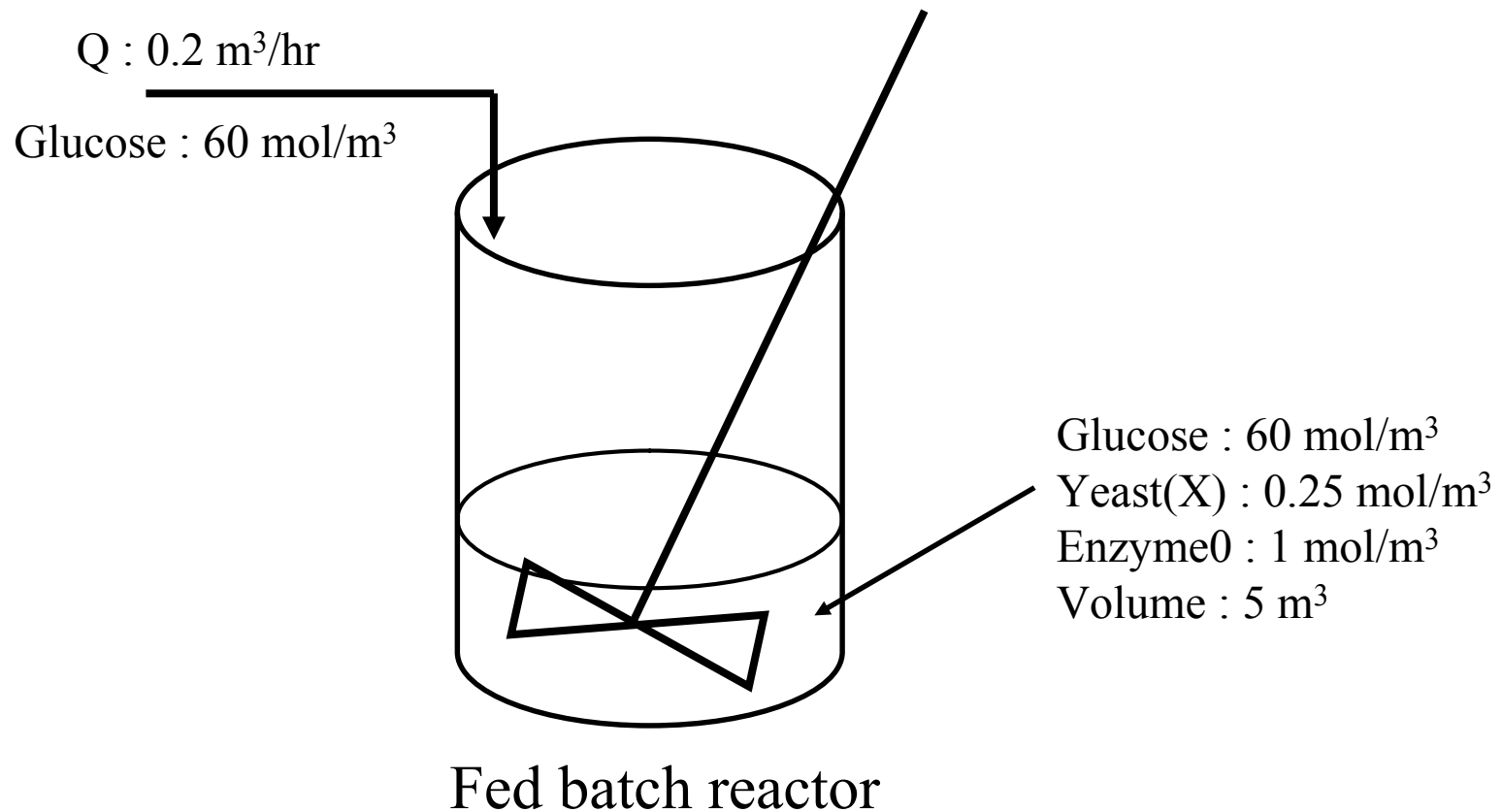


# Ethanol Fed Batch Diauxic Fermentation

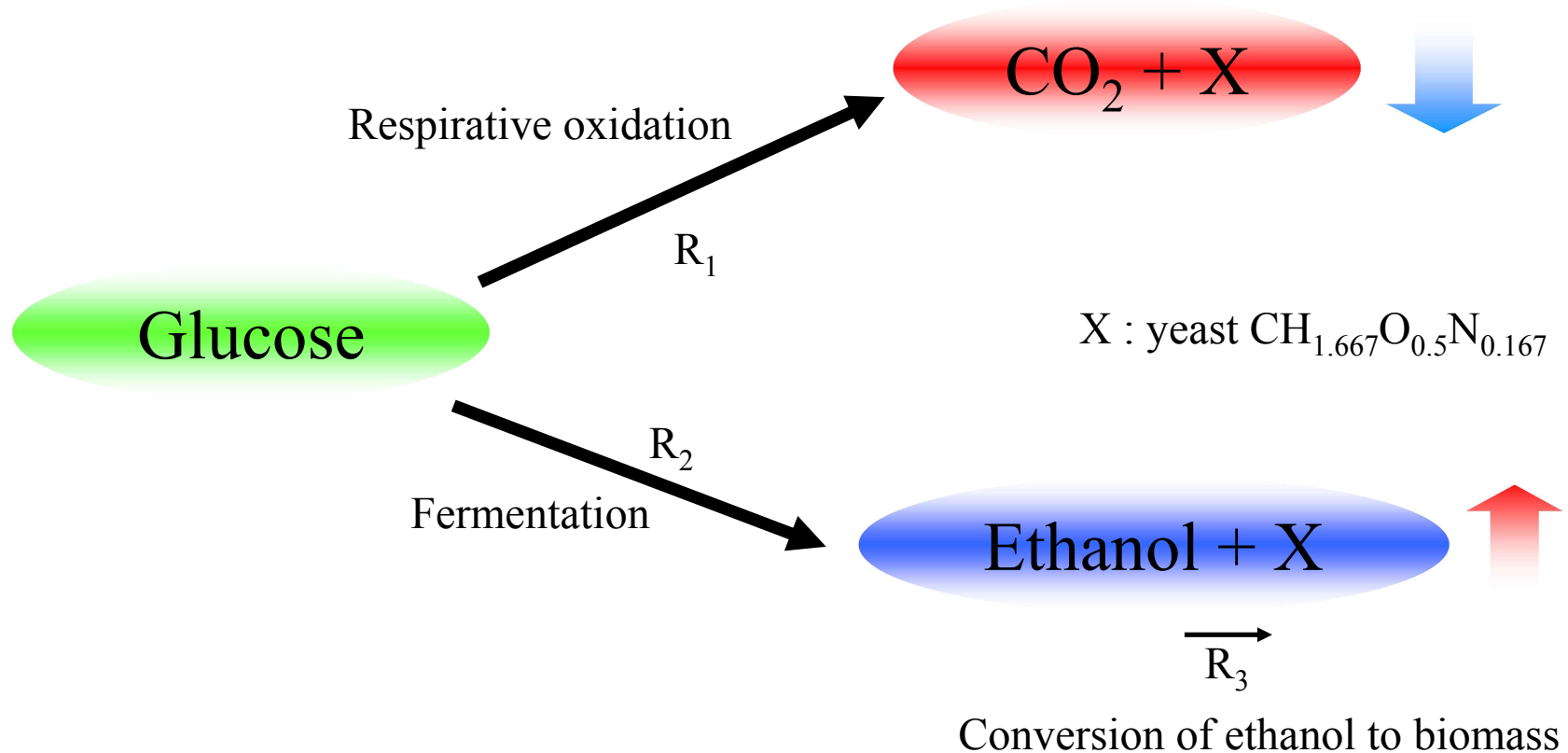
# Introduction

## ➡ Ethanol Fed Batch Diauxic Fermentation



# Introduction

↪ Ethanol Fed Batch Diauxic Fermentation



Pathway of aerobic ethanol fermentation

# Introduction

## Rate of the process

Respirative oxidation on glucose

$$R_1 = \frac{Glu}{Glu + K_{S1}} K_1 \alpha X$$

Fermentation to ethanol

$$R_2 = \frac{Glu}{Glu + K_{S2}} K_1 (1 - \alpha) X$$

Conversion of ethanol to biomass

$$R_3 = \frac{EtOH}{EtOH + K_{S3}} K_3 E_2 X$$

Production rate of enzyme E<sub>1</sub>

$$R_4 = \frac{K_4}{K_{S4} + Glu^3} X E_0$$

Production rate of enzyme E<sub>2</sub>

$$R_5 = K_5 X E_1$$

# Introduction

Mass and component balance of the biomass

