc(start = 0);

//VDK model
Real VDK(start = 0);
Real AAL(start = 0);

//
Real miuG;
Real miuM;
Real miuN;

Real KG;
Real KM;
Real KN;

Real KdashG;
Real KdashM;
```

```
Real miu1;
Real miu2;
Real miu3;
Real miuX;

Real D;
Real KL;
Real KV;

Real miuL;
Real miuI;
Real miuV;

Real miuIA;

Real KVDK;
Real KAAL;
```



```
equation
//Growth Model
//Temparature dependancy
miuG=miuG0*exp(-EmiuG/(R*(T+273.15)));
miuM=miuM0*exp(-EmiuM/(R*(T+273.15)));
miuN=miuN0*exp(-EmiuN/(R*(T+273.15)));



KG=KG0*exp(-EKG/(R*(T+273.15)));
KM=KM0*exp(-EKM/(R*(T+273.15)));
KN=KN0*exp(-EKN/(R*(T+273.15)));
```

```
KdashG=KdashG0*exp(-EKdashG/(R*(T+273.15)));
KdashM=KdashM0*exp(-EKdashM/(R*(T+273.15)));

miu1=miuG*G/(KG+G);
miu2=(miuM*M/(KM+M))*(KdashG/(KdashG+G));
miu3=(miuN*N/(KN+N))*(KdashG/(KdashG+G))*(KdashM/(KdashM+M));
miuX=(YXG*miu1+YXM*miu2+YXN*miu3)*Kx/(Kx+(X-X0)^2);

//Differential equations

der(G) = -miu1*X;
der(M) = -miu2*X;
der(N) = -miu3*X;
der(X) = miuX*X;
der(E) = (YEG*miu1+YEM*miu2+YEN*miu3)*X;

//heart balance
der(T)=(1/(rho*Cp))*(-X*(deltaHFG*miu1+deltaHFM*miu2+deltaHFN*miu3));

//-------------------------------------------------------------------
//Nutrient model
D = 1-exp(-time/toud); //time delay

KL=KL0*exp(-EKL/(R*(T+273.15)));
KV=KV0*exp(-EKV/(R*(T+273.15)));



//Differential equations

der(L) = -YLX*der(X)*(L/(KL+L))*D;
der(I) = -YIX*der(X)*(I/(KI+I))*D;
```

```
der(V) = -YVX*der(X)*(V/(KV+V))*D;

//------------------------------------------------------------------

//Falvour model

//Fusel alcohol%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

miuL = -(1/X)*der(L);
miuI = -(1/X)*der(I);
miuV = -(1/X)*der(V);

//Didderential equations

der(IB) = YIB*miuV*X;
der(IA) = YIA*miuL*X;
der(MB)= YMB*miuI*X;
der(P) = YPE*(miuV+miuI)*X;

//Esters%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

miuIA = miuL; //Assamption

//Defferential equations

der(EA) = YEA*(miu1+miu2+miu3)*X;
der(EC) = YEC*miuX*X;
der(IAc) = YIAc*miuIA*X;

//Vicinal diketones & Acetaldehyde Model%%%%%%%%%%%%%%%%%%%%%%%%%%%
```

```
//Temperature depandancy
KVDK=KVDK0*exp(-EVDK/(R*(T+273.15)));
KAAL=KAAL0*exp(-EAAL/(R*(T+273.15)));

//Differential equation
der(VDK) = YVDK*miuX*X - KVDK*VDK*X;
der(AAL) = YAAL*(miu1+miu2+miu3)*X - KAAL*AAL*X;

end FermReact;
```

Python code

FermReact.py

```
from jmodelica import simulate

import pylab as p


##Simulating

res_object = simulate(model='FermReact', file_name='FermReact.mo',

      alg_args={'start_time':0.0,'final_time':250.0,'num_communicati
on_points':0})


res = res_object.get_result_data()


##Etracting data from result object


G = res.get_variable_data('G')

M = res.get_variable_data('M')

N = res.get_variable_data('N')

