

# FINAL REPORT ON PH MODELING AND CONTROL

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## **Overview of The Final Report**

This final report details problems, their description and the solutions implemented against them. While the solutions are being explained, the approach to how problems should be solved are mentioned as well. When trying to tackle the problems arose, some sources like books, theses and codes are used. Furthermore, comparisons are made between existing codes and final codes and, their relation is given, whenever possible. The report follows the timeline, that is to say, the first problem encountered is discussed before the subsequent one. The ultimate aim of this final report is to explain everything in detail and give a holistic approach for developed models.

## **Acknowledgment**

I would like to thank my supervisor doc. Ing. Pavel Hrnčířík, Ph.D. for his support and his guidance during my internship. I strongly believe that the experience I gained from this internship will be immeasurably beneficial for me in any endeavor I want to take on.

# Problem Statement 1 – Variables for pH modeling

The program did not have any pH modeling and control which is very crucial for some species during the fermentation process. pH affects maximum specific growth rate directly and it also affects yield and productivity in an indirect way. The old version lacks some variables for pH model and control. To construct pH model before controlling, first it is needed that new manipulated, state and output variables must be added. They are going to be the building blocks of the entire system.

## Solution to Problem 1 – Adding new variables into yeast\_simcon

New manipulated variables are acid and base flow rate. In Figure 1, the acid flow rate is fourth manipulated variable, while the base flow rate is fifth manipulated variable. All manipulated variables are going to change with time when control action is taken. As it can be seen, they are not separated into strong or weak acid or base. Reason for that is it is convenient to use this way.

```
%%
% u(:,1) ... feed flowrate (F, ml/s) (according to a specific feeding strategy)
% u(:,2) ... air flowrate (Fv, ml/s) (in a laboratory fermenter typically 10 l/min, i.e. 167 ml/s)
% u(:,3) ... stirrer speed (n, 1/s) (in a laboratory fermenter typically 600 1/min, i.e. 10 1/s)
%%
% u(:,4) ... flow rate of acid which is either strong or weak (ml/s)
% u(:,5) ... flow rate of base which is either strong or weak (ml/s)
```

Figure 1 Addition of Acid and Base Flow Rates.

There will be either strong acid strong base scenario or weak acid weak base scenario. The strong base and acid are NaOH and H<sub>2</sub>SO<sub>4</sub>, respectively. For the weak acid weak base, the agents are H<sub>3</sub>PO<sub>4</sub> and NH<sub>4</sub>OH [1].

As for new state variables, they are NaOH, H<sub>2</sub>SO<sub>4</sub>, H<sub>3</sub>PO<sub>4</sub>, NH<sub>4</sub>OH and NH<sub>3</sub> concentrations in the bioreactor since they will be added continuously into the system. When creating differential equations, they are going to be used. But the main reason why they are incorporated into state variables is that they are going to be used when pH model is implemented. In other words, pH model needs these variables. In Figure 2, they are clearly displayed with units.

```
% x(:,10) ... NaOH concentration in the fermentation broth (cnaoh, mol/ml)
% x(:,11) ... H2SO4 concentration in the fermentation broth (ch2so4, mol/ml)
% x(:,12) ... NH4OH concentration in the fermentation broth (cnh4oh, mol/ml)
% x(:,13) ... H3PO4 concentration in the fermentation broth (ch3po4, mol/ml)
% x(:,14) ... NH3 concentration in the fermentation broth (cnh3, mol/ml)
```

Figure 2 Addition of New State Variables.

The only output variable added here is pH. Its value will be calculated with the help of pH modeling. In Figure 3, pH addition is given.

```
% y(:,1) ... ethanol mol fraction in the fermentation broth (xe, %)
% y(:,2) ... O2 mol fraction in the bioreactor off-gas (xoog, %)
% y(:,3) ... CO2 mol fraction in the bioreactor off-gas (xcog, %)
% y(:,4) ... dissolved O2 concentration in the fermentation broth (DO, % saturation)
%%
% y(:,5) ... pH value (unitless)
```

Figure 3 Addition of pH.



## Problem Statement 2 – Necessary equilibrium constants for pH modeling

For pH to be modeled, there are necessary equilibrium constants for each reaction. These constants are going to be used in the final equations for pH modeling for both strong and weak scenarios. They must be stored in `get_par` code because it is where all parameters reside.

## Solution to Problem 2 – Storing equilibrium constants in `get_par` code

In Figure 4, it can be seen that they are logged in `get_par` code. They are from the thesis [1].

```
p(42) = 1.047e-3; % equilibrium constant for first carbonic acid reaction Kh0
p(43) = 4.074e-4; % equilibrium constant for second carbonic acid reaction Kh1
p(44) = 5.6e-11; % equilibrium constant for third carbonic acid reaction Kh2
p(45) = 1.3e-16; % equilibrium constant for ethanol Ke1
p(46) = 1e-14; % equilibrium constant for water Kw
p(47) = 6.9e-3; % equilibrium constant for first phosphoric acid reaction ka1
p(48) = 6.2e-8; % equilibrium constant for second phosphoric acid reaction ka2
p(49) = 4.8e-13; % equilibrium constant for third phosphoric acid reaction ka3
p(50) = 5.5e-10; % equilibrium constant for ammonium hydroxide kb1
```

Figure 4 Equilibrium Constants.



## **Problem Statement 3 – Necessary constant concentration values for NaOH, H<sub>2</sub>SO<sub>4</sub>, H<sub>3</sub>PO<sub>4</sub>, NH<sub>4</sub>OH and NH<sub>3</sub>**

In order for pH model to work, some constant concentration values must be stored in `get_par` code. These constant concentration values are needed to solve differential equations in `f` code. The logic behind this is that differential equations are going to calculate the state variables, for example NaOH, and then these state variables will determine the pH value.

## **Solution to Problem 3 – Storing constant concentration values for NaOH, H<sub>2</sub>SO<sub>4</sub>, H<sub>3</sub>PO<sub>4</sub>, NH<sub>4</sub>OH and NH<sub>3</sub> in `get_par` code**

In Figure 5, it can be seen that they are stored in `get_par` code. They are from the thesis [1].

```
p(51) = 0.0026;          % NaOH concentration at the base vessel (mol/ml)
p(52) = 0.00132;         % H2SO4 concentration at the acid vessel (mol/ml)
p(53) = 0.0019;          % H3PO4 concentration at the acid vessel (mol/ml)
p(64) = 0.0039;          % NH4OH concentration in the base tank
p(65) = 0.0039;          % NH3 concentration at the base vessel (mol/ml)
```

Figure 5 Constant Concentration Values.



## Problem Statement 4 – Coefficients for NH<sub>3</sub> in each reaction

So far, parameters for differential equations and pH model have been logged since they will give us pH values in return. After the differential equations, pH modeling will be carried out. In differential equations, NH<sub>3</sub> has a reaction term. To construct that, every coefficient for NH<sub>3</sub> in every reaction should be known. Only then the differential equation for NH<sub>3</sub> is complete.

## Solution to Problem 4 – Calculating coefficients for NH<sub>3</sub> in each reaction in get\_par

The procedure and results are given below. This procedure depends on simple atomic balance between reactants and products. y(i)xs coefficients are for the biomass for each reaction. The coefficients y(i)xs are from the existing model [2]. Results are also given in Figure 6. y(i)ns are separate coefficients for ammonia in reaction 1,2 or 3.

- $y(i)ns = y(i)xs * N \text{ atoms in biomass}$
- $y1ns = -0.584 * 0.17 = -0.1$
- $y2ns = -0.083 * 0.17 = -0.014$
- $y3ns = -0.658 * 0.17 = -0.112$

```
p(57) = -0.1;          % y1ns
p(58) = -0.014;        % y2ns
p(59) = -0.112;        % y3ns
```

Figure 6 Calculated Coefficients for NH<sub>3</sub>.



## Problem Statement 5 – Other parameters for NH<sub>3</sub> for mass transfer

So as to further develop NH<sub>3</sub> behavior in the differential equation, concentration of ammonia in the inlet gas and Henry's constant must be known. They are going to contribute to the mass transfer rate.

### Solution to Problem 5 – Setting other parameters for NH<sub>3</sub> for mass transfer in get\_par

While Henry's constant for ammonia is found to be 9.49e+4 from a source, the concentration of ammonia in the inlet gas is assumed to be 0 [3]. Parameters can be seen in Figure 7. Now, caw value, which is the equilibrium concentration value, can be calculated with the help of these parameters. caw is particularly going to be needed because it will further help develop evaporating NH<sub>3</sub>. To get an idea of how caw is calculated, please refer to f code.

```
p(60) = 0;          % concentration of ammonia in the inlet gas (mol/ml)
p(61) = 9.49e+4;    % Ha (Pa)
```

Figure 7 Other Parameters for Ammonia.



## **Problem Statement 6 – Ammonia evaporation**

Ammonia needs to be modeled with evaporation. Since it is highly volatile compound, it is imperative that the differential equation for ammonia should include evaporation term in its mass transfer.

### **Solution to Problem 6 – $K_{alvol}$ coefficient in calc\_Kalvol code**

One book suggested its proper way of modeling with  $K_{alvol}$  coefficient [4]. This equation is shown in Figure 8. This coefficient accounts for the evaporation phenomenon. All variables can be measured except for Kalvol which going to be calculated with the help of this code. Further description is given below.

- $F_{nG}$  is air flowrate into the bioreactor (ml/s),
- $V_l$  is the volume of the bioreactor (ml),
- $K_w$  is the ion product of the water ( $\text{mol}^2/\text{l}^2$ )
- $C_{alLtot}$  is the concentration of ammonia in the bioreactor (mol/ml)
- $M_{al}$  is the molar mass of ammonia, but this variable is not used.
- $K_{al}$  is the value of ammonia dissociation constant (mol/l)
- $C_{hl}$  is the concentration value of hydrogen ions in the bioreactor (mol/l)
- $K_{alvol}$  is a dimensionless parameter to be found by ‘calc\_Kalvol’ code.
- It is assumed that,
- $akla*(caw-ca)=AITR(t)$ , for only estimation.

- $t = 0$ , which means we have constant values of all concentration, volume of the bioreactor and air flowrate into the bioreactor. As a result, the equation above is solved in an algebraic way.

This code provides  $K_{alvol}$  values with respect to Henry's constants. In this work, Henry's constant for ammonia is assumed to be  $9.49e+5$  which corresponds to  $K_{alvol}$  of 137. From now on  $AlTR(t)$  equation is going to be used. For more detail, please check out `calc_Kalvol` code.

$$AlTR(t) = - \frac{K_{Alvol} \cdot F_{nG}(t)}{V_L(t)} \cdot \frac{K_W \cdot C_{AlLtot}(t) \cdot M_{Al}}{K_{Al} \cdot C_{HL}^+(t) + K_W}$$

Figure 8 Mass Transfer Equation of Ammonia [4].



## Problem Statement 7 – Absence of reaction term for NH<sub>3</sub>

Ammonia needs reaction terms for each three reaction. Without it, differential equation for ammonia is incomplete.

## Solution to Problem 7 – Addition of reaction term for NH<sub>3</sub>

Reaction kinetics follow the same logic as described in the previous paper [2]. It needs to be multiplication of coefficients by rs(i). At the end, what matters is summation of each three reactions individually. After that, the ammonia reaction term is complete. In Figure 9, they are shown.

```
rs1=-qs1*cx;
rx1=p(27)*rs1;
ro1=(1+1.05*p(27))*rs1;
rc1=(-1-p(27))*rs1;
ra1=p(57)*rs1;

rs2=-qs2*cx;
rx2=p(28)*rs2;
re2=(-2/3-0.7*p(28))*rs2;
rc2=(-1/3-0.3*p(28))*rs2;
ra2=p(58)*rs2;

re3=-qe3*cx;
rx3=p(29)*re3;
ro3=(1.5+1.05*p(29))*re3;
rc3=(-1-p(29))*re3;
ra3=p(59)*re3;

rx=rx1+rx2+rx3;
rs=rs1+rs2;
re=re2+re3;
ro=ro1+ro3;
rc=rc1+rc2+rc3;
ra=ra1+ra2+ra3;
```

Figure 9 Reaction Term for Ammonia.