$$\frac{dV}{dt} = Q, \quad \rho = \text{constant} \quad \frac{d(VC)}{dt} = \frac{VdC}{dt} + \frac{CdV}{dt} = \frac{VdC}{dt} + CQ$$

Glucose 의 농도변화

$$\frac{dGlu}{dt} = -(R_1 + R_2) + \frac{Q(Glu_0 - Glu)}{V}$$

Yeast 의 농도변화

$$\frac{dX}{dt} = Y_1R_1 + Y_2R_2 + Y_4R_3 - \frac{XQ}{V}$$

EtOH 의 농도변화

$$\frac{dEtOH}{dt} = Y_3R_2 - R_3 - \frac{EtOHQ}{V}$$

Enzyme 의 농도변화

$$\frac{dE_0}{dt} = -R_4 - \frac{E_0Q}{V}$$

$$\frac{dE_1}{dt} = R_4 - R_5 - \frac{E_1Q}{V}$$

$$\frac{dE_2}{dt} = R_5 - \frac{E_2Q}{V}$$

# Methods

## ➤ 수치해석을 위해 기호화

- Volume  $\rightarrow V \rightarrow y1$ ,      Glucose  $\rightarrow$  Glu  $\rightarrow y2$
- Yeast  $\rightarrow X \rightarrow y3$ ,      Ethanol  $\rightarrow$  EtOH  $\rightarrow y4$
- Enzyme0  $\rightarrow E0 \rightarrow y5$ ,      Enzyme1  $\rightarrow E1 \rightarrow y6$ ,
- Enzyme2  $\rightarrow E2 \rightarrow y7$