D = res.get_variable_data('D')


X = res.get_variable_data('X')

E = res.get_variable_data('E')

T = res.get_variable_data('T')


L = res.get_variable_data('L')

I = res.get_variable_data('I')

V = res.get_variable_data('V')


IB = res.get_variable_data('IB')

IA = res.get_variable_data('IA')

MB = res.get_variable_data('MB')
```

```
P = res.get_variable_data('P')

EA = res.get_variable_data('EA')
EC = res.get_variable_data('EC')
IAc = res.get_variable_data('IAc')

VDK = res.get_variable_data('VDK')
AAL = res.get_variable_data('AAL')

##plotting graphs
p.figure(1)
p.clf()

p.subplot(311)
p.plot(G.t,G.x)
p.grid()
p.ylabel('Glucose')

p.subplot(312)
p.plot(M.t,M.x)
p.grid()
p.ylabel('Maltose')

p.subplot(313)
p.plot(N.t,N.x)
p.grid()
p.ylabel('Maltotriose')
p.xlabel('Time (h)')
```

```
p.figure(2)
p.clf()

p.subplot(311)
p.plot(X.t,X.x)
p.grid()
p.ylabel('Yeast Growth')

p.subplot(312)
p.plot(E.t,E.x)
p.grid()
p.ylabel('Ethanol')

p.subplot(313)
p.plot(T.t,T.x)
p.grid()
p.ylabel('Temperature')
p.xlabel('Time (h)')

p.figure(3)
p.clf()

p.subplot(311)
p.plot(L.t,L.x)
p.grid()
p.ylabel('Leucine')

p.subplot(312)
p.plot(I.t,I.x)
p.grid()
p.ylabel('Isoleucine')
```

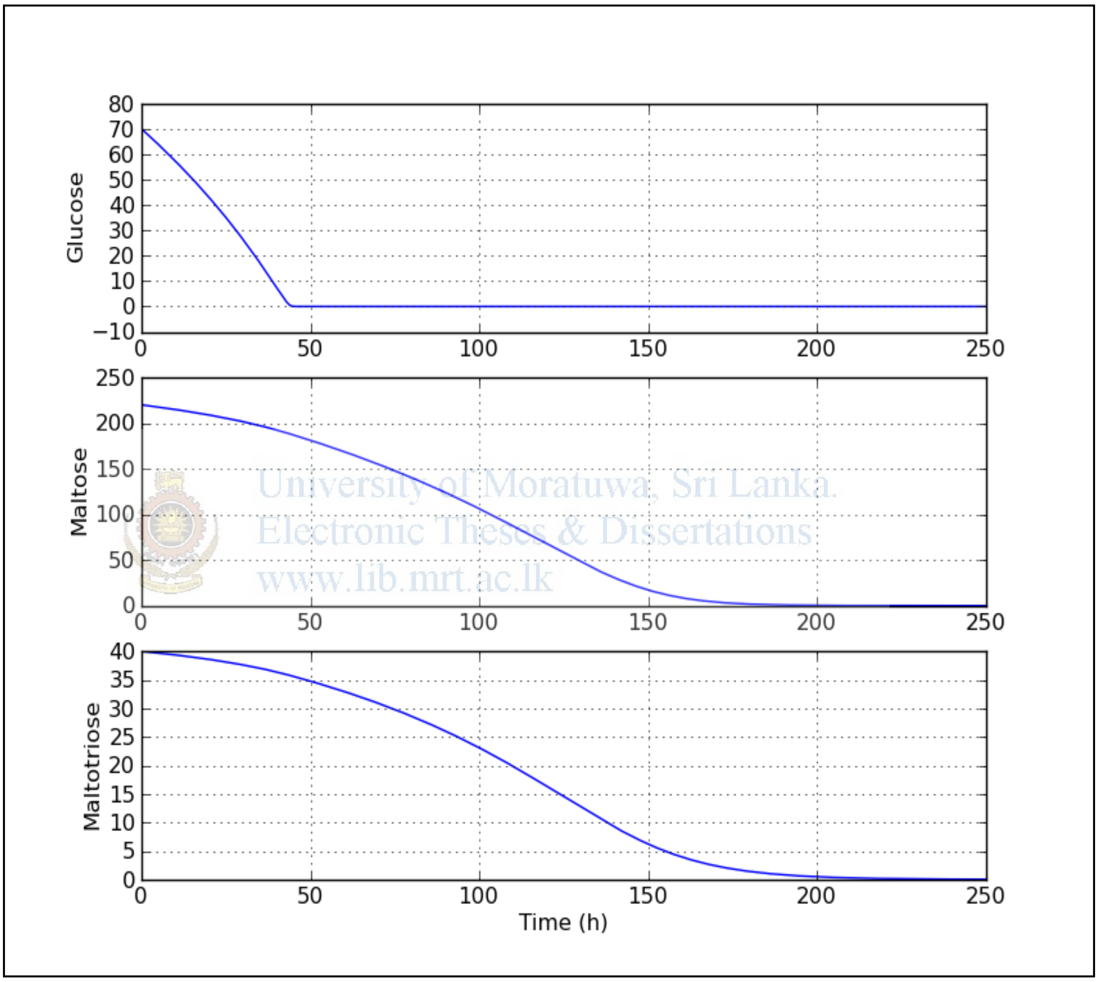
```
p.subplot(313)
p.plot(V.t,V.x)
p.grid()
p.ylabel('Valine')
p.xlabel('Time (h)')