## **Problem Statement 8 – Absence of new flow rates in f code**

Different species will need different flow rates because some species are not present in some flow rates. In previous model, the only flow rate for species was glucose feed rate. However, this will not be the case from now on.

## **Solution to Problem 8 – Addition of new flow rates in f code**

Acid and base flow rates are added in f code because they are going to be needed when some species are being modeled. It is done because now the model does not only have glucose feed flow rate, but also acid and base flow rate. Also, F\_in variable is given which is the summation of each three flow rates. In Figure 10, they are shown.

```
vvi=u(1);
F_a = u(4);
F_b = u(5);

F_in = vvi + F_a + F_b;
```

Figure 10 Manipulated Variables in f Code.



## Problem Statement 9 – Old differential equations

Old model took into account only glucose feed flow when creating differential equation. But now, since there are new flow rates, differential equations themselves have to change according to that.

## Solution to Problem 9 – Reconstructing the differential equations in f code

Before reconstructing, some assumptions must be made. General equation for each species is given below in Figure 11 [4]. For example,  $c_i^{vvi}$  means i-th species' concentration value in vvi stream, in this case glucose feed stream.  $F_a$  is acid stream and  $F_b$  is base stream. Note that they are all for liquid phase.

- Biomass

No biomass in either acid or base stream so,  $c_i^{F\_a} = c_i^{F\_b} = 0$

No mass transfer

- Glucose

No glucose in either acid or base stream so,  $c_i^{F\_a} = c_i^{F\_b} = 0$

No mass transfer

- Ethanol

No ethanol in either acid or base stream so,  $c_i^{F\_a} = c_i^{F\_b} = 0$

With mass transfer

- Oxygen

No oxygen in either acid or base stream so,  $c_i^{F-a} = c_i^{F-b} = 0$

With mass transfer

- Carbon Dioxide

No carbon dioxide in either acid or base stream so,  $c_i^{F-a} = c_i^{F-b} = 0$

With mass transfer

- Volume of the bioreactor

It is the sum of all flow rates into the bioreactor.

- NaOH

No NaOH in glucose feed stream and acid stream so,  $c_i^{vvi} = c_i^{F-a} = 0$

No mass transfer

No reaction rate

- H<sub>2</sub>SO<sub>4</sub>

No H<sub>2</sub>SO<sub>4</sub> in glucose feed stream and base stream so,  $c_i^{vvi} = c_i^{F-b} = 0$

No mass transfer

No reaction rate

- NH4OH

No NH4OH in glucose feed stream and acid stream so,  $c_i^{vvi} = c_i^{F-a} = 0$

No mass transfer

No reaction rate

- H3PO4

No H3PO4 in glucose feed stream and base stream so,  $c_i^{vvi} = c_i^{F-b} = 0$

No mass transfer

No reaction rate

- NH3

No NH3 in glucose feed stream and acid stream so,  $c_i^{vvi} = c_i^{F-a} = 0$

With mass transfer and reaction rate

$$\frac{dc_i}{dt} = \frac{vvi(t) * c_i^{vvi}}{V_L(t)} + \frac{(F_a(t) * c_i^{Fa})}{V_L(t)} + \frac{(F_b(t) * c_i^{Fb})}{V_L(t)} - \frac{F_{in}(t)}{V_L(t)} * c_i(t) + r_i + iTR$$

Figure 11 General Equation for All Species [4].

The final equation for each species are given below in Figure 12. Commented lines are for old equation. New added variables here have initial value of 0 for all species which are from 10 to 14.

```

yout(1)=rx+(vvi*p(13)/vt)-(F_in*cx/vt);
yout(2)=rs+(vvi*p(14)/vt)-(F_in*cs/vt); % changed
%yout(3)=re+(F_in)/vt*(p(15)-ce)+akla*(cew-ce);
yout(3)=re+(vvi*p(15)/vt)-(F_in*ce/vt)+akla*(cew-ce);
yout(4)=ro+(vvi*p(16)/vt)-(F_in*co/vt)+akla*(cow-co); % changed
%yout(5)=rc+(F_in)/vt*(p(17)-cc)+akla*(ccw-cc);
yout(5)=rc+(vvi*p(17)/vt)-(F_in*cc/vt)+akla*(ccw-cc);
yout(6)=F_in;
yout(7)=kon2*(-qocap+max([min([qodes qou1]) p(36)])); % min max
yout(8)=kon1*(-help-sup);
yout(9)=1/p(39)*(p(38)/(p(38)+ce)-1-sup);

yout(10)=F_b/vt*p(51) - F_in*cnaoh/vt;
% yout(10)=0;
yout(11)=F_a/vt*p(52) - F_in*ch2so4/vt;
% yout(11)=0;
yout(12)=F_b/vt*p(63) - F_in*cnh4oh/vt;
yout(13)=F_a/vt*p(53) - F_in*ch3po4/vt;
yout(14)=ra+(F_b*p(65)/vt)-(F_in*ca/vt) + (-Kalvol*u(2)/vt)*(Kw*ca/(Kal*ch_ion+Kw)); % changed

```

Figure 12 Final Equations in f Code.



## **Problem Statement 10 – pH modeling for weak acid weak base scenario**

Now that differential equations which give the concentration values of acid or base agents are implemented, pH can be modeled. The existing model does not have any pH model for weak scenario. In order to have an idea of how pH changes over time, the model must be included. That way, the control action could be implemented afterwards.

## **Solution to Problem 10 – Using ionic balance equations for weak acid weak base scenario to create wawb code**

In the construction of the code, all state variables and parameters are included in case they are needed. The thesis will be referred to because it has comprehensive final equations for both scenarios. This thesis uses several dissociation constants so they are stored in a vector called p. Static modeling is used for pH where these models are only valid when there is an equilibrium [1]. This static modeling is going to be coupled with dynamic models which involve differential equations for strong or weak acid or base agents. This code is derived from charge2.m code which was used for the thesis [5]. It includes some tweaks to the original code charge 2.m but they are essentially serve same purpose. The final ionic balance is given in Figure 13. Its MATLAB equivalence is shown in Figure 14. In the g code, the equation will be made equal to 0 in order to get H ion denoted as h in the code. As you can see, new state variables  $H_3PO_4$  and  $NH_4OH$  are used. For more detail and variables in the equation, please check out the thesis, wawb and charge2 codes.

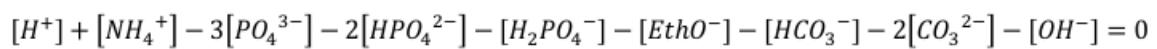


Figure 13 The Ionic Balance for Weak Acid Weak Base Scenario [1].

```
y = h - p(46)/h ...
+ (cNH4/pseudoalphaA)*cnh4oh ...
- (cH2P04/pseudoalphaP)*ch3po4 - 2*(cHP04/pseudoalphaP)*ch3po4 - 3*(cP04/pseudoalphaP)*ch3po4 ...
- (cHC03/pseudoalphaC)*cc - 2*(cC03/pseudoalphaC)*cc ...
- ((p(45)/h)/pseudoalphaE)*ce;
```

Figure 14 The Final Equation for Weak Acid Weak Base Scenario in MATLAB.



## **Problem Statement 11 – pH modeling for strong acid strong base scenario**

Now that differential equations which give the concentration values of acid or base agents are implemented, pH can be modeled. The existing model does not have any pH model for strong scenario. In order to have an idea of how pH changes over time, the model must be included. That way, the control action could be implemented afterwards.

## **Solution to Problem 11 – Using ionic balance equations for strong acid strong base scenario to create sasb code**

In the construction of the code, all state variables and parameters are included in case they are needed. The thesis will be referred to because it has comprehensive final equations for both scenarios. This thesis uses several dissociation constants so they are stored in a vector called p. Static modeling is used for pH where these models are only valid when there is an equilibrium [1]. This static modeling is going to be coupled with dynamic models which involve differential equations for strong or weak acid or base agents. This code is derived from charge.m code which was used for the thesis [6]. It includes some tweaks to the original code charge.m but they are essentially serve same purpose. The final ionic balance is given in Figure 15. Its MATLAB equivalence is shown in Figure 16. In the g code, the equation will be made equal to 0 in order to get H ion denoted as h in the code. As you can see, new state variables NaOH and H<sub>2</sub>SO<sub>4</sub> are used. For more detail and variables in the equation, please check out the thesis, sasb and charge codes.

$$\begin{aligned}
[H^+] + X - \frac{k_w}{[H^+]} - \frac{\frac{k_{a0}H_2CO_3k_{a1}H_2CO_3}{[H^+]} + 2\frac{k_{a0}H_2CO_3k_{a1}H_2CO_3k_{a2}H_2CO_3}{[H^+]}}{\left(1 + k_{a0}H_2CO_3 + \frac{k_{a0}H_2CO_3k_{a1}H_2CO_3}{[H^+]} + \frac{k_{a0}H_2CO_3k_{a1}H_2CO_3k_{a2}H_2CO_3}{[H^+]^2}\right)} [CO_{2(aq)}]_{Total} - \\
-\frac{\frac{k_{a1}EthOH}{[H^+]}}{\left(1 + \frac{k_{a1}EthOH}{[H^+]}\right)} [EthOH]_{Total} = 0
\end{aligned}$$

Figure 15 The Ionic Balance for Strong Acid Strong Base Scenario [1].

```
%% charge balance
y = h - p(46)/h + (cnaoh-2*ch2so4) - (cHCO3/alphaC)*cc - 2*(cCO3/alphaC)*cc - ((p(45)/h)/alphaE)*ce;
```

Figure 16 The Final Equation for Strong Acid Strong Base Scenario in MATLAB.



## Problem Statement 12 – pH output absence in g code

Now that pH is modeled, pH value can be a variable in g code as an output. A built-in function is needed to get H ion concentration value in the bioreactor.

## Solution to Problem 12 – Providing g code with pH value in g code

Finally, pH is able to be plotted as a function of time. It is fifth output variable. Before calculating pH, fzero built-in function should be used since the ultimate equation in either wawb or sasb code must be equal to zero in order to get H ion concentration. The implementation is given in Figure 17.

```
% pH
fun = @(h) wawb(h,x,p);
z = fzero(fun,[1e-20;100000]);
yout(5)=-log10(z);
ph_values=yout(5)
```

Figure 17 The implementation of pH value in g code.



## **Problem Statement 13 – Initial concentration values**

If the initial concentration values are entered wrong, the system behaves differently. So, what is needed is entering the new state variable's initial concentration values.

### **Solution to Problem 13 – Providing RUN\_YEAST\_SIMCON code with new initial conditions**

There are five new state variables, namely two strong and weak acid and base agents and ammonia concentration. Their initial value in the bioreactor is assumed to be 0. The last five values are represented in Figure 18.

```
x0=[4e-5 0 0 2.3e-7 0 5000 5.5556e-5 0 0 0 0 0 0 0];
```

Figure 18 Initial Values of New State Variables.



## Problem Statement 14 – Absence of relationship between maximum specific growth rate and pH

Maximum growth rate is an important parameter for the species involved in the bioreactor. This in return requires a modeling of it against pH value.