$$R1 = \left( \frac{y2}{y2 + KS1} \right) * K1 * ALPHA * y3;$$

$$R2 = \left( \frac{y2}{y2 + KS2} \right) * K2 * (1 - ALPHA) * y3;$$

$$R3 = \left( \frac{y4}{y4 + KP13} \right) * K3 * y7 * y3;$$

$$R4 = \left( \frac{K4}{KS4 + y2 * y2 * y2} \right) * y3 * y5;$$

$$R5 = K5 * y3 * y6;$$

# Methods

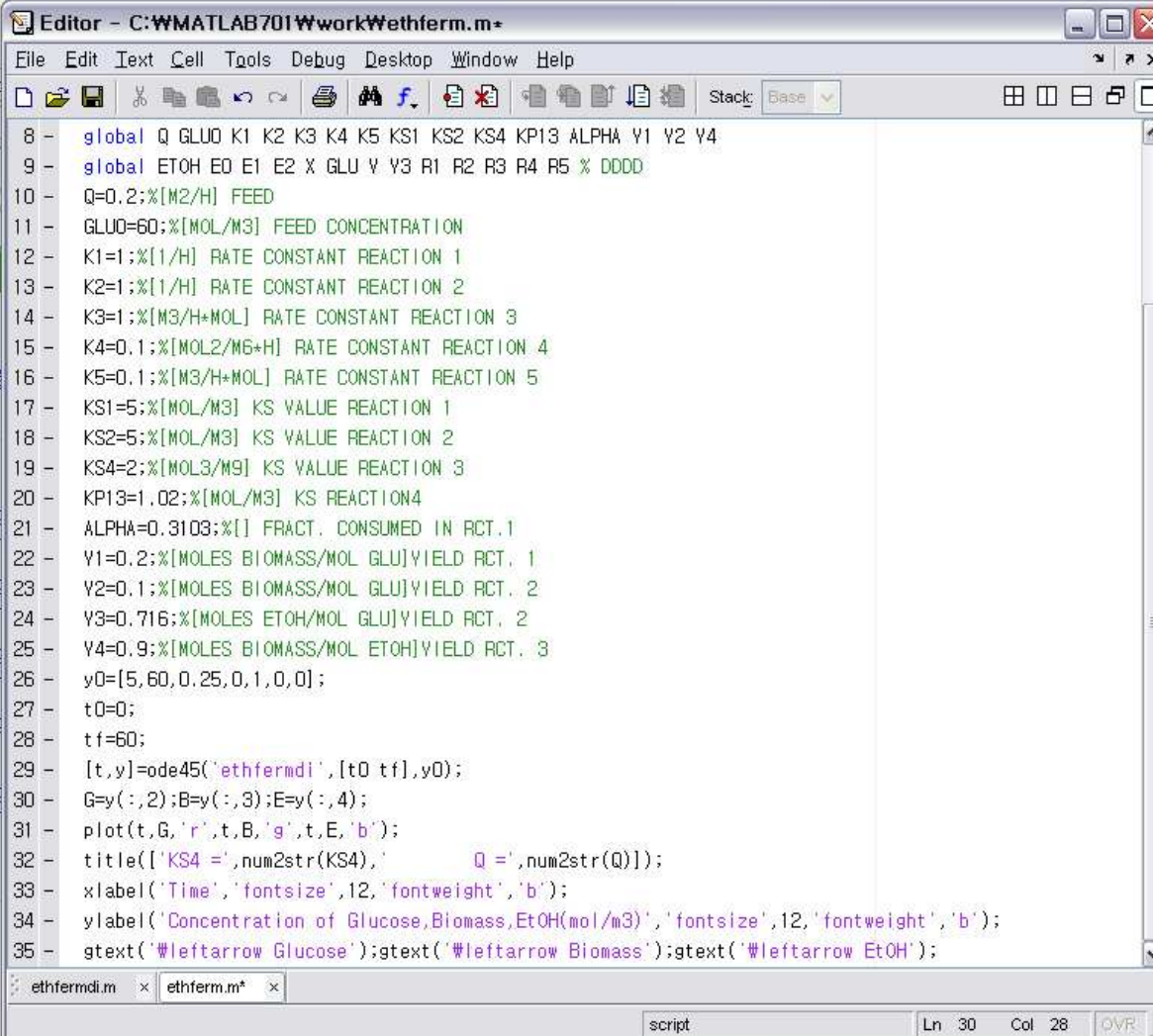
## ➔ 초기값 설정

- ➔  $Q=0.2; \%[M^2/H]$  FEED
- ➔  $GLU_0=60; \%[MOL/M^3]$  FEED CONCENTRATION
- ➔  $K_1=1; \%[1/H]$  RATE CONSTANT REACTION 1
- ➔  $K_2=1; \%[1/H]$  RATE CONSTANT REACTION 2
- ➔  $K_3=1; \%[M^3/H * MOL]$  RATE CONSTANT REACTION 3
- ➔  $K_4=0.1; \%[MOL^2/M^6 * H]$  RATE CONSTANT REACTION 4
- ➔  $K_5=0.1; \%[M^3/H * MOL]$  RATE CONSTANT REACTION 5
- ➔  $KS_1=5; \%[MOL/M^3]$  KS VALUE REACTION 1
- ➔  $KS_2=5; \%[MOL/M^3]$  KS VALUE REACTION 2
- ➔  $KS_4=2; \%[MOL^3/M^9]$  KS VALUE REACTION 3
- ➔  $KP_{13}=1.02; \%[MOL/M^3]$  KS REACTION 4
- ➔  $ALPHA=0.3103; \%[ ]$  FRACT. CONSUMED IN RCT. 1
- ➔  $Y_1=0.2; \%[MOLES BIOMASS/MOL GLU]$  YIELD RCT. 1
- ➔  $Y_2=0.1; \%[MOLES BIOMASS/MOL GLU]$  YIELD RCT. 2
- ➔  $Y_3=0.716; \%[MOLES ETOH/MOL GLU]$  YIELD RCT. 2
- ➔  $Y_4=0.9; \%[MOLES BIOMASS/MOL ETOH]$  YIELD RCT. 3

