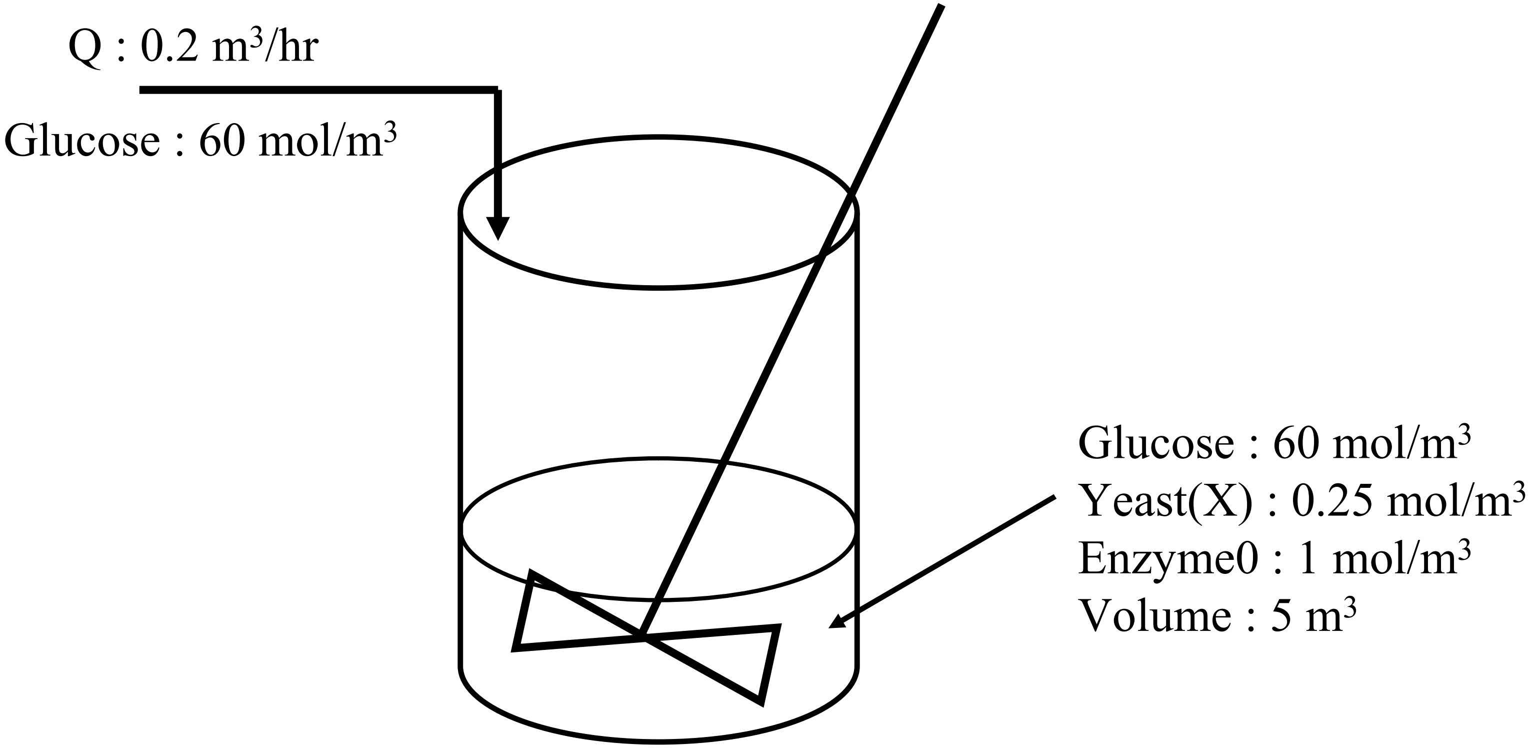
Ethanol Fed Batch Diauxic Fermentation

Introduction

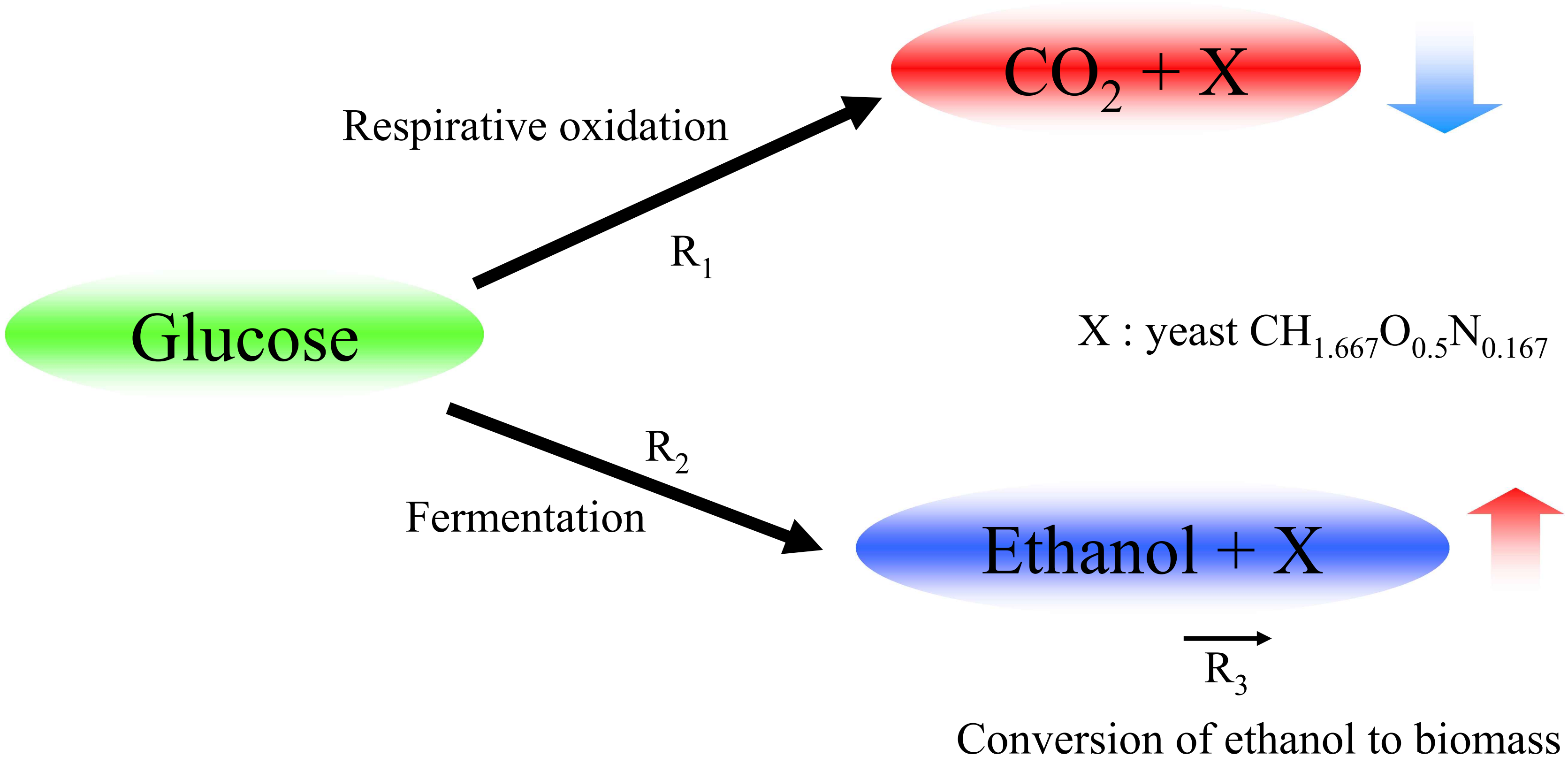
- Ethanol Fed Batch Diauxic Fermentation



Fed batch reactor

Introduction

- Ethanol Fed Batch Diauxic Fermentation



Pathway of aerobic ethanol fermentation

Introduction

Rate of the process

Respiritive 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_1

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

Production rate of enzyme E_2

$$R_5 = K_5 X E_1$$

Introduction

Mass and component balance of the biomass

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

Glucose 의 농도변화