p.figure(4)
p.clf()

p.subplot(221)
p.plot(IB.t,IB.x)
p.grid()
p.ylabel('Isobutyl Alcohol')

p.subplot(222)
p.plot(IA.t,IA.x)
p.grid()
p.ylabel('Isoamyl Alcohol')
p.xlabel('Time (h)')

p.subplot(223)
p.plot(MB.t,MB.x)
p.grid()
p.ylabel('2-methyl-1-butanol')

p.subplot(224)
p.plot(P.t,P.x)
p.grid()
p.ylabel('Propanol')
p.xlabel('Time (h)')
p.figure(5)
```

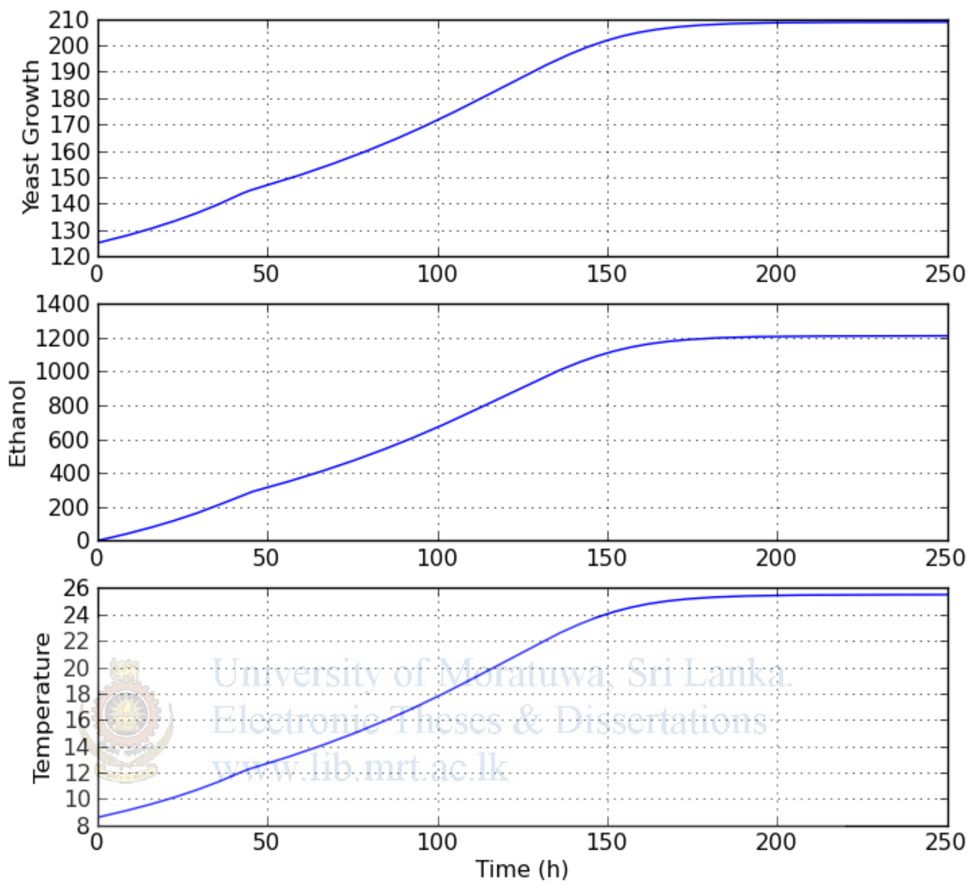
```
p.clf()
p.subplot(311)
p.plot(EA.t,EA.x)
p.grid()
p.ylabel('Ethyl Acetate')