# Methods

## ➔ M파일 작성

- ➔ 초기값
- ➔ 출력설정
- ➔ 풀이법 등

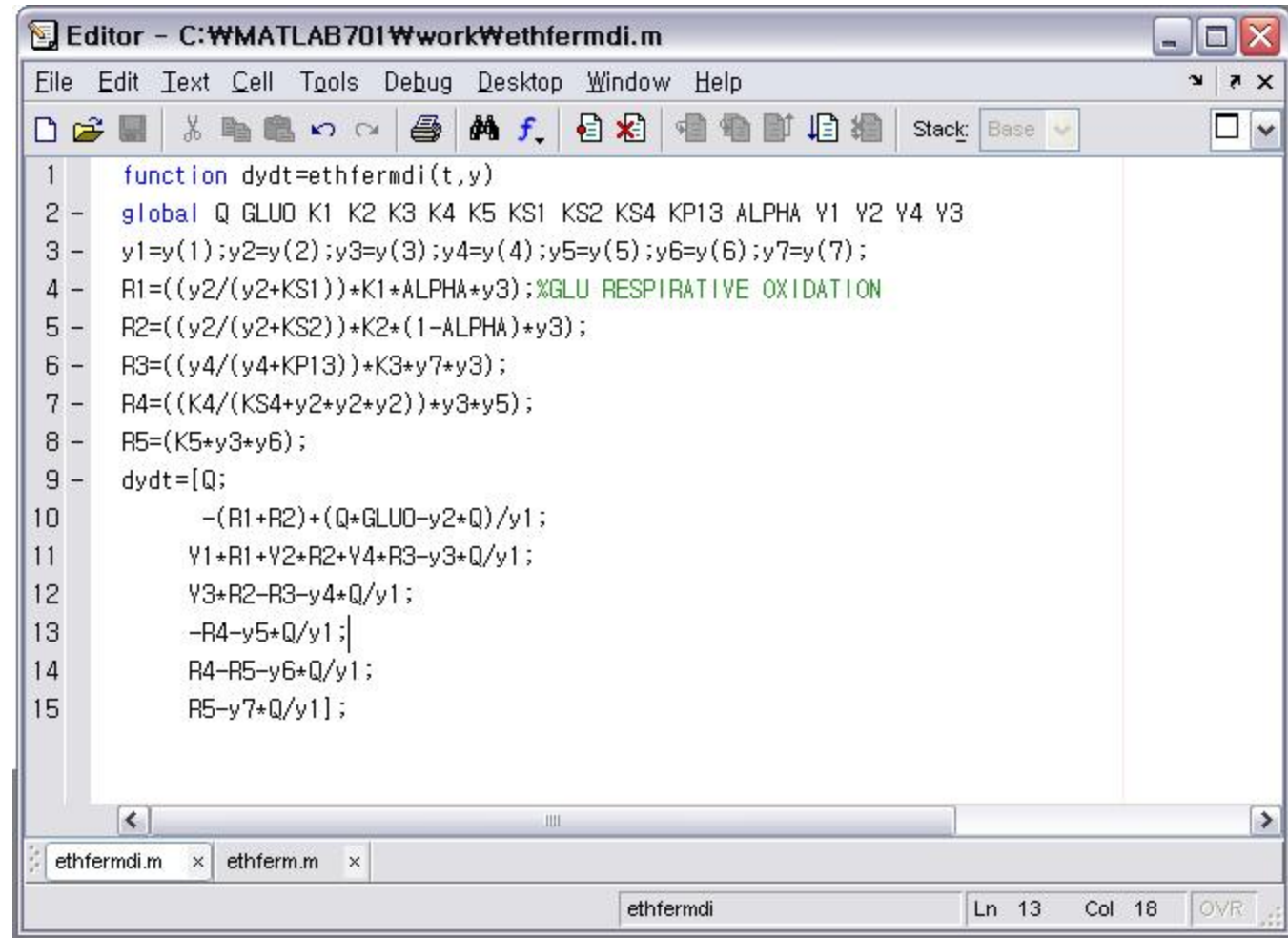


```
Editor - C:\WMATLAB701\work\Wethferm.m*
File Edit Text Cell Tools Debug Desktop Window Help
[Icons] Stack: Base
8 - global Q GLU0 K1 K2 K3 K4 K5 KS1 KS2 KS4 KP13 ALPHA Y1 Y2 Y4
9 - global ETOH EO E1 E2 X GLU V Y3 R1 R2 R3 R4 R5 % DDDD
10 - Q=0.2; %[M2/H] FEED
11 - GLU0=60; %[MOL/M3] FEED CONCENTRATION
12 - K1=1; %[1/H] RATE CONSTANT REACTION 1
13 - K2=1; %[1/H] RATE CONSTANT REACTION 2
14 - K3=1; %[M3/H+MOL] RATE CONSTANT REACTION 3
15 - K4=0.1; %[MOL2/M6+H] RATE CONSTANT REACTION 4
16 - K5=0.1; %[M3/H+MOL] RATE CONSTANT REACTION 5
17 - KS1=5; %[MOL/M3] KS VALUE REACTION 1
18 - KS2=5; %[MOL/M3] KS VALUE REACTION 2
19 - KS4=2; %[MOL3/M9] KS VALUE REACTION 3
20 - KP13=1.02; %[MOL/M3] KS REACTION4
21 - ALPHA=0.3103; %[] FRACT. CONSUMED IN RCT.1
22 - Y1=0.2; %[MOLES BIOMASS/MOL GLU]YIELD RCT. 1
23 - Y2=0.1; %[MOLES BIOMASS/MOL GLU]YIELD RCT. 2
24 - Y3=0.716; %[MOLES ETOH/MOL GLU]YIELD RCT. 2
25 - Y4=0.9; %[MOLES BIOMASS/MOL ETOH]YIELD RCT. 3
26 - y0=[5,60,0,25,0,1,0,0];
27 - t0=0;
28 - tf=60;
29 - [t,y]=ode45('ethfermdi',[t0 tf],y0);
30 - G=y(:,2); B=y(:,3); E=y(:,4);
31 - plot(t,G,'r',t,B,'g',t,E,'b');
32 - title(['KS4 =',num2str(KS4), ' Q =',num2str(Q)]);
33 - xlabel('Time','fontsize',12,'fontweight','b');
34 - ylabel('Concentration of Glucose,Biomass,EtOH(mol/m3)','fontsize',12,'fontweight','b');
35 - gtext('#leftarrow Glucose');gtext('#leftarrow Biomass');gtext('#leftarrow EtOH');
```



# Methods

- ➔ M파일 작성
- ➔ 미분방정식



```
Editor - C:\WMATLAB701\work\ethfermdi.m
File Edit Text Cell Tools Debug Desktop Window Help
Stack: Base
1 function dydt=ethfermdi(t,y)
2 - global Q GLU0 K1 K2 K3 K4 K5 KS1 KS2 KS4 KP13 ALPHA Y1 Y2 Y4 Y3
3 - y1=y(1);y2=y(2);y3=y(3);y4=y(4);y5=y(5);y6=y(6);y7=y(7);
4 - R1=((y2/(y2+KS1))+K1+ALPHA+y3);%GLU RESPIRATIVE OXIDATION
5 - R2=((y2/(y2+KS2))+K2*(1-ALPHA)+y3);
6 - R3=((y4/(y4+KP13))+K3+y7+y3);
7 - R4=((K4/(KS4+y2+y2+y2))+y3+y5);
8 - R5=(K5+y3+y6);
9 - dydt=[Q;
10 -     -(R1+R2)+(Q+GLU0-y2+Q)/y1;
11 -     Y1+R1+Y2+R2+Y4+R3-y3+Q/y1;
12 -     Y3+R2-R3-y4+Q/y1;
13 -     -R4-y5+Q/y1;
14 -     R4-R5-y6+Q/y1;
15 -     R5-y7+Q/y1];
ethfermdi.m x ethferm.m x
ethfermdi Ln 13 Col 18 OVR
```