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

Yeast 의 농도변화

$$\frac{dX}{dt} = Y_1 R_1 + Y_2 R_2 + Y_4 R_3 - \frac{XQ}{V}$$

EtOH 의 농도변화

$$\frac{dEtOH}{dt} = Y_3 R_2 - R_3 - \frac{EtOHQ}{V}$$

Enzyme 의 농도변화

$$\frac{dE_0}{dt} = -R_4 - \frac{E_0 Q}{V}$$

$$\frac{dE_1}{dt} = R_4 - R_5 - \frac{E_1 Q}{V}$$

$$\frac{dE_2}{dt} = R_5 - \frac{E_2 Q}{V}$$

Methods

- 수치해석을 위해 기호화
  - Volume -> V -> y1, Glucose -> Glu -> y2
  - Yeast -> X -> y3, Ethanol -> EtOH -> y4
  - Enzyme0 -> E0 -> y5, Enzyme1 -> E1 -> y6,
  - Enzyme2 -> E2 -> y7

R1=((y2/(y2+KS1))*K1*ALPHA*y3);

R2=((y2/(y2+KS2))*K2*(1-ALPHA)*y3);

R3=((y4/(y4+KP13))*K3*y7*y3);

R4=((K4/(KS4+y2*y2*y2))*y3*y5);