p.subplot(312)
p.plot(EC.t,EC.x)
p.grid()
p.ylabel('Ethyl Caproate')

p.subplot(313)
p.plot(IAc.t,IAc.x)
p.grid()
p.ylabel('Isoamyl Acetate')
p.xlabel('Time (h)')

p.figure(6)
p.clf()

p.subplot(211)
p.plot(VDK.t,VDK.x)
p.grid()
p.ylabel('Vicinal Diketones')

p.subplot(212)
p.plot(AAL.t,AAL.x)
p.grid()
p.ylabel('Acetaldehyde')
p.xlabel('Time (h)')
p.show()
```

APPENDIX E

JModelica simulations under no temperature control conditions.

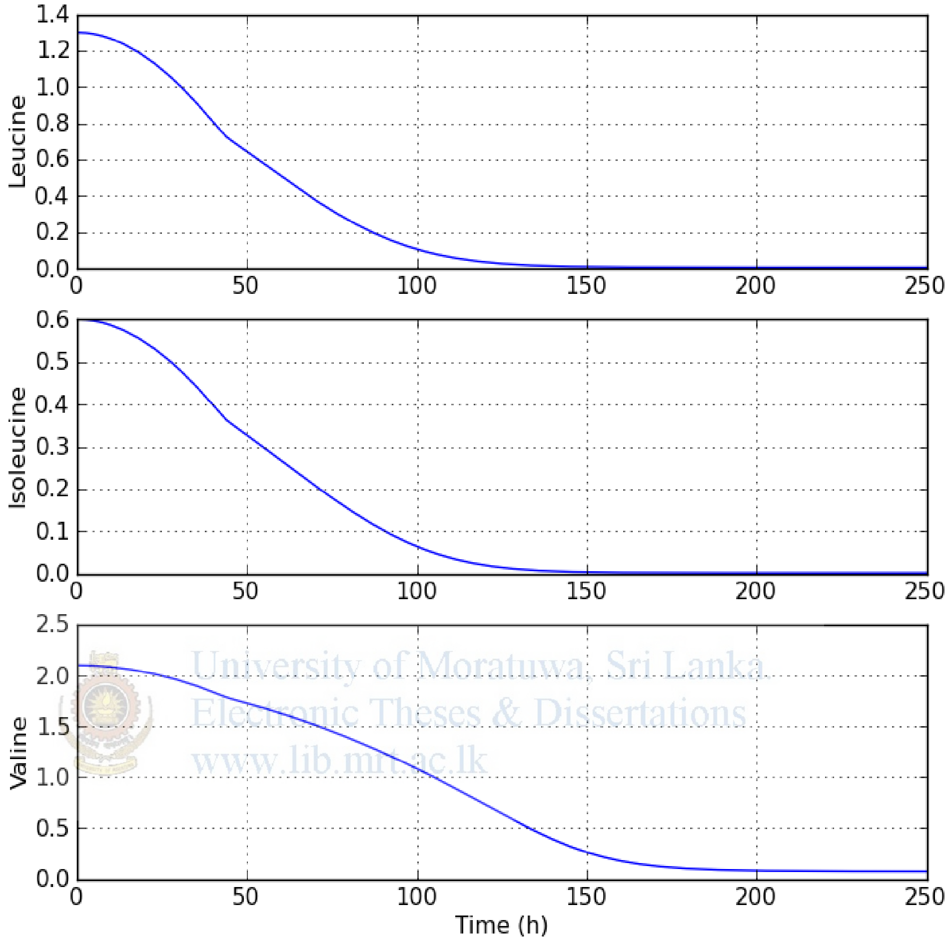
- Growth model simulation results



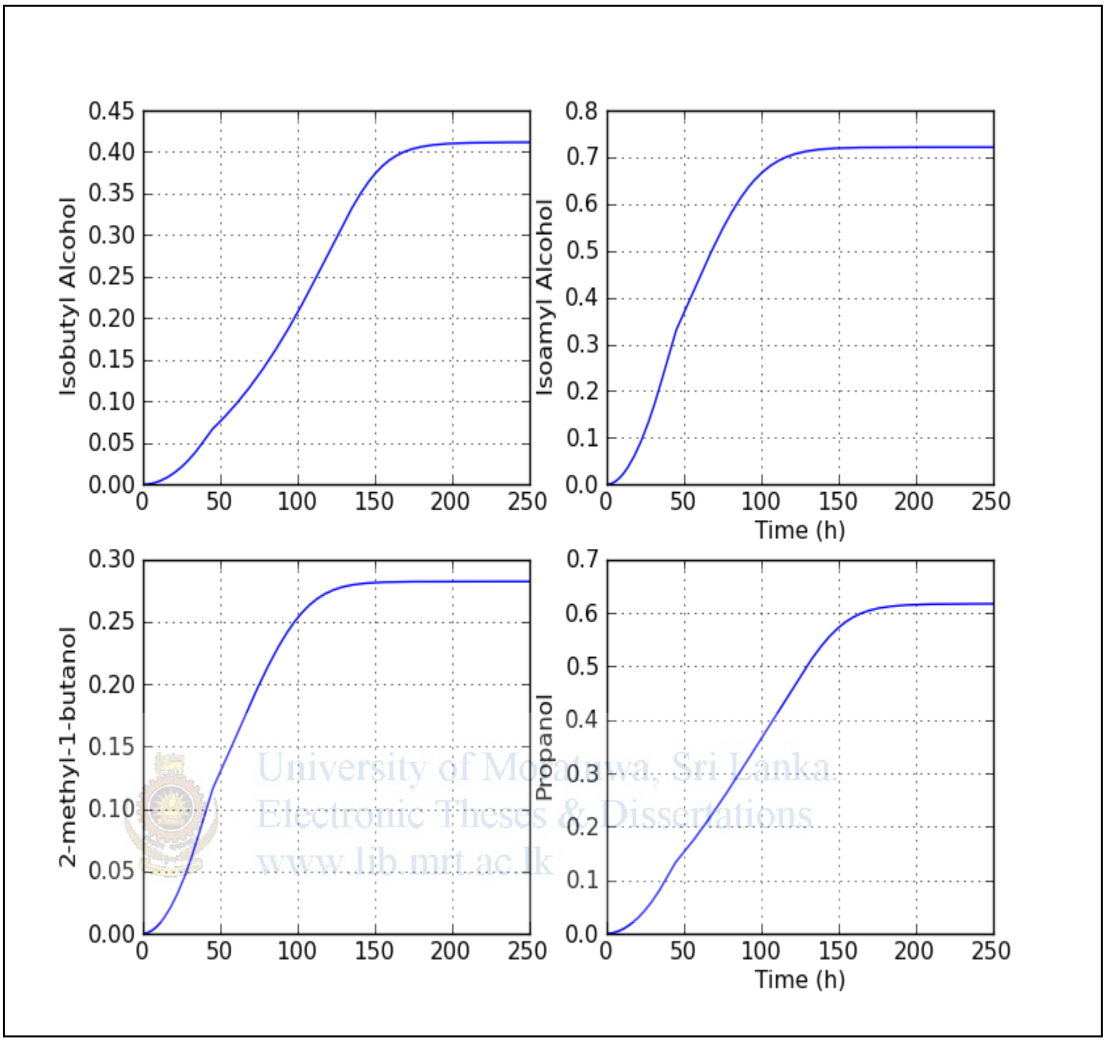


Yeast Growth
210
200
190
180
170
160
150
140
130
120
0
50
100