# Methods

## ↘ 조건 변화 변수와 예측

### ↘ KS4

◆ EtOH의 생성과 밀접한 연관이 있음. → EtOH의 증가 예상

### ↘ Q

◆ 유입되는 Glucose양의 변화에 따른 반응 정도 → 속도가 느려지고 반응저하 예상

### ↘ Glu0

◆ 유입되는 Glucose의 농도에 따른 양의 변화 → EtOH 생성 저하 예상

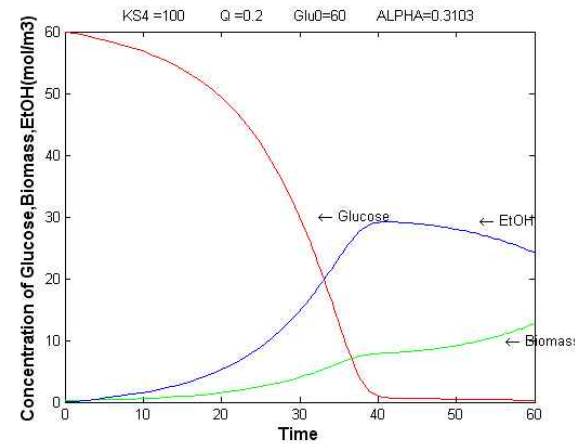
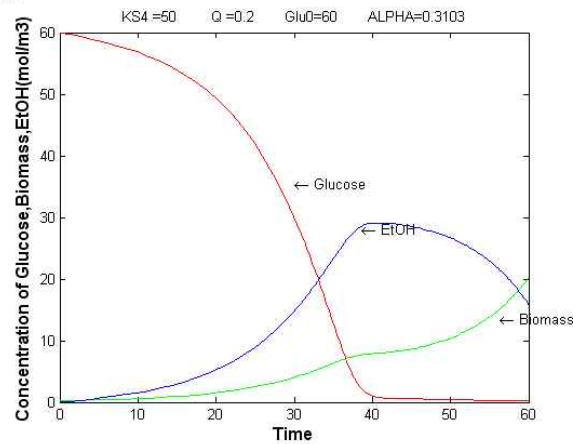
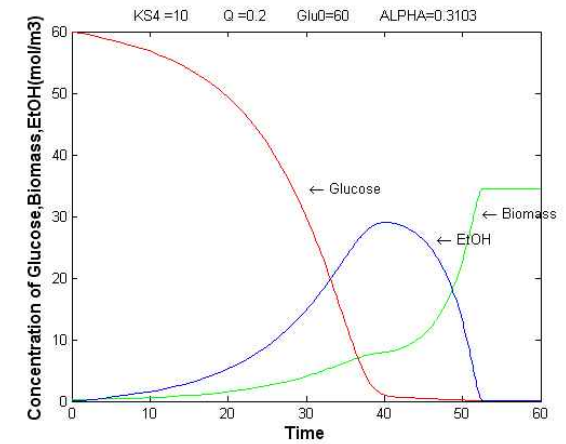
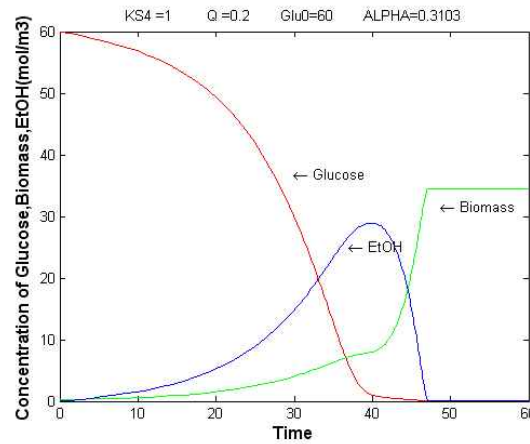
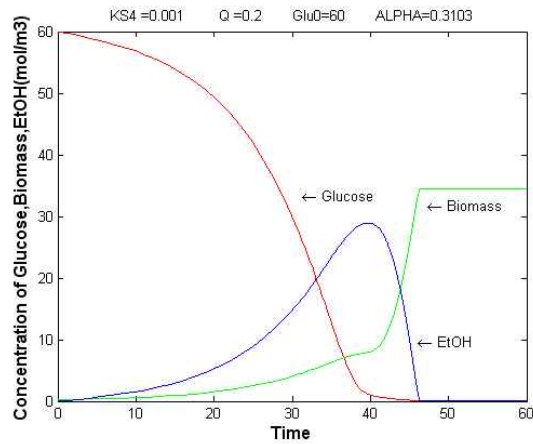
### ↘ ALPHA

◆ 작으면 작을 수록 EtOH 생성량 증가 예상

# Results and Discussion

## 결과

### KS4값의 변화

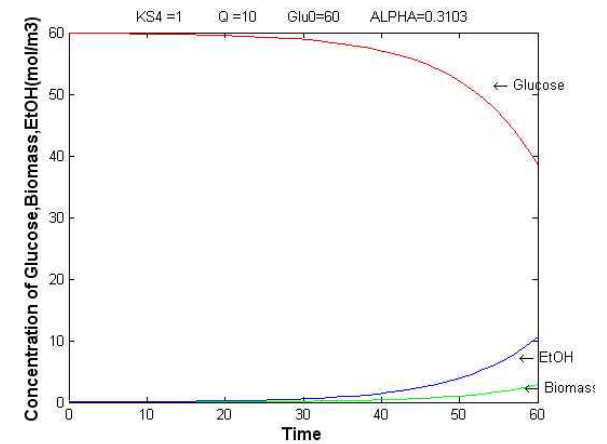
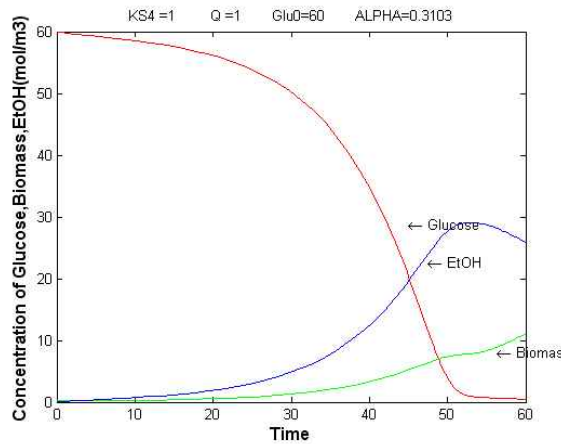
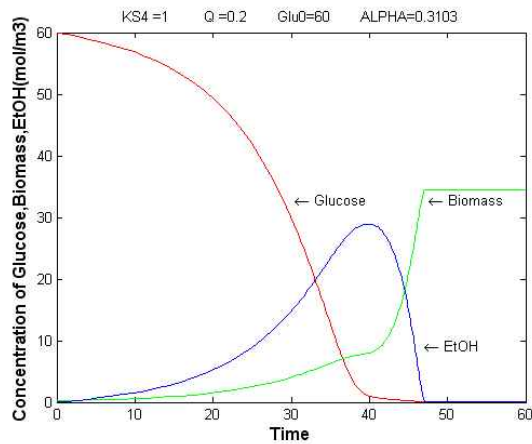
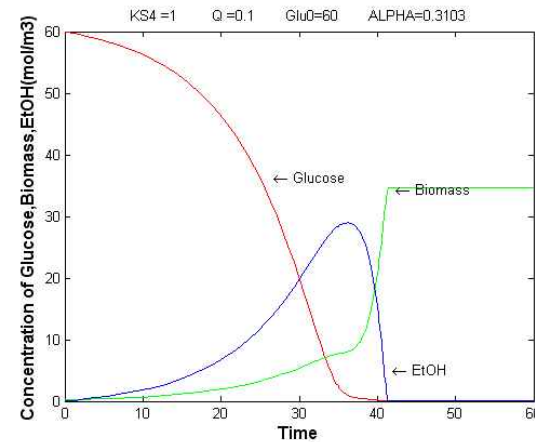
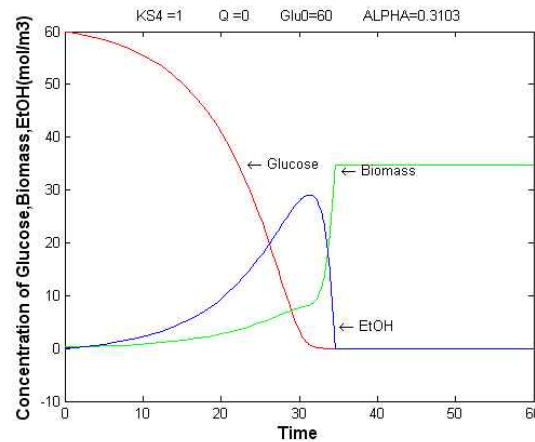