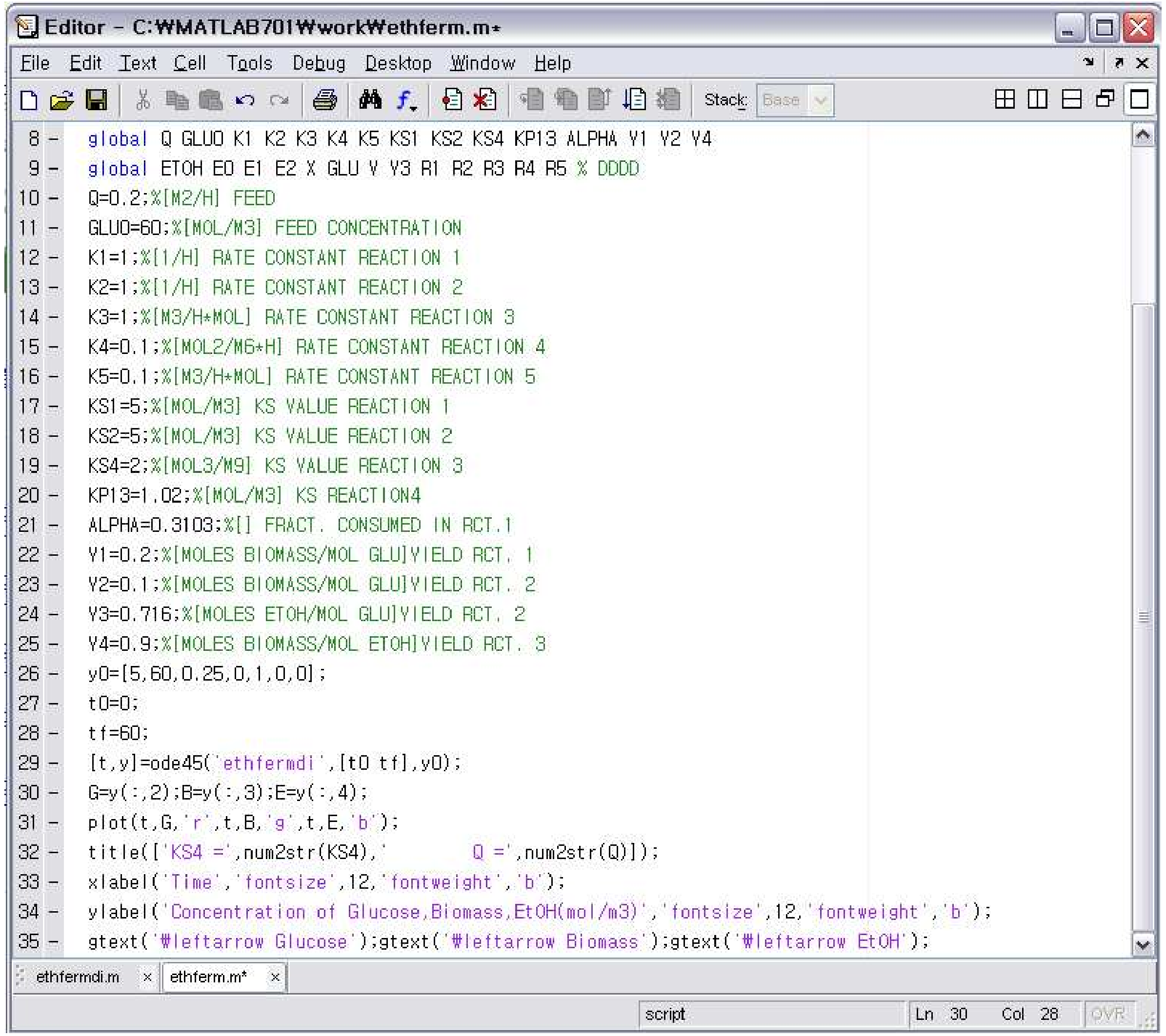
R5=(K5*y3*y6);

Methods

- 초기값 설정
  - Q=0.2;%[M2/H] FEED
  - GLU0=60;%[MOL/M3] FEED CONCENTRATION
  - K1=1;%[1/H] RATE CONSTANT REACTION 1
  - K2=1;%[1/H] RATE CONSTANT REACTION 2
  - K3=1;%[M3/H*MOL] RATE CONSTANT REACTION 3
  - K4=0.1;%[MOL2/M6*H] RATE CONSTANT REACTION 4
  - K5=0.1;%[M3/H*MOL] RATE CONSTANT REACTION 5
  - KS1=5;%[MOL/M3] KS VALUE REACTION 1
  - KS2=5;%[MOL/M3] KS VALUE REACTION 2
  - KS4=2;%[MOL3/M9] KS VALUE REACTION 3
  - KP13=1.02;%[MOL/M3] KS REACTION4
  - ALPHA=0.3103;%[] FRACT. CONSUMED IN RCT.1
  - Y1=0.2;%[MOLES BIOMASS/MOL GLU]YIELD RCT. 1
  - Y2=0.1;%[MOLES BIOMASS/MOL GLU]YIELD RCT. 2
  - Y3=0.716;%[MOLES ETOH/MOL GLU]YIELD RCT. 2
  - Y4=0.9;%[MOLES BIOMASS/MOL ETOH]YIELD RCT. 3