## Solution to Problem 14 – Implementation of mathematical model for maximum specific growth rate and pH

To model, cardinal parameters such as optimal, minimum and maximum pH values are used [7]. Also, alpha parameter is introduced as a fine tuning option for the fitness of the graph, in case it is subjected to any experiment. The final parameter in the code in Figure 19 is to show that the maximum specific growth rate occurs at the optimal pH value. Please note that peak value is the value stored in get\_par code. The output of the code is a bell curve. The parameters for the code are shown in Figure 20. As can be seen, only glucose and ethanol species are simulated for this purpose as they are the only species whose the maximum specific growth rates are stored in get\_par code. Optimal pH value is selected to be 4.8 [8].

```
% Define gammamapH function
function gamma_pH = gammamapH(pH, pHopt, pHmin, pHmax, alfa, qmax)
    % First coefficient K1
    num = alfa;
    denom1 = (alfa - alfa * ((pHopt - pHmin) / (pHmax - pHmin))) / ((pHopt - pHmin) / (pHmax - pHmin));
    denom = alfa + denom1;
    K1 = (num / denom)^(-alfa);

    % Second coefficient K2
    K2 = (1 - (alfa / denom ))^-(denom1);

    K3 = ((pH-pHmin)/(pHmax-pHmin)).^alfa;
    K4 = (1 - ((pH-pHmin)/(pHmax-pHmin))).^(denom1);

    % Final gamma_pH result
    gamma_pH = K1 * K2 .* K3 .* K4*qmax;
end
```

Figure 19 Mathematical Model for Maximum Growth Rate vs. pH.

```

pHmin = min(yc(:,5));
pHmax = max(yc(:,5));
pHopt = 4.8;           % Optimal pH
alfa = 2;              % Alpha parameter

% Normalize gamma_pH to have a maximum value of 1
%gamma_pH = gamma_pH / max(gamma_pH);
pH_value = yc(:,5);
gamma_pH = gammamapH(pH_value, pHopt, pHmin, pHmax, alfa, 2.94/3600);
figure;
plot(pH_value, gamma_pH, 'b-', 'LineWidth', 2);
xlabel('pH');
ylabel('\gamma_{pH}');
title('\gamma_{pH} for Glucose as a Function of pH');
grid on;

gamma_pH = gammamapH(pH_value, pHopt, pHmin, pHmax, alfa, 0.22/3600);
figure;
plot(pH_value, gamma_pH, 'b-', 'LineWidth', 2);
xlabel('pH');
ylabel('\gamma_{pH}');
title('\gamma_{pH} for Ethanol as a Function of pH');
grid on;

```

Figure 20 Parameters for The Model.



## Problem Statement 15 – Absence of relationship between temperature and time

Temperature is an important parameter for the species involved in the bioreactor. This in return requires a modeling of it against time.

## Solution to Problem 15 – Implementation of mathematical model for temperature and time

Temperature of baker's yeast cultivation is carried out approximately at 30C, so in the code depicted in Figure 21, it is set constant 30. Whereas the process follows the constant 30C, a comparison is made by plotting a sinus wave with a peak value of 34.1C and the lowest value of 13.9C [8]. Frequency is set arbitrarily.

```
peak_value = 34.1;
low_value = 13.9;
frequency = 1 / 200; % arbitrary frequency in Hz

% Time vector
time=[t0:ts:t1]';
time=time./60;

% Amplitude and offset
amplitude = (peak_value - low_value) / 2;
offset = (peak_value + low_value) / 2;

% Sinusoidal function
sinusoidal = amplitude * sin(2 * pi * frequency * time) + offset;

% Straight line
straight_line = 30 * ones(size(time));

% Plot
figure;
plot(time, sinusoidal, 'b', 'LineWidth', 1.5); hold on;
plot(time, straight_line, 'r--', 'LineWidth', 1.5);
title('Sinusoidal Function and Straight Line');
xlabel('Time (minutes)');
ylabel('Value');
legend('Sinusoidal Function', 'Straight Line (y=30)');
grid on;
```

Figure 21 The Code for Temperature vs. Time.



## **Problem Statement 16 – Absence of relationship between maximum specific growth rate and temperature**

Temperature is an important parameter for the species involved in the bioreactor. This time growth rate vs. temperature is to be modeled.

## **Solution to Problem 16 – Implementation of mathematical model for maximum specific growth rate and temperature**

To model, cardinal parameters such as optimal, minimum and maximum T values are used [7]. Also, alpha parameter is introduced as a fine tuning option for the fitness of the graph, in case it is subject to any experiment. Maximum specific growth rate occurs at the optimal T value. Please note that peak value is the value that is constant 30C [8]. The output of the code is a bell curve. The parameters for the code are shown in Figure 22. Optimal T value is selected to be 30C [8]. Maximum temperature and minimum temperature values are 35.9C and 13C, respectively [8]. Mathematical implementation is given in Figure 23 [7].

```
% gammamaT Function and Plot
% Parameters
Tmin = 13.9;           % Minimum T
Tmax = 35;             % Maximum T
Topt = 30;              % Optimal T
alfa = 4;               % Alpha parameter

% Normalize gamma_T to have a maximum value of 1
gamma_T = gamma_T / max(gamma_T);
T_value = linspace(Tmin,Tmax,100); % 100 pH values between Tmin and Tmax
gamma_T = gammamaT(T_value, Topt, Tmin, Tmax, alfa);
figure;
plot(T_value, gamma_T, 'b-', 'LineWidth', 2);
xlabel('T');
ylabel('\gamma_{\{T\}}');
title('(\gamma_{\{T\}}) as a Function of T (Normalized to 1)');
grid on;
```

Figure 22 Parameters for Maximum Specific Growth Rate vs. Temperature.

```
%%
% Define gammamaT function
function gamma_T = gammamaT(T, Topt, Tmin, Tmax, alfa)
    % First coefficient K1
    num = alfa;
    denom1 = (alfa - alfa * ((Topt - Tmin) / (Tmax - Tmin))) / ((Topt - Tmin) / (Tmax - Tmin));
    denom = alfa + denom1;
    K1 = (num / denom)^(-alfa);

    % Second coefficient K2
    K2 = (1 - (alfa / denom ))^-(denom1);

    K3 = ((T-Tmin)/(Tmax-Tmin)).^alfa;
    K4 = (1 - ((T-Tmin)/(Tmax-Tmin))).^(denom1);

    gamma_T = K1 * K2 .* K3 .* K4;
end
% Plot the results
```

Figure 23 Mathematical Implementation of Maximum Growth Rate vs. Temperature.



## **Problem Statement 17 – Absence of a control action for pH in weak case**

There is no control action in old model. So it is needed that a control action should be implemented.

## **Solution to Problem 17 – Reconstructing the REGULAR\_DOCONT\_v4 for pH control**

While the control action for glucose feed flowrate stays the same, pH control is incorporated at the end of the code. This code specifically designed for weak acid weak base scenario as it is multiplied by 1.5 after controller output for base addition. It starts with calculating the error between setpoint and current value. The setpoint here is stored in auxt array. The whole code is constructed from an existing code and thesis [1,9]. In thesis the, there are SIMULINK files. These SIMULINK files are converted into MATLAB files.

In the case of  $e > 0$ , the base stream will enter the system.  $kP$  is set by trial and error method. For integral part, cumulative errors are needed. To carry this out, trapezoidal rule is used and the output of integral part is given.  $kI$  is set by trial and error method. Initially, base stream steady state value is kept 0. Finally, the flowrate of base is set by multiplying the summation of proportional and integral part by 1.5. If there is a base flow, there should not be an acid flow into the system.

The same logic applies to the situation where error is less than zero. In this situation, acid is added. The things that are different from base addition is  $kP$  value, cumulative error,  $kI$  and controller output multiplier.  $kP$  value is -0.000036. It is negative because there is a reverse relationship between pH and acid addition. The

control output is not multiplied by 1.5 but rather 1. Lastly, the volume of the bioreactor is kept at 7500 maximum. For more information, please check out REGULAR\_DOCONT\_v4.

As it can be seen, the same PID parameters are not used in this case. If the same parameters were used, the model would behave very strange, making the feed glucose rate less than zero.



## **Problem Statement 18 – Absence of a control action for pH in strong case**

There is no control action in old model. So it is needed that a control action should be implemented.

### **Solution to Problem 18 – Creating the REGULAR\_DOCONT\_v4\_v2 for pH control**

This code specifically designed for strong acid strong base scenario as it is multiplied by 1 after controller output for base addition. The only differences from previous control code is control output of base addition is not multiplied by 1.5.



## Problem Statement 19 – Choosing between the cases

There are lots of cases. One should be picked.

### Solution to Problem 19 – Creating the productivity and yield table for each case

The table is shown in Figure 24. In weak acid weak base scenario as setpoint increases, the yield increases too. As for strong acid strong base scenario, the yield reaches a constant value around 0.4830 gX/gS at 4.8 and 5.5 pH values. On the other hand, productivity peaks at 4.8 pH with 0.9599 gX/gS in weak acid weak base scenario. But it is shown to continue going up with increasing pH value in strong acid strong base scenario. The ideal pick would be 5.5 pH and strong scenario since the productivity is the highest and its yield is comparable to the value in weak scenario and 4.8 pH value.

The reason why 4 is simulated is it is needed to see how the system behaves under optimal conditions which is 4.8. And the reason why 5.5 is simulated is that it is imperative to see how the system behaves above optimal conditions.

	Weak Acid Weak Base Scenario			Strong Acid Strong Base Scenario		
	4	4.8	5.5	4	4.8	5.5
Yield (gX/gS)	0.4794	0.4830	0.4851	0.4806	0.4830	0.4829
Productivity (gX/1/h)	0.9224	0.9599	0.9454	0.9459	0.9602	0.9752

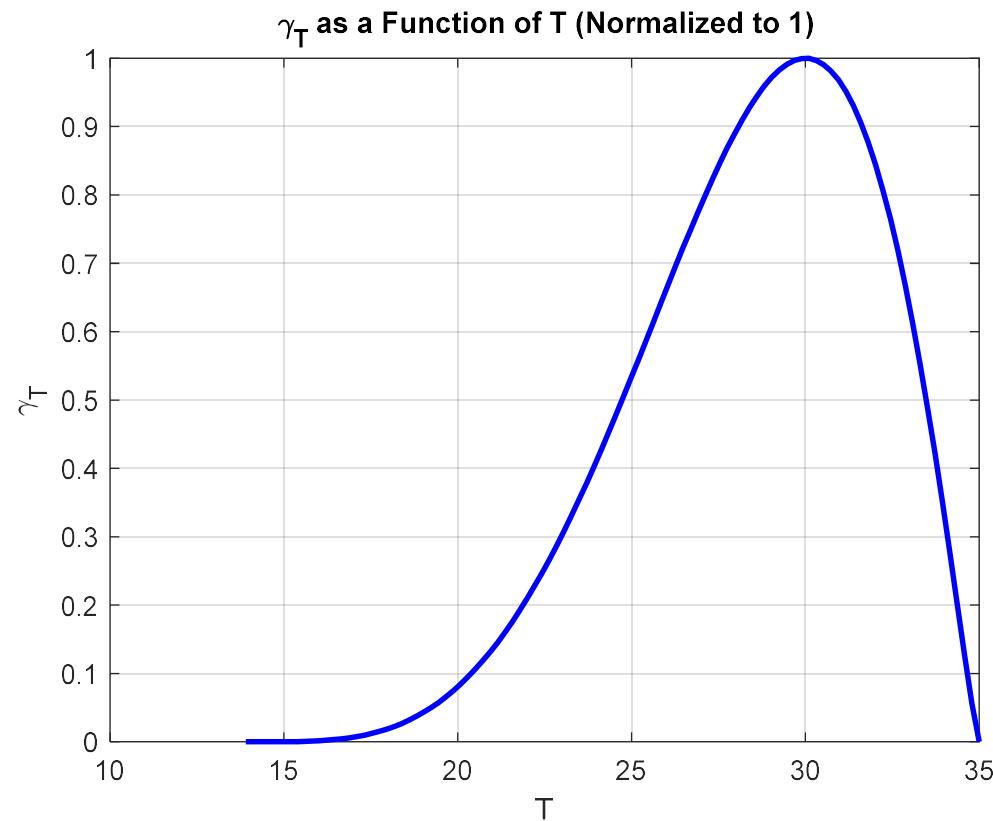
Figure 24 Productivity and Yield Chart.