KS4 값이 클수록 EtOH의 양 변화가 적음.

# Results and Discussion

## 결과

### Q값의 변화

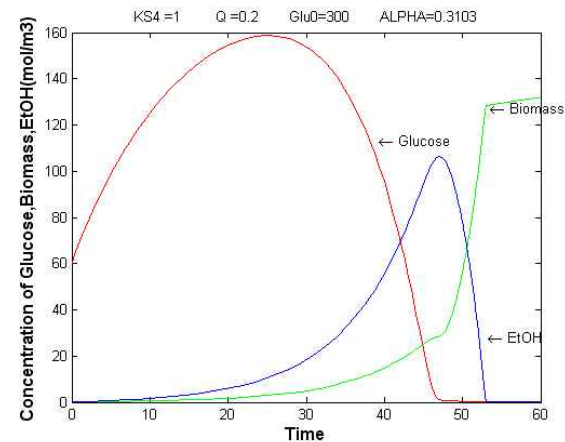
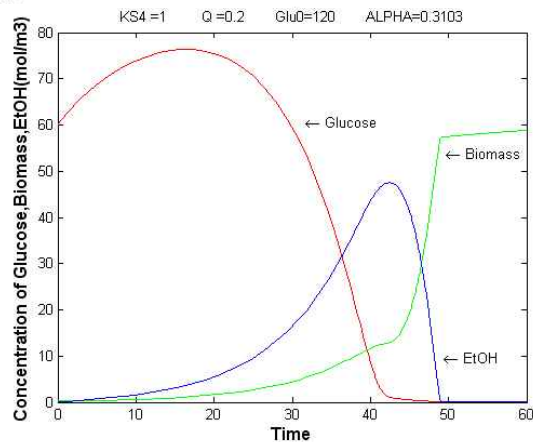
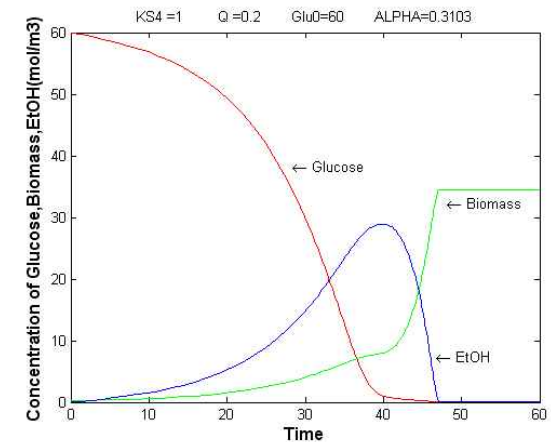
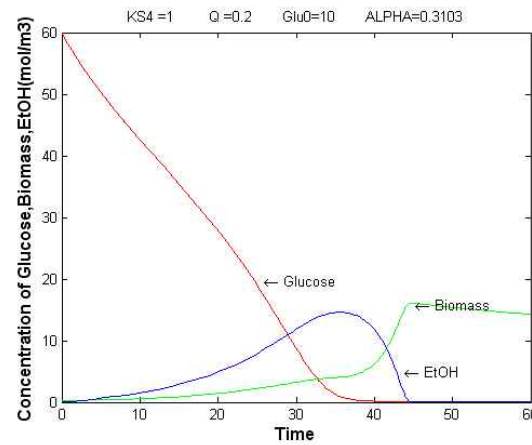
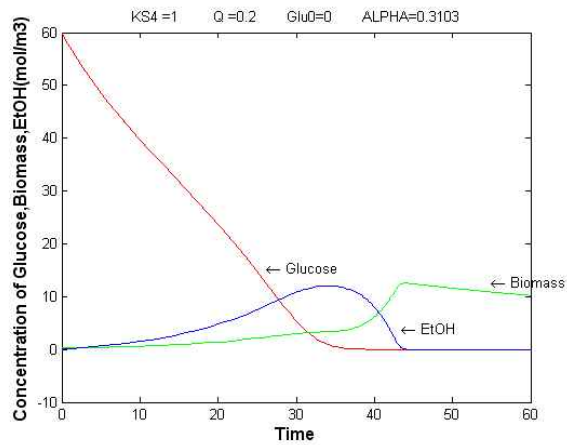