Methods

- M파일 작성
  - 초기값
  - 출력설정
  - 풀이법 등



Methods

- M파일 작성
  - 미분방정식

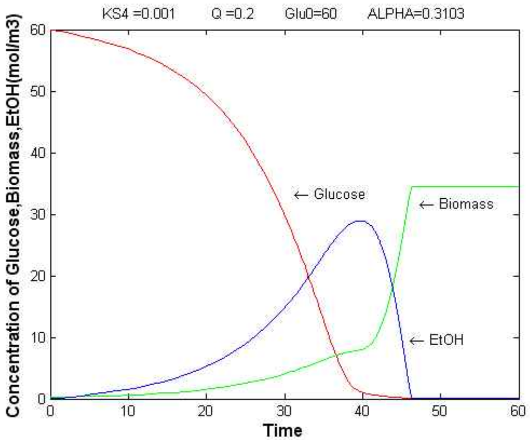
```
function dydt=ethfermdi(t,y)
global Q GLUO K1 K2 K3 K4 K5 KS1 KS2 KS4 KP13 ALPHA Y1 Y2 Y4 Y3
y1=y(1);y2=y(2);y3=y(3);y4=y(4);y5=y(5);y6=y(6);y7=y(7);
R1=((y2/(y2+KS1))*K1*ALPHA*y3);%GLU RESPIRATIVE OXIDATION
R2=((y2/(y2+KS2))*K2*(1-ALPHA)*y3);
R3=((y4/(y4+KP13))*K3*y7*y3);
R4=((K4/(KS4+y2*y2*y2))*y3*y5);
R5=(K5*y3*y6);
dydt=[Q;
       -(R1+R2)+(Q*GLUO-y2*Q)/y1;
      Y1*R1+Y2*R2+Y4*R3-y3*Q/y1;
      Y3*R2-R3-y4*Q/y1;
      -R4-y5*Q/y1;
      R4-R5-y6*Q/y1;
      R5-y7*Q/y1];
```

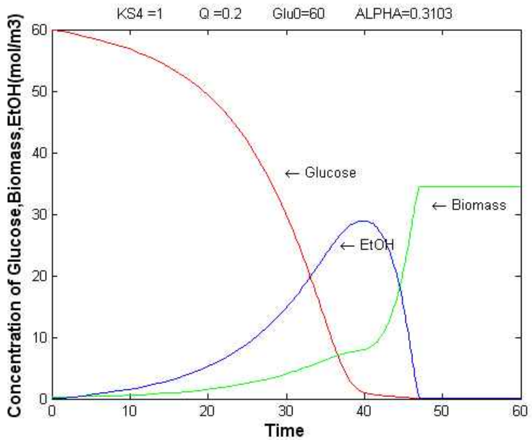
Methods

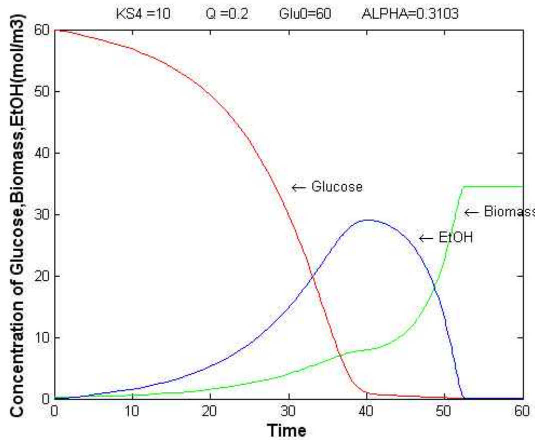
- 조건 변화 변수와 예측
  - KS4
    - EtOH의 생성과 밀접한 연관이 있음. -> EtOH의 증가 예상
  - Q
    - 유입되는 Glucose양의 변화에 따른 반응 정도 -> 속도가 느려지고 반응저하 예상
  - GluO
    - 유입되는 Glucose의 농도에 따른 양의 변화 -> EtOH 생성 저하 예상
  - ALPHA
    - 작으면 작을 수록 EtOH 생성량 증가 예상