## REFERENCES

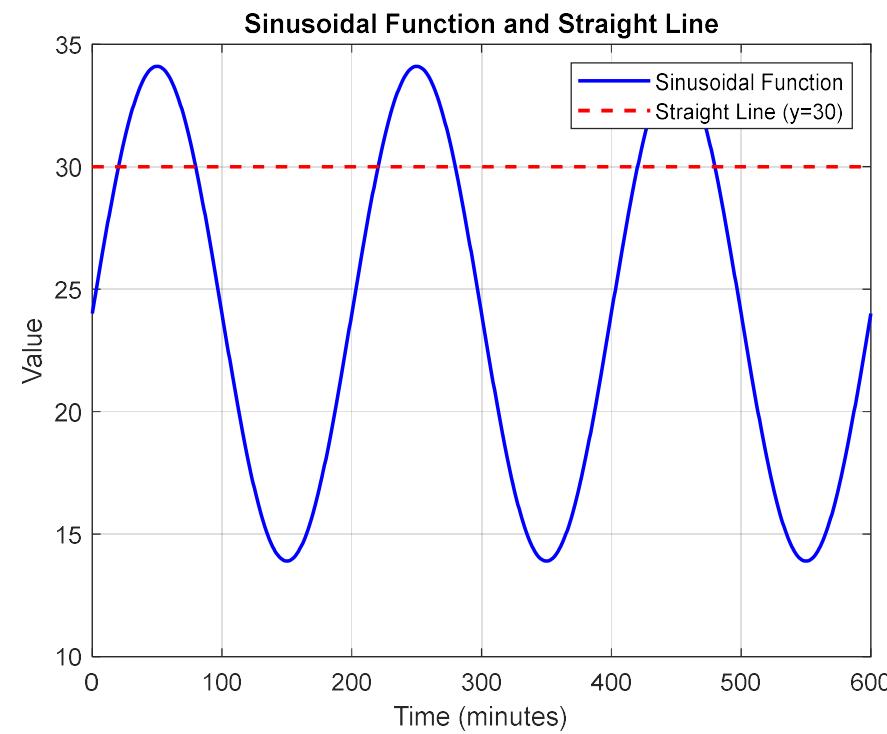
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- [2] YEASTsim: a Matlab-based simulator for the study of process control of fed-batch yeast fermentations, Pavel Hrnčířík, Jan Kohout, UCT Prague. Accessed: Nov. 25, 2024.
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## SIMULATION RESULTS

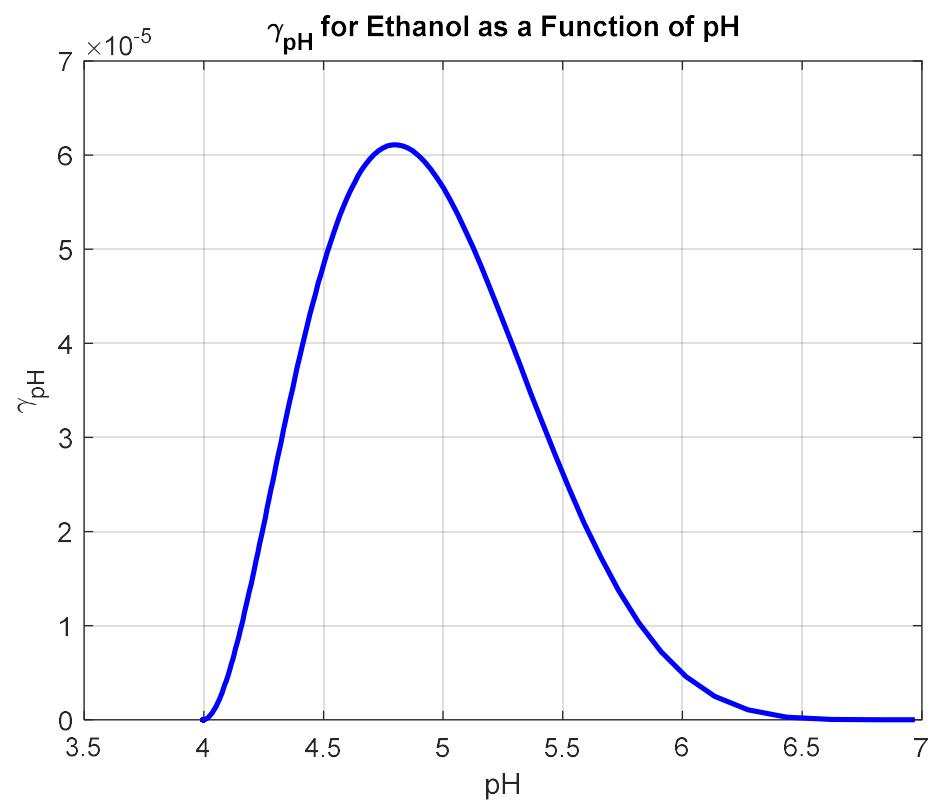
# Simulation Results for Weak Acid Weak Base and Set Point of 4 with Steady State Value of 3.9998



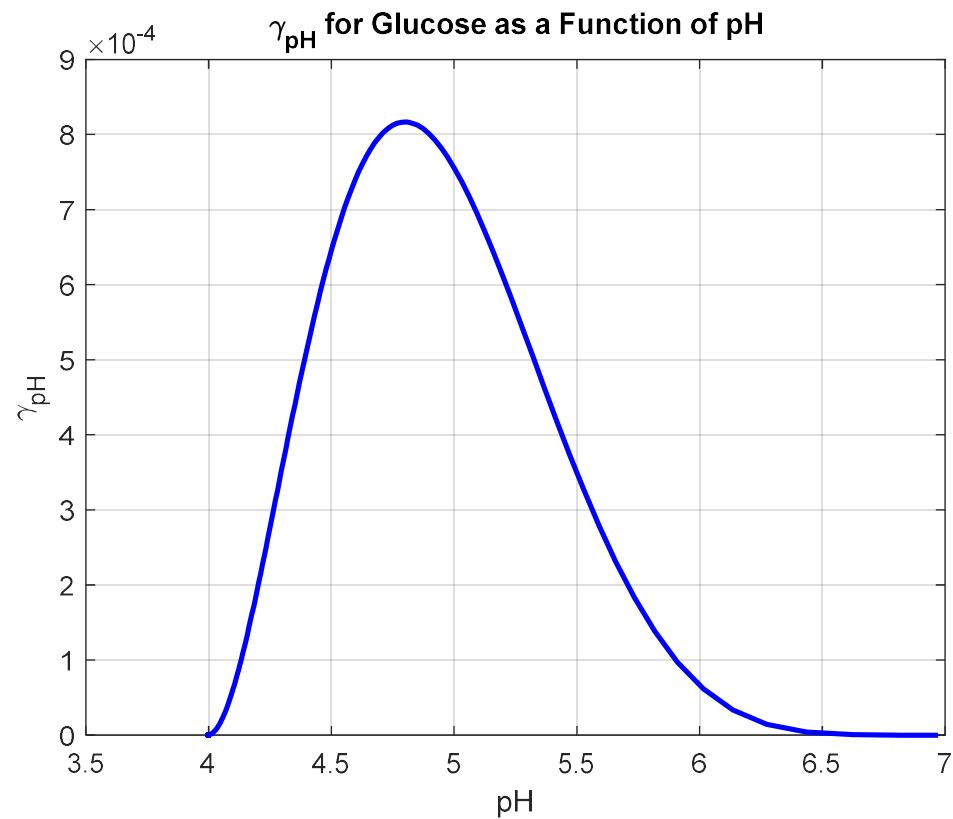
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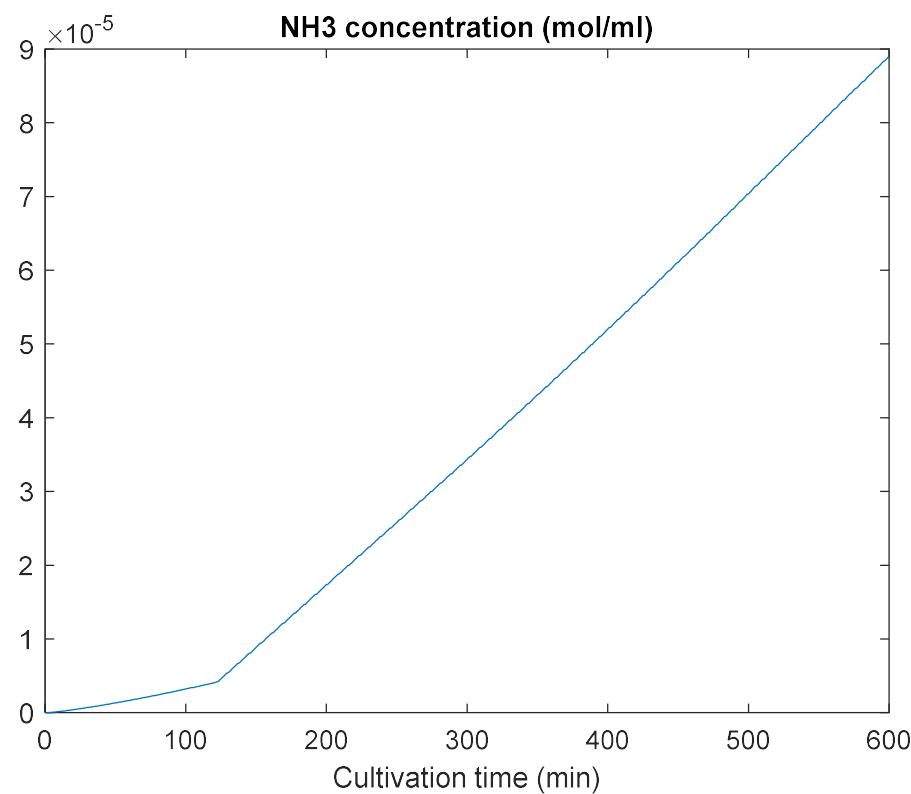
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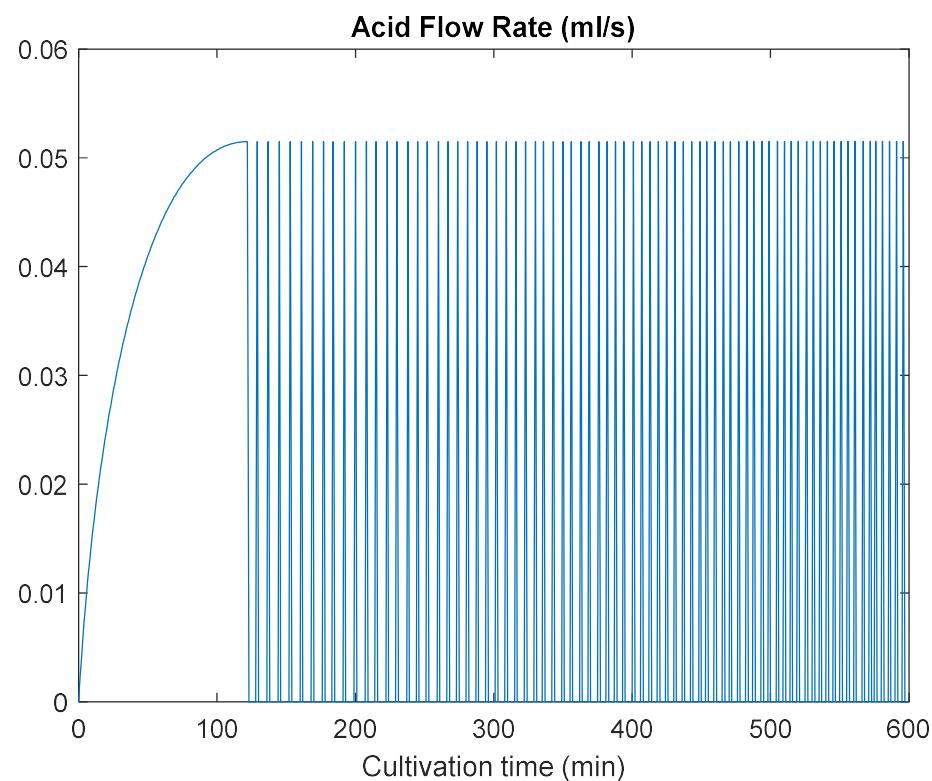
# Simulation Results for Weak Acid Weak Base and Set Point of 4