150
200
250
Ethanol
1400
1200
1000
800
600
400
200
0
Temperature
26
24
22
20
18
16
14
12
10
8
Time (h)

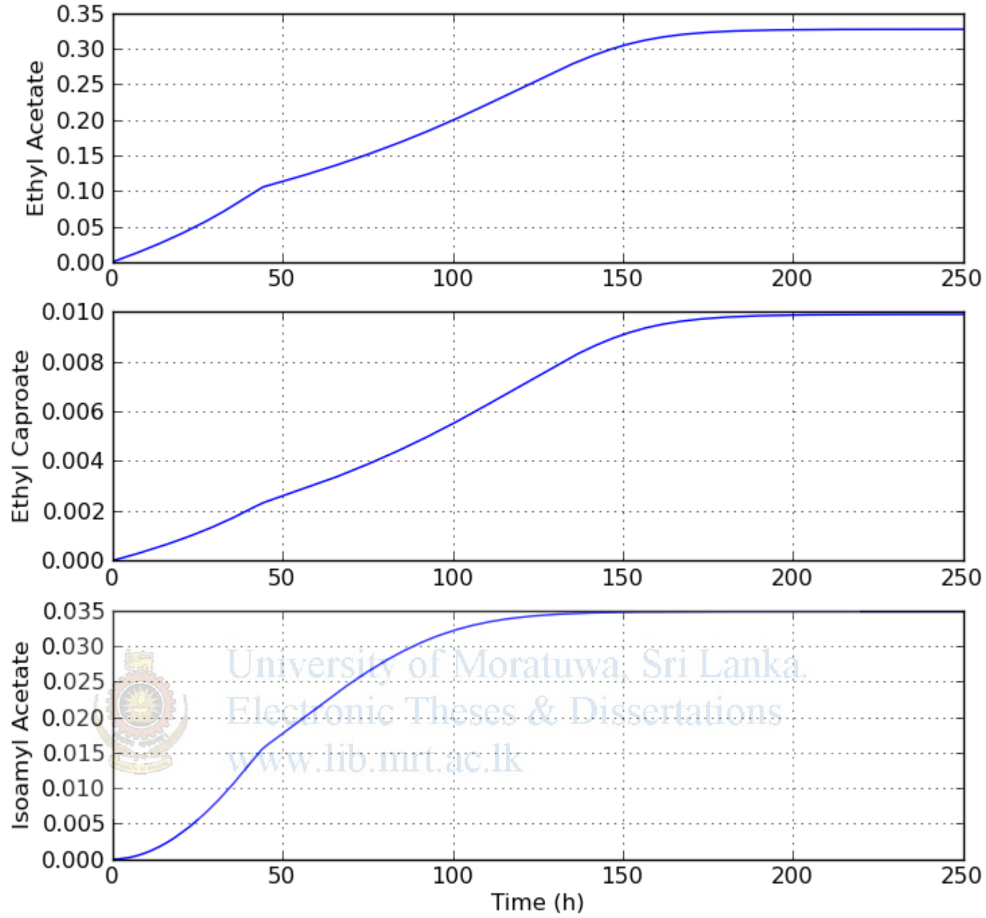
- Nutrient model simulation results



- Fusel alcohol model simulation results



- Ester model simulation results



- VDK and acetaldehyde model simulation results