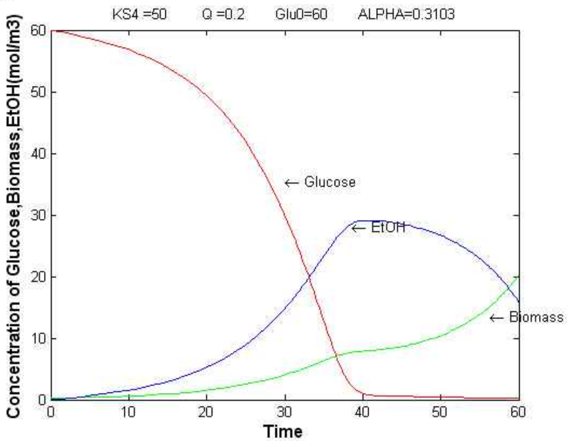
Results and Discussion

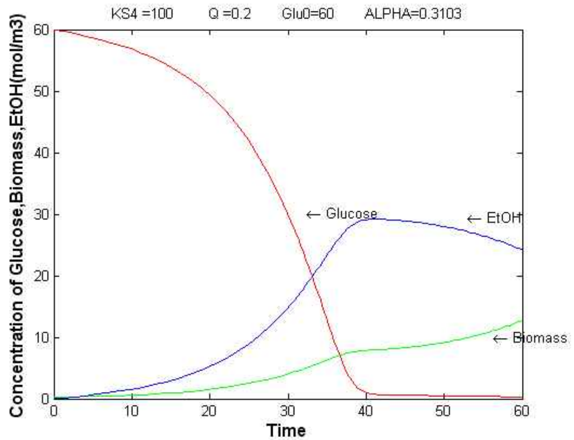
- 결과
  - KS4값의 변화







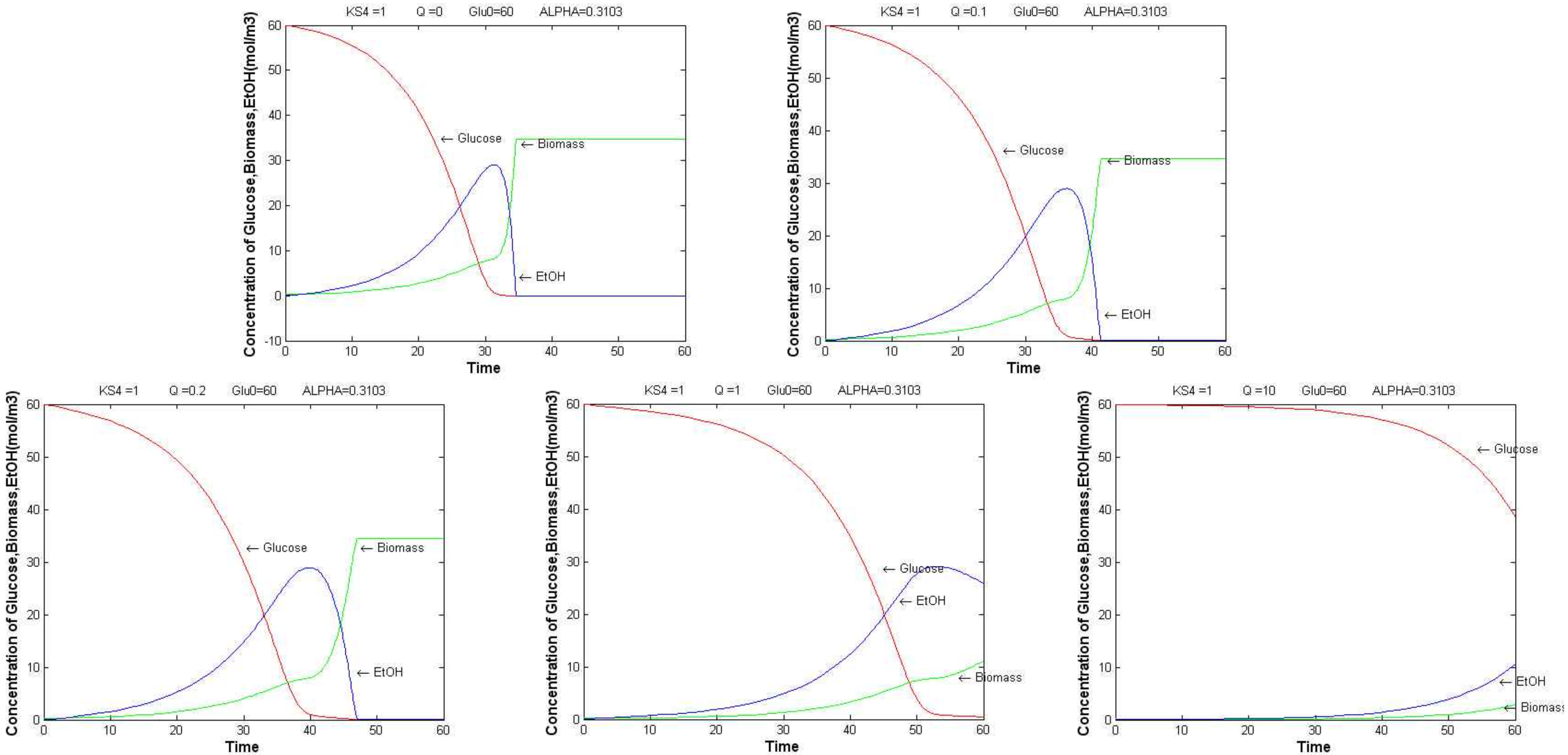




KS4 값이 클수록 EtOH의 양 변화가 적음.