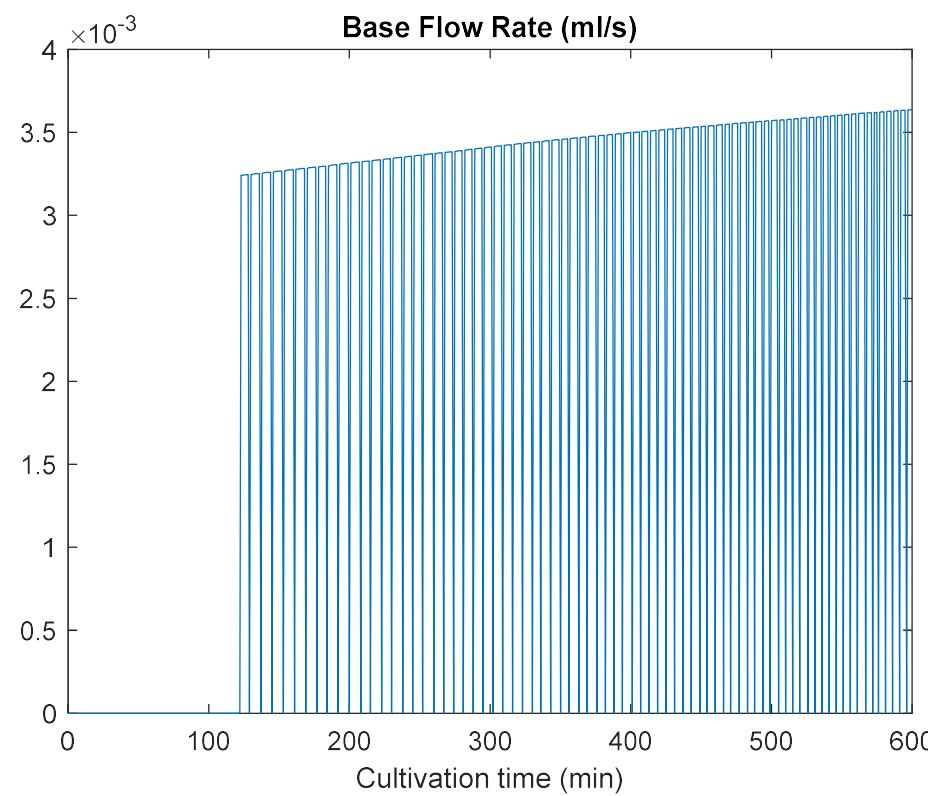
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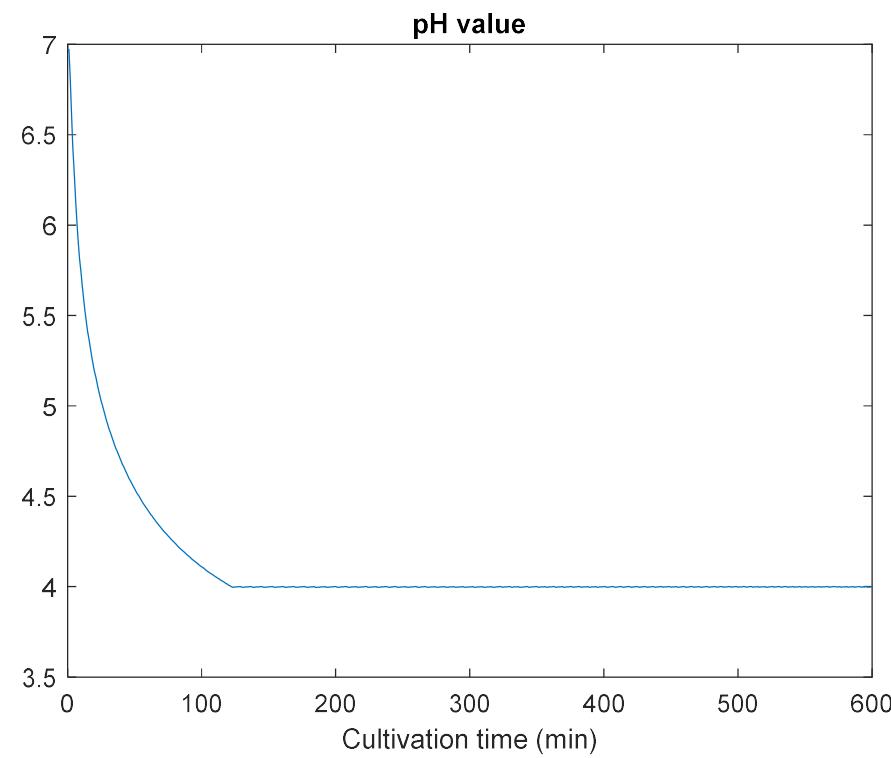
# Simulation Results for Weak Acid Weak Base and Set Point of 4



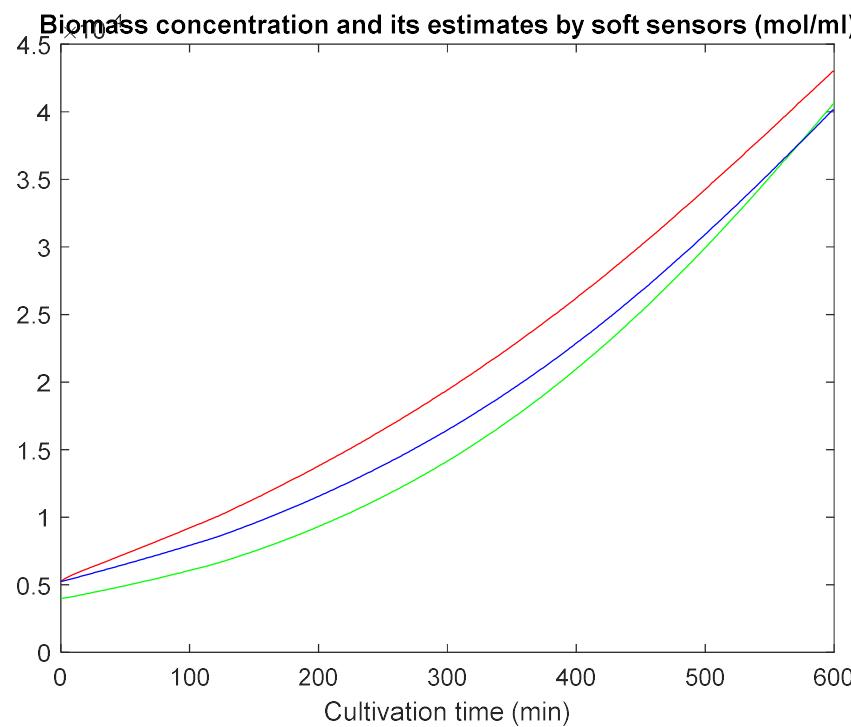
# Simulation Results for Weak Acid Weak Base and Set Point of 4



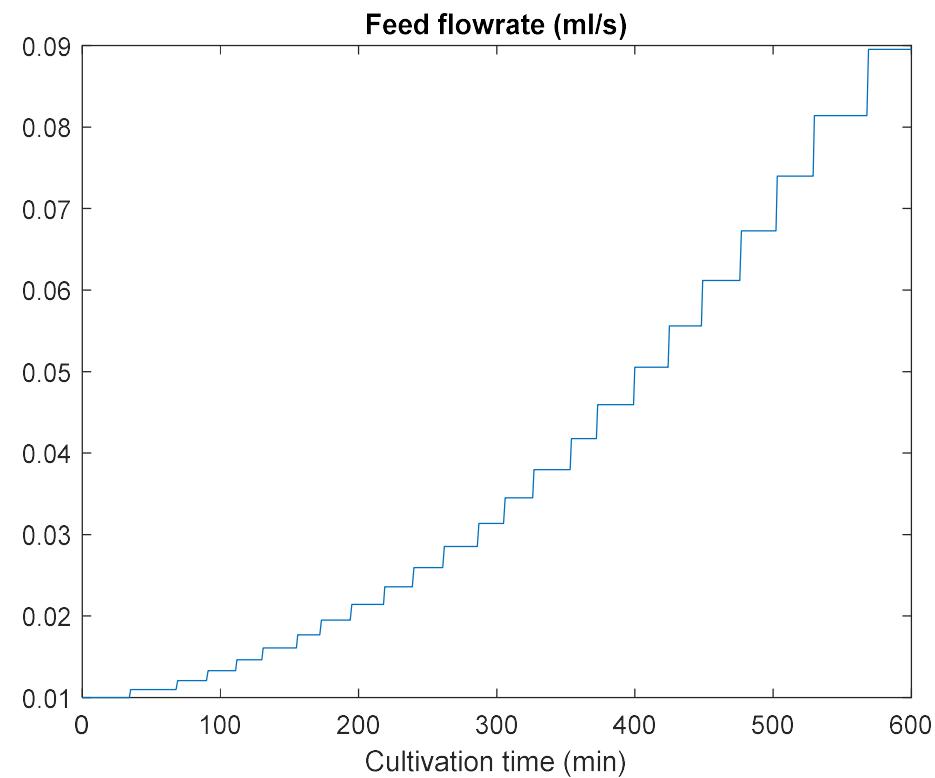
# Simulation Results for Weak Acid Weak Base and Set Point of 4



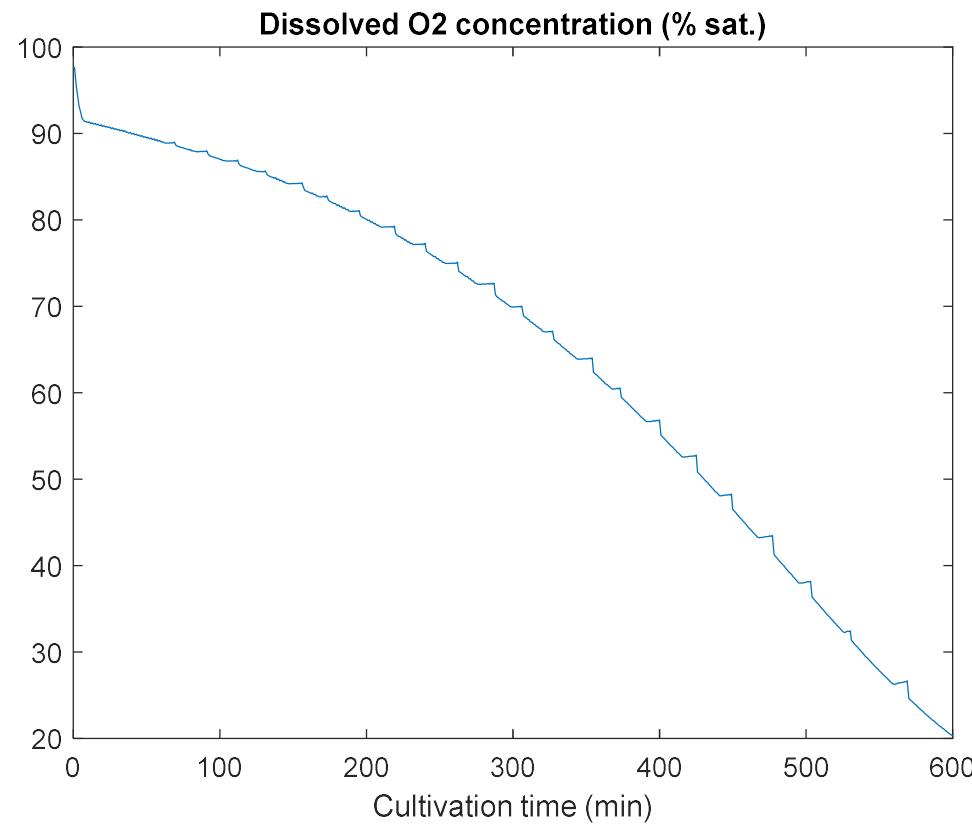
# Simulation Results for Weak Acid Weak Base and Set Point of 4