Q 값이 클수록 반응시간이 길어지며, EtOH의 수율도 나쁨

# Results and Discussion

## 결과

### Glu0 값의 변화

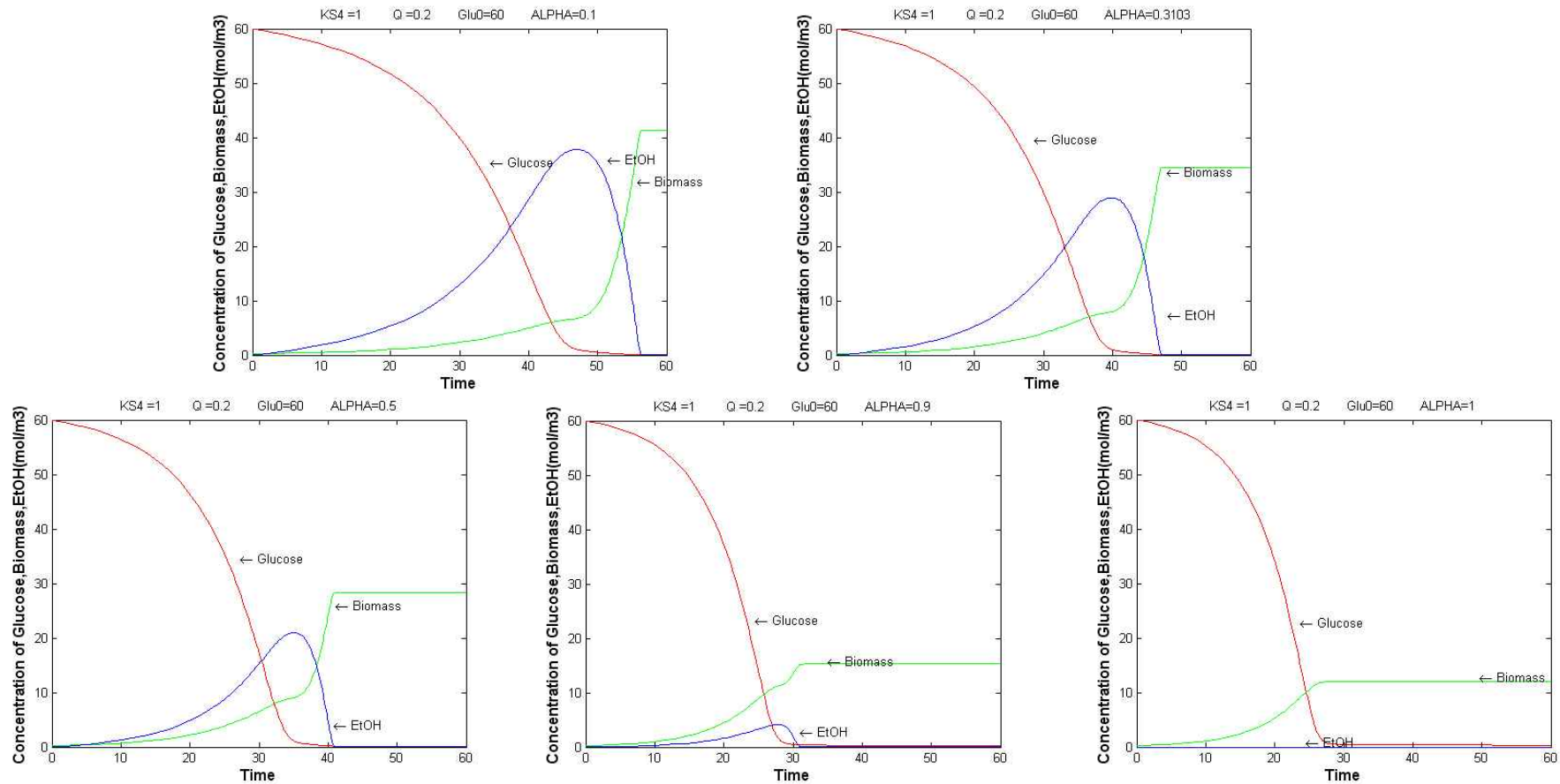


Glu0 값이 클수록 생성되는 EtOH의 양이 늘어남

# Results and Discussion

## 결과

### ALPHA 값의 변화

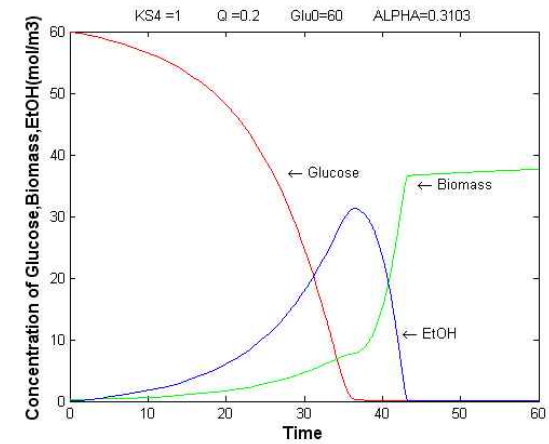
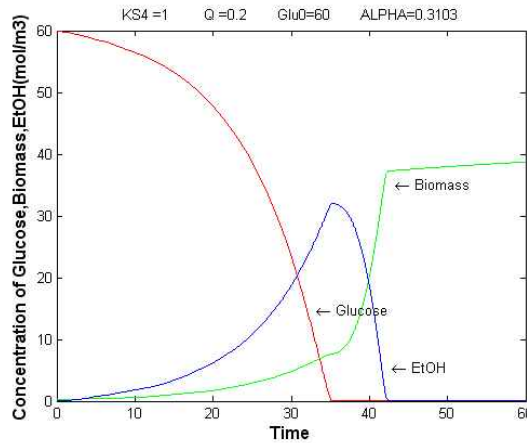
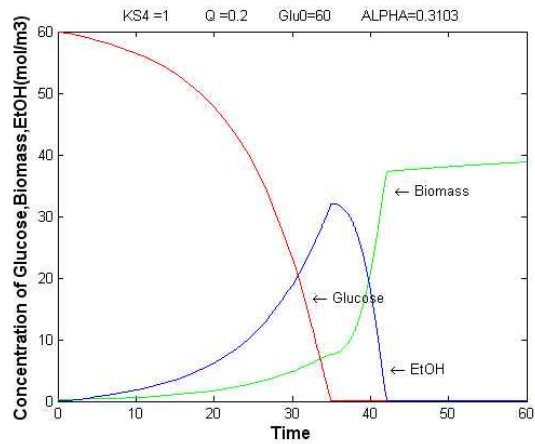