Results and Discussion

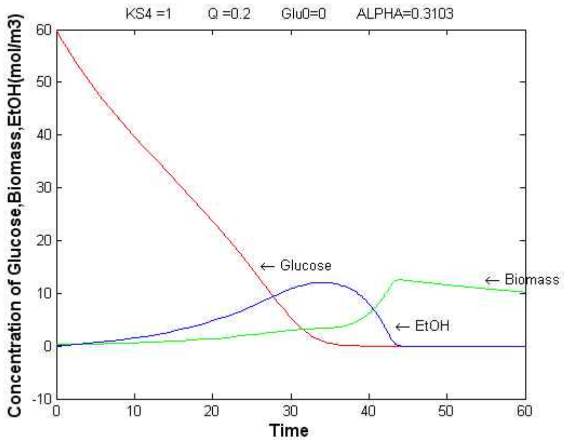
- 결과
  - Q값의 변화

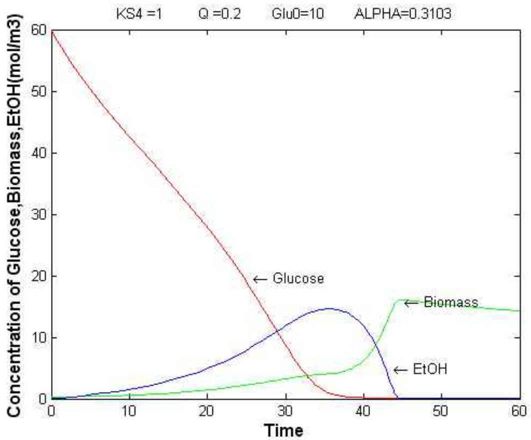


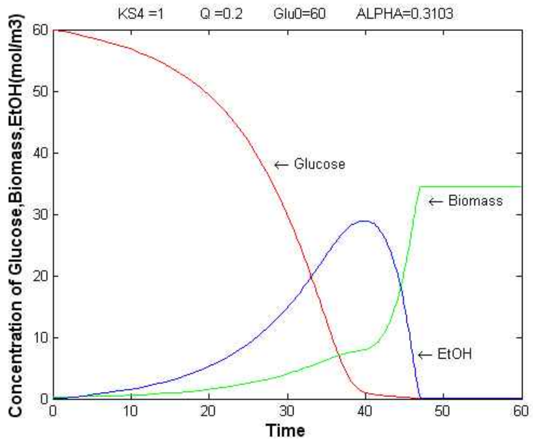
Q 값이 클수록 반응시간이 길어지며, EtOH의 수율도 나쁨

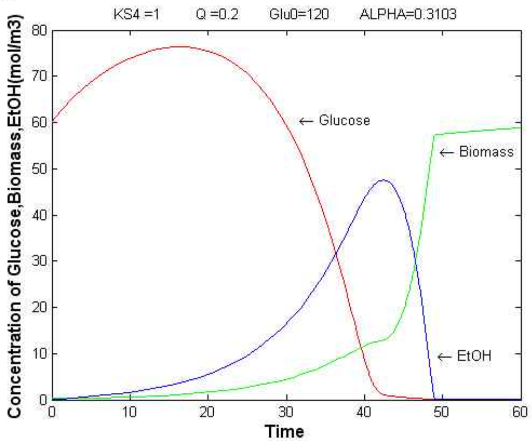
Results and Discussion

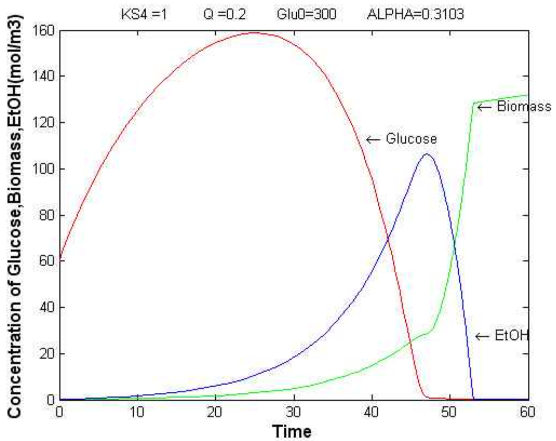
- 결과
  - Glu0 값의 변화







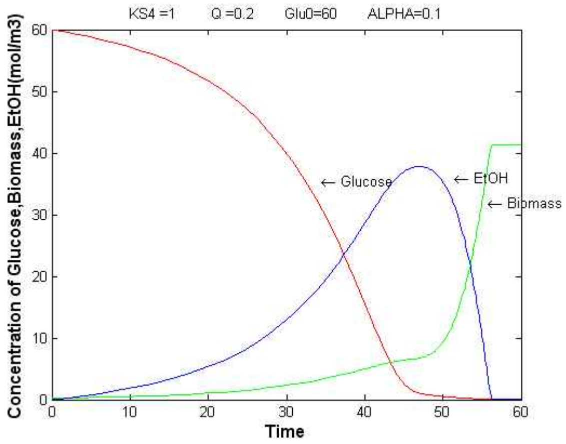


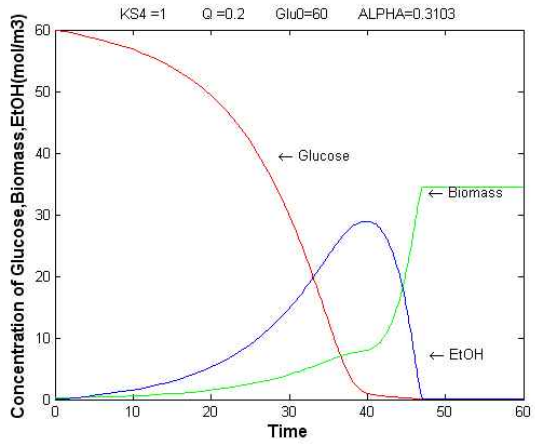