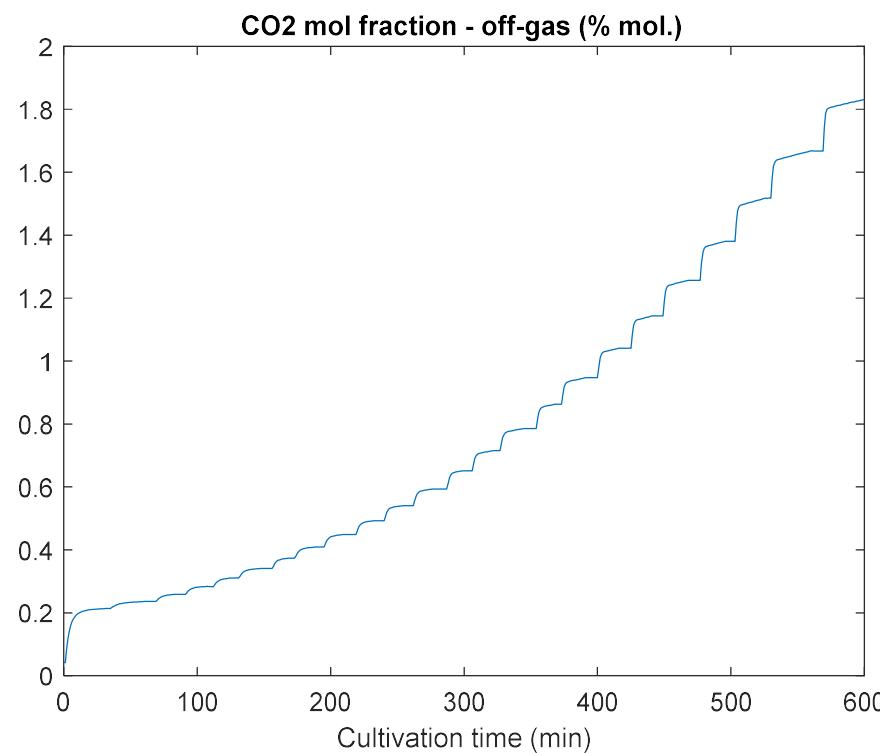
# Simulation Results for Weak Acid Weak Base and Set Point of 4



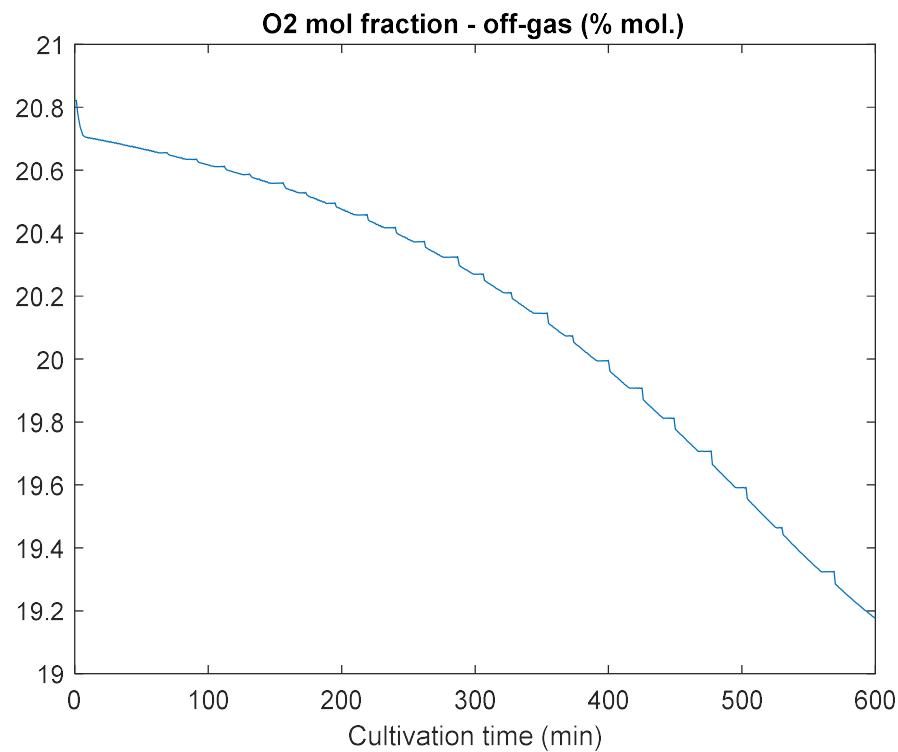
# Simulation Results for Weak Acid Weak Base and Set Point of 4



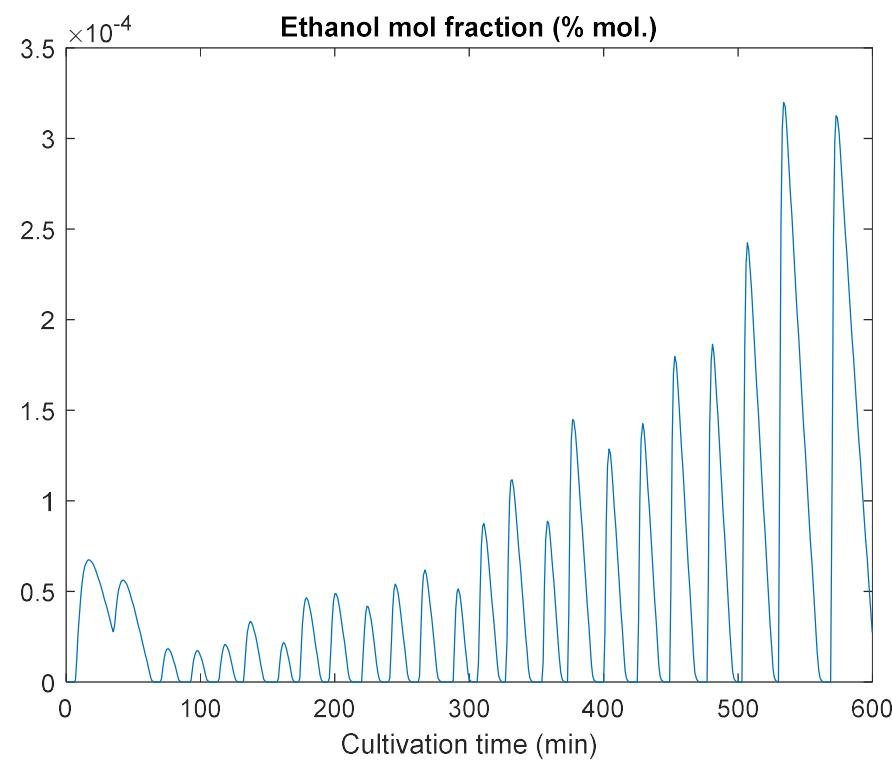
# Simulation Results for Weak Acid Weak Base and Set Point of 4



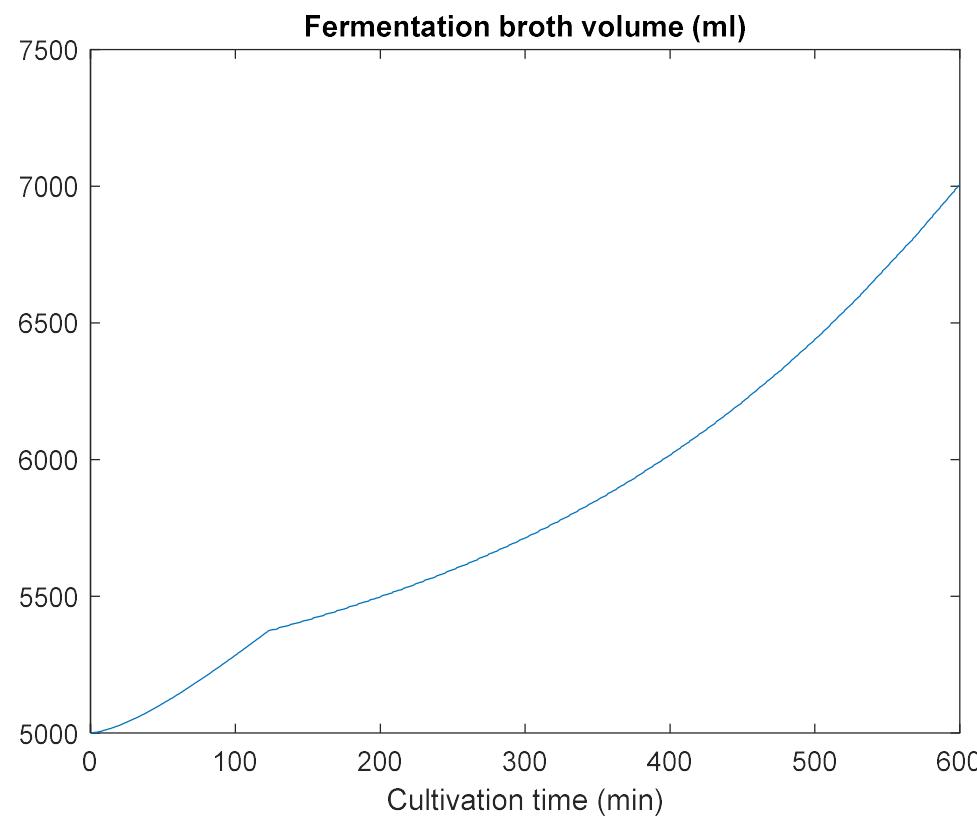
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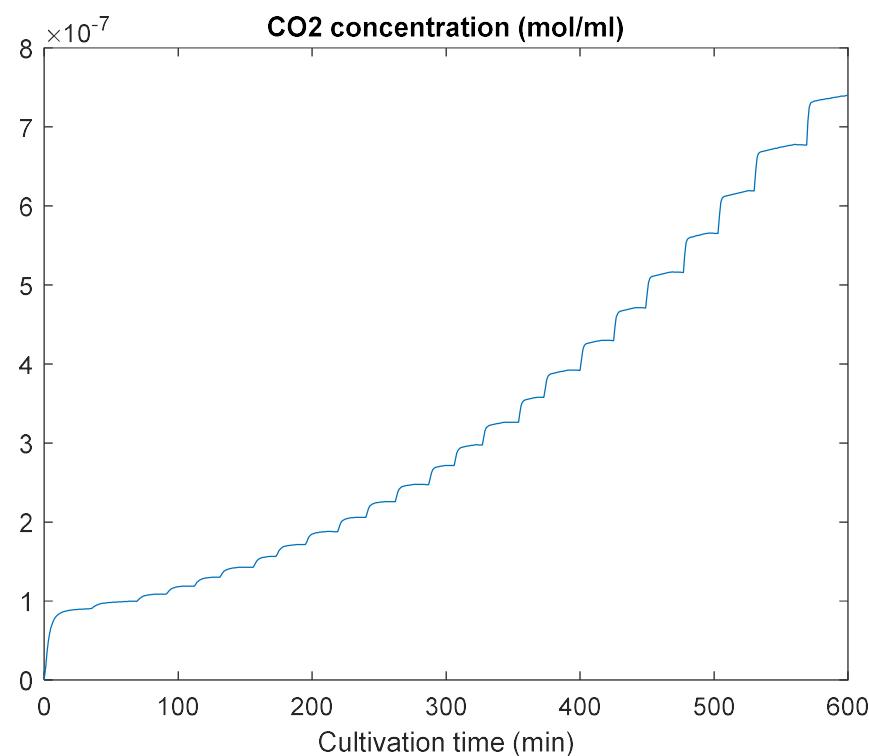
# Simulation Results for Weak Acid Weak Base and Set Point of 4



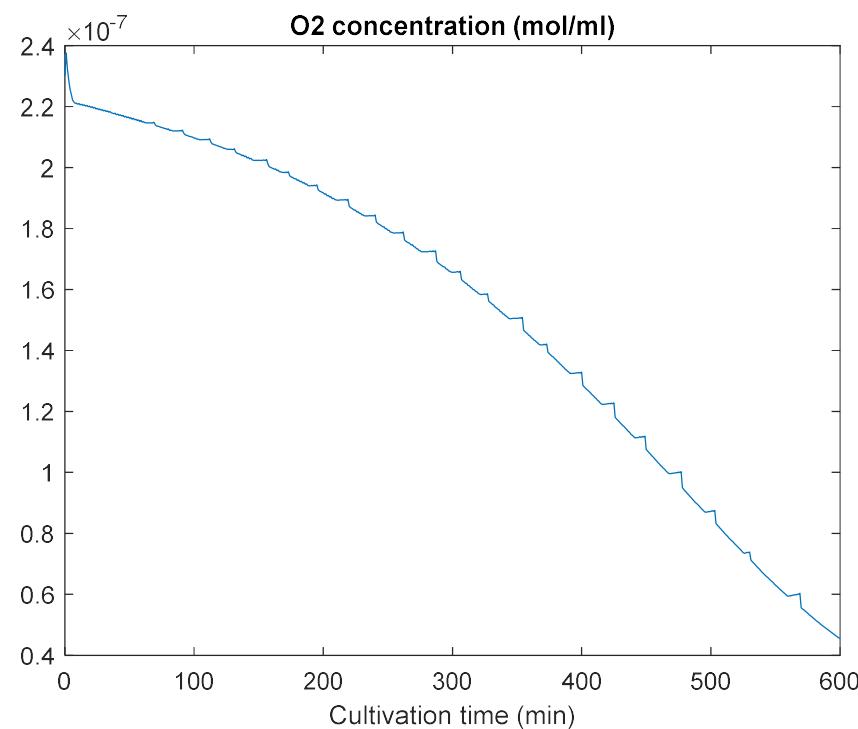
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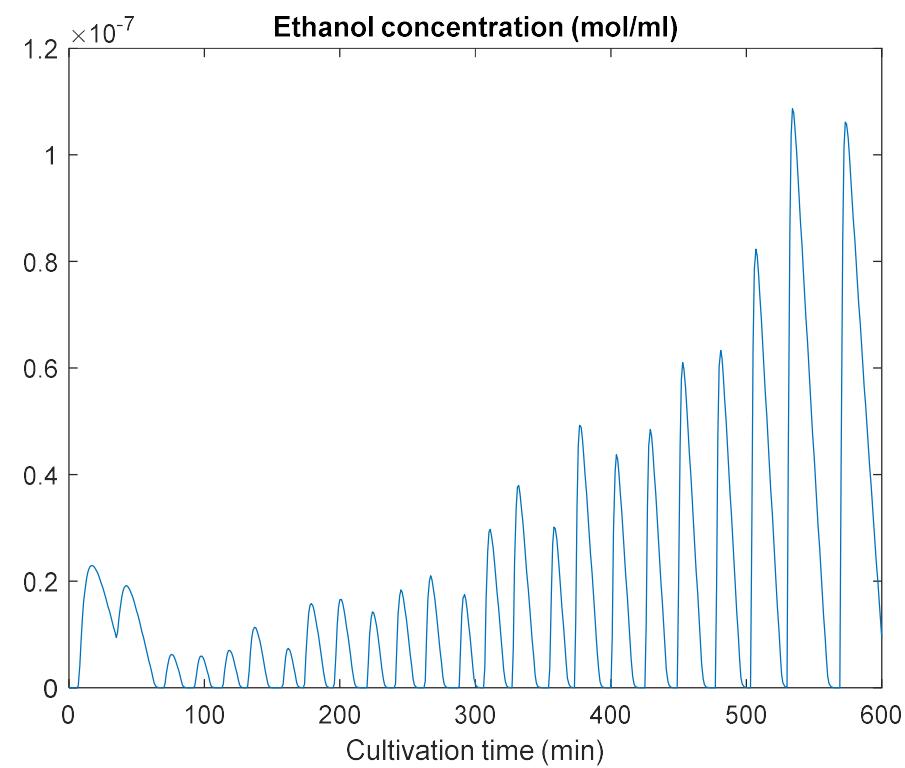
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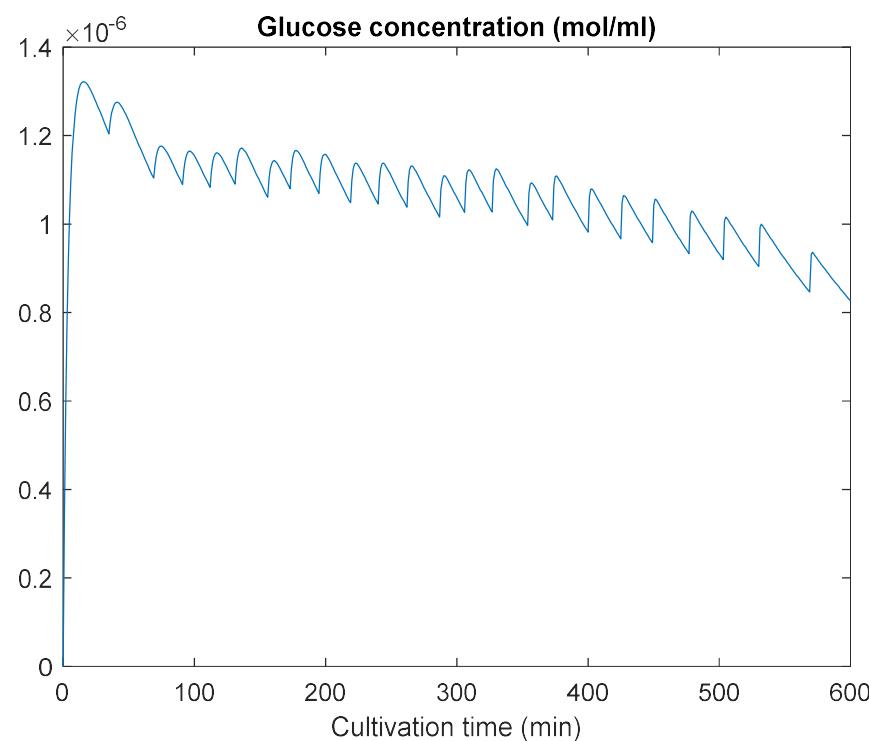
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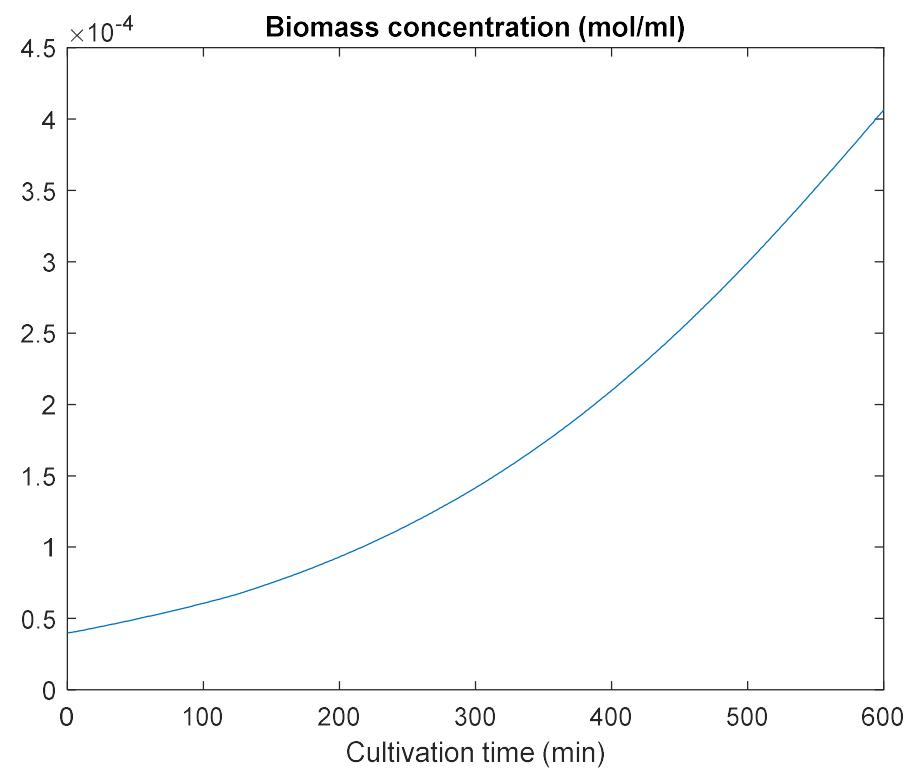
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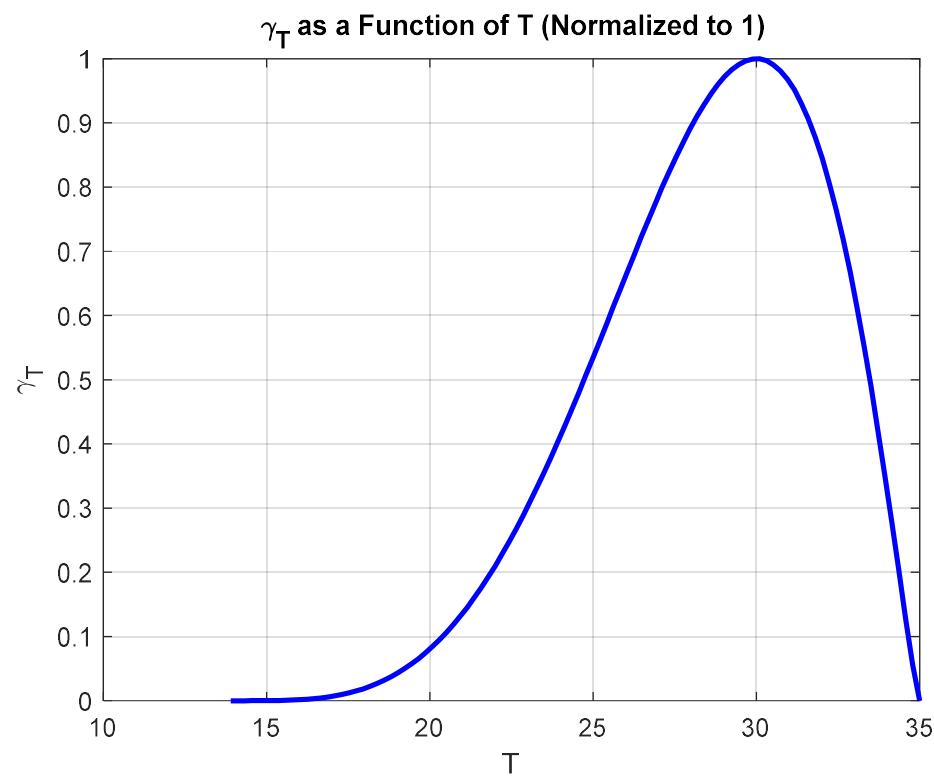
# Simulation Results for Weak Acid Weak Base and Set Point of 4



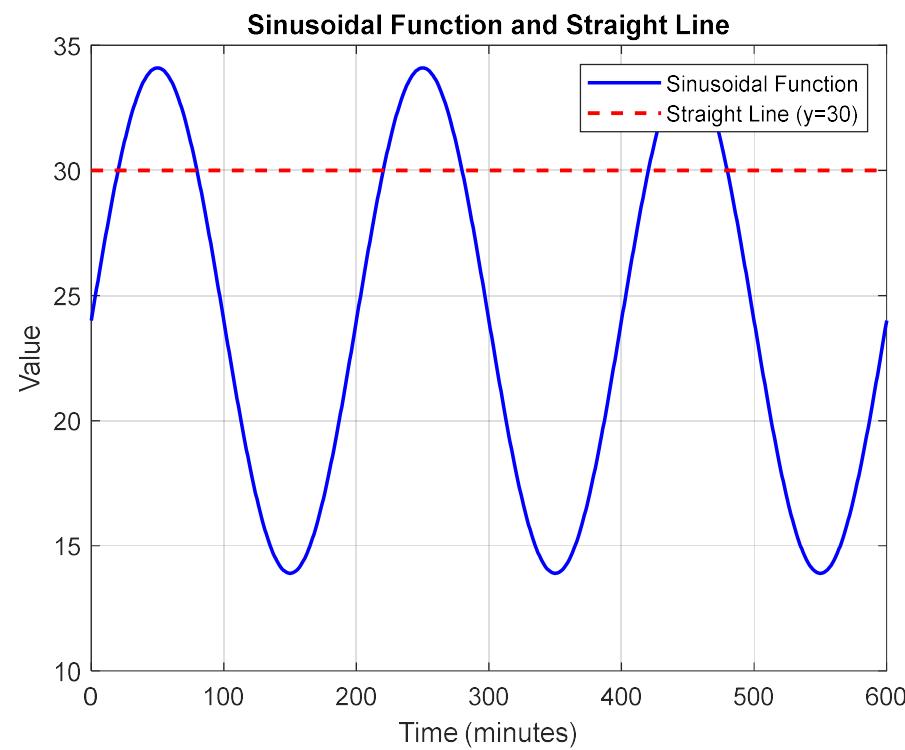
# Simulation Results for Weak Acid Weak Base and Set Point of 4



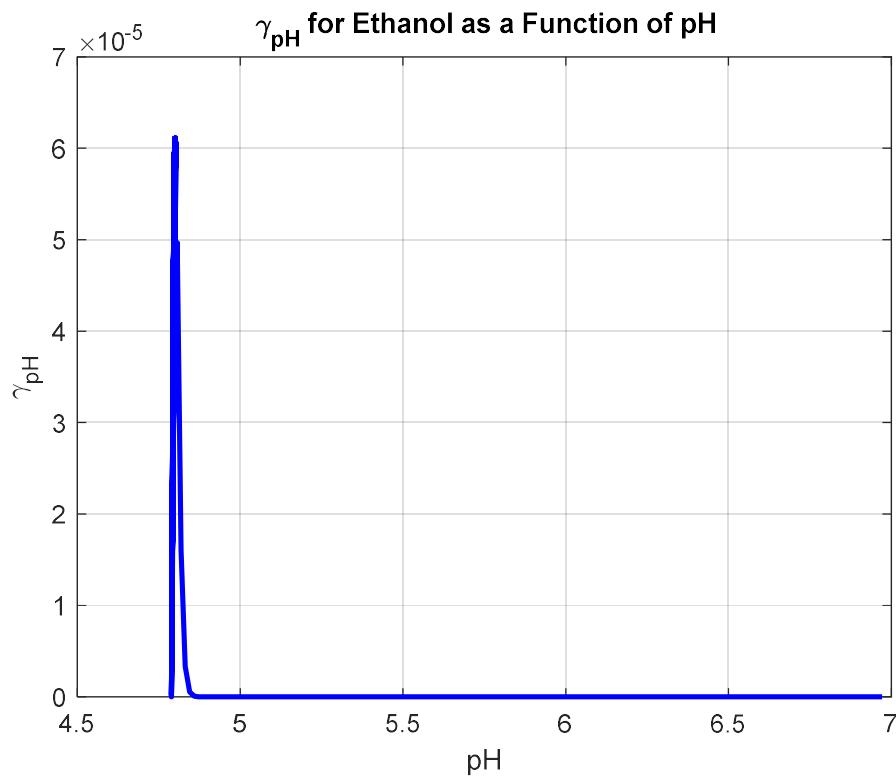
# Simulation Results for Weak Acid Weak Base and Set Point of 4.8 with Steady State Value of 4.7988



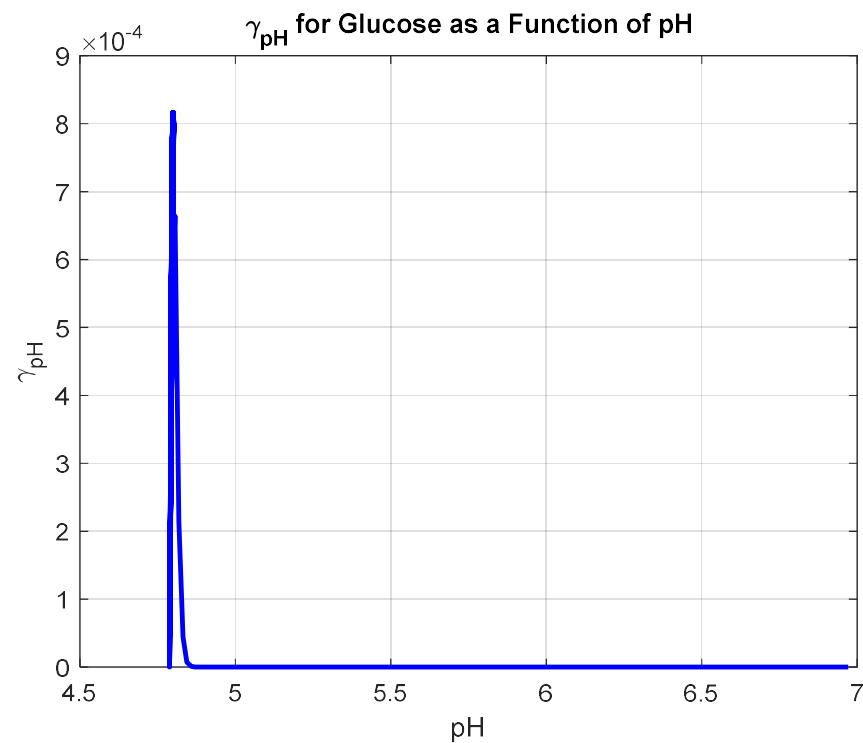
# Simulation Results for Weak Acid Weak Base and Set Point of 4.8



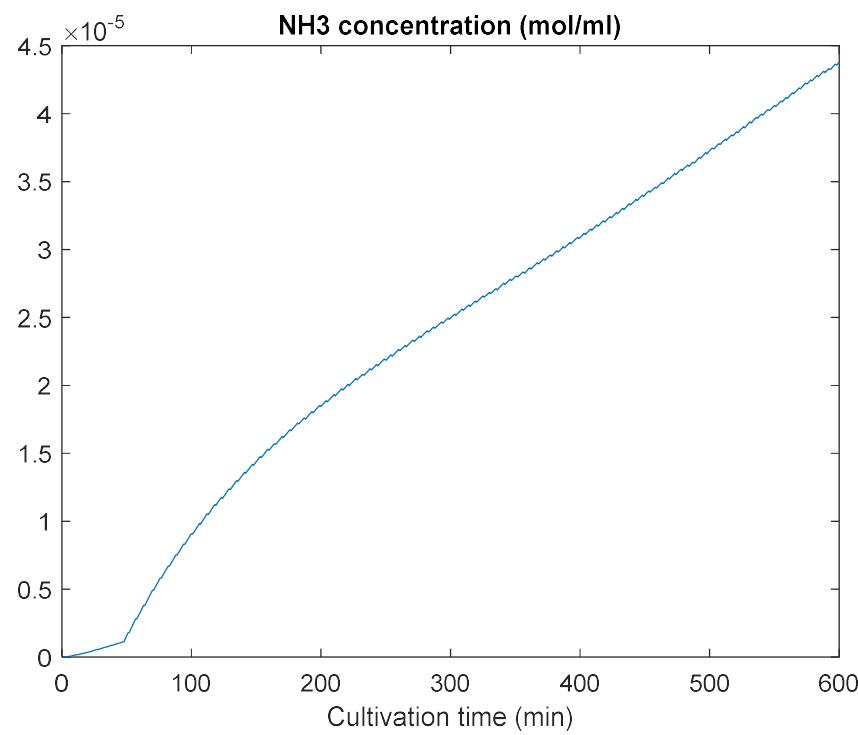
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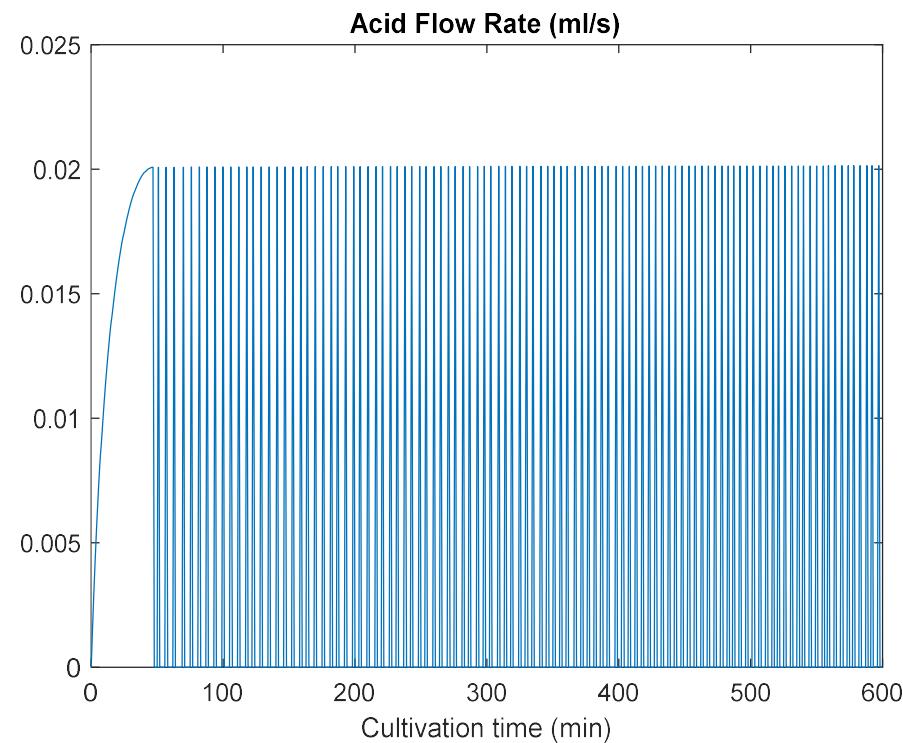
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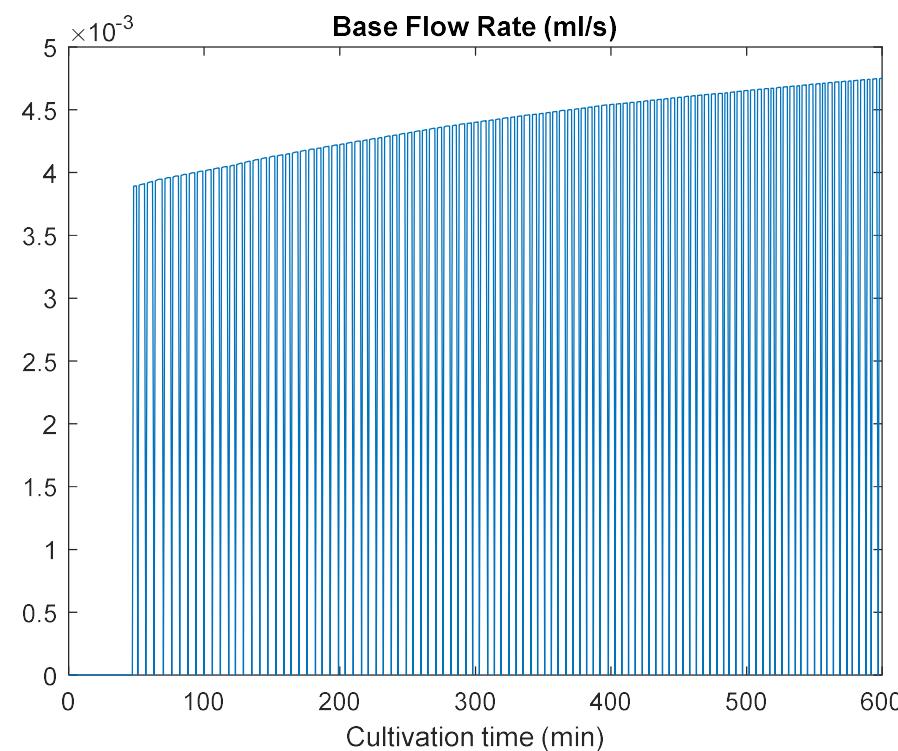
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