ALPHA 값이 클수록 생성되는 EtOH의 양이 적어짐

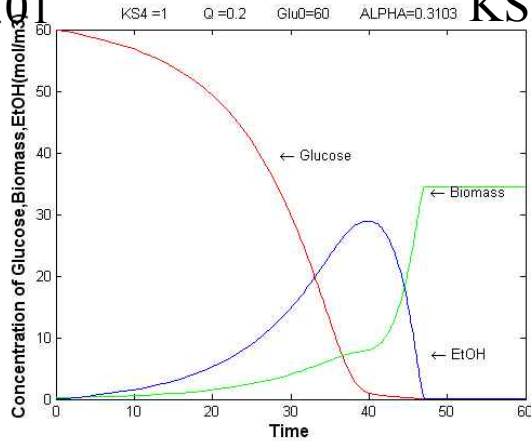
# Result and Discussion

## 결과

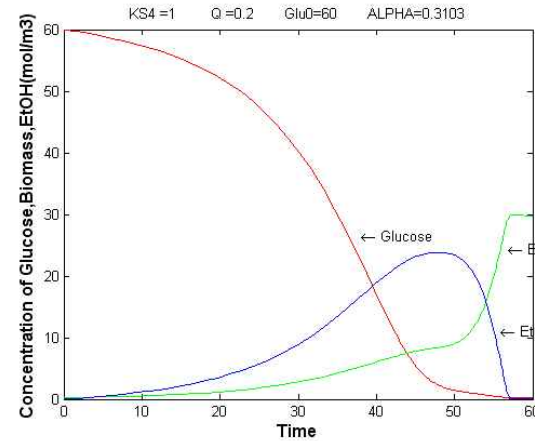
### KS4 와 KS2 값의 변화사이



KS2 : 0.01

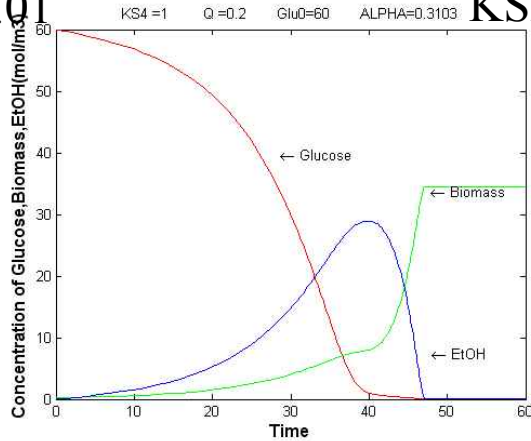


KS2 : 0.1



KS2 : 1

KS2 : 5



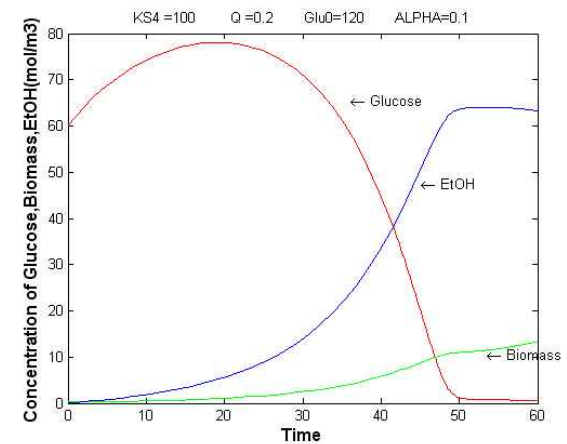
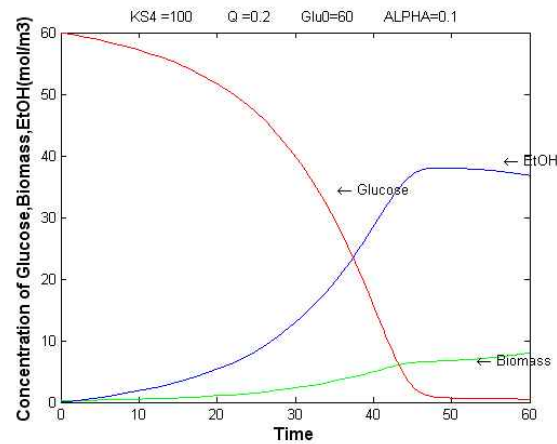
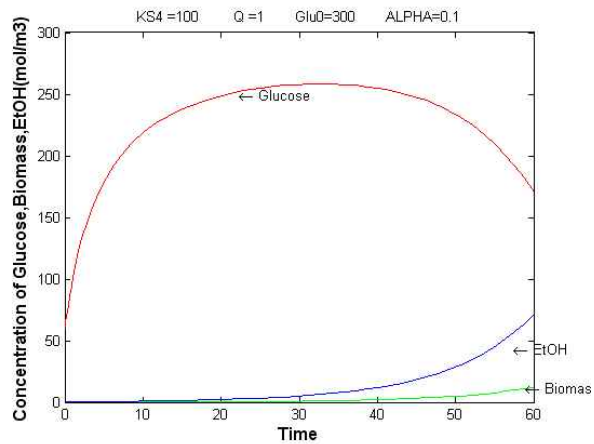
KS2 : 20

KS4의 변화에서는 EtOH의 양은 차이 없었으나, KS2는 약간 차이 있음.

# Result and Discussion

## 결과

결과값이 가장 좋았을 경우를 혼합시켜서



- 가장 많은 양을 얻기 위해 각 과정에서 제일 좋은 조건만 넣었지만  
처음과 같은 그래프가 나왔음
- 비율을 맞추는 것도 중요한 문제임.



# Conclusions

## ➔ 결론

- ➔ KS4 값이 커지면 EtOH의 수율이 증가한다.
- ➔ Q 값이 커지면 반응하는 시간이 더 오래 걸린다.
- ➔ Glu0의 값이 증가함에 따라서 생성되는 EtOH가 증가한다.
- ➔ Alpha값은 작을 수록 좋다.
- ➔ KS2 값은 생성되는 EtOH의 양에 영향을 준다.
- ➔ 반응기 설치 및 운전조건 확립시에는 전체적인 균형을 생각에 주어야한다.