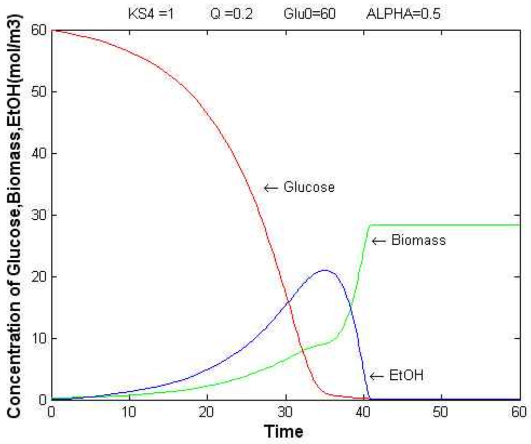
Glu0 값이 클수록 생성되는 EtOH의 양이 늘어남

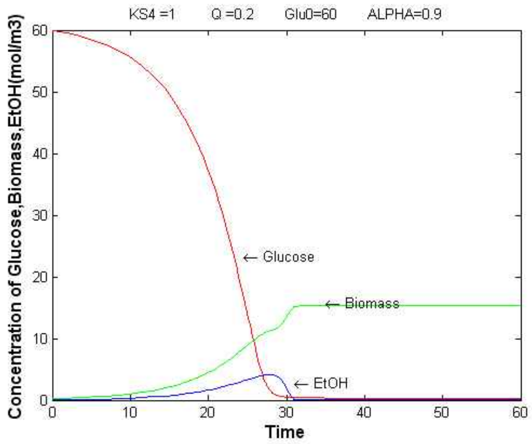
Results and Discussion

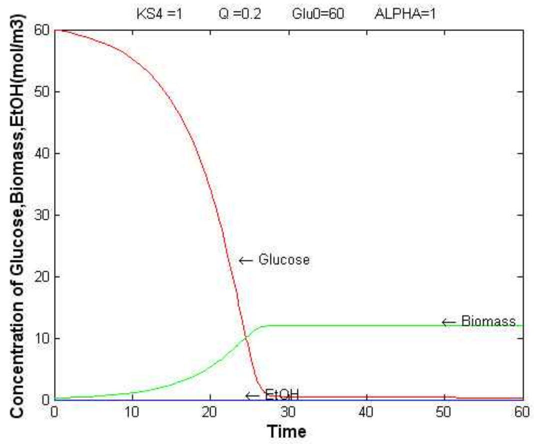
- **결과**
  - **ALPHA 값의 변화**









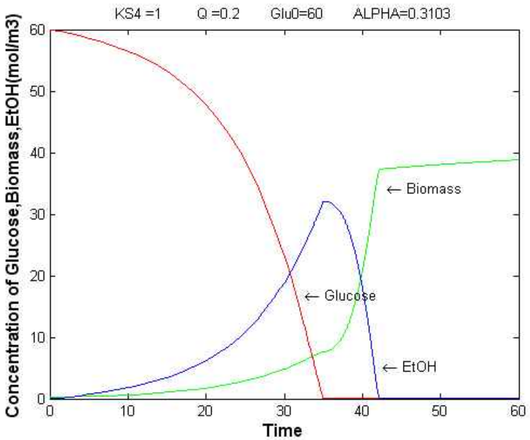


ALPHA 값이 클수록 생성되는 EtOH의 양이 적어짐

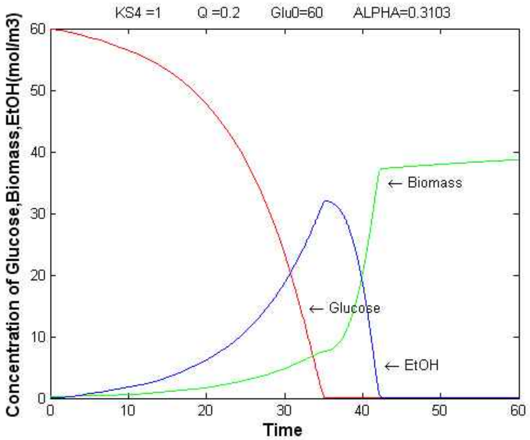
Result and Discussion

결과

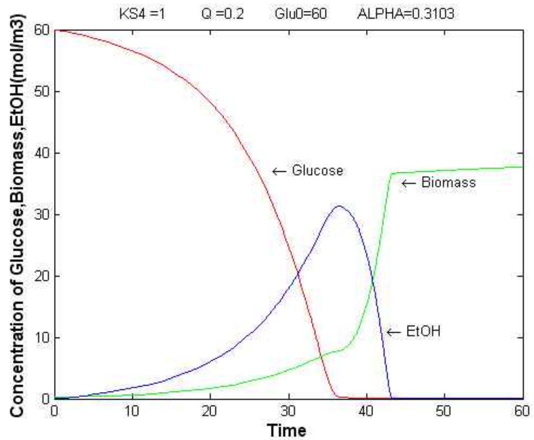
KS4 와 KS2 값의 변화차이



KS2 : 0.01

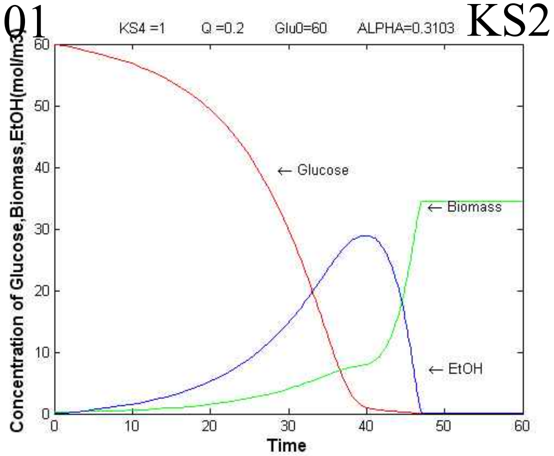


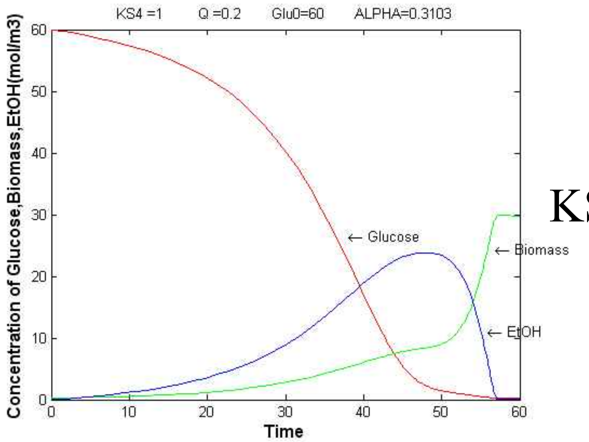
KS2 : 0.1



KS2 : 1

KS2 : 5



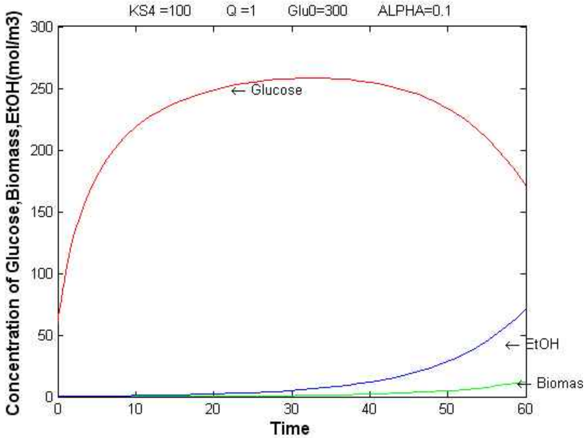


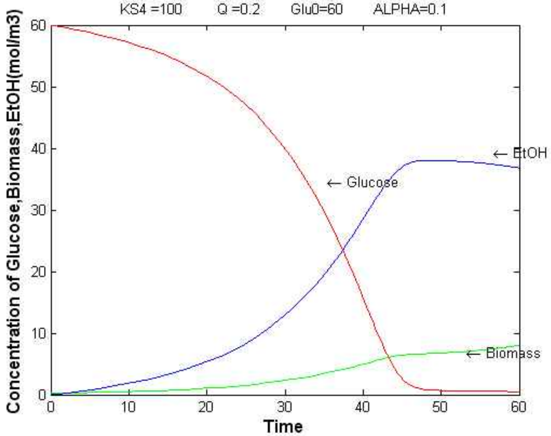
KS2 : 20

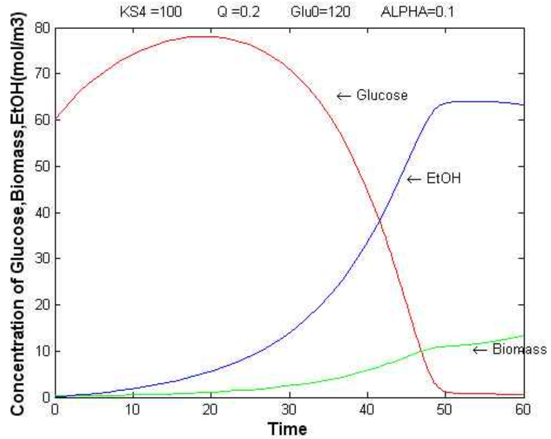
KS4의 변화에서는 EtOH의 양은 차이 없었으나, KS2는 약간 차이 있음.

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 생각해 주어야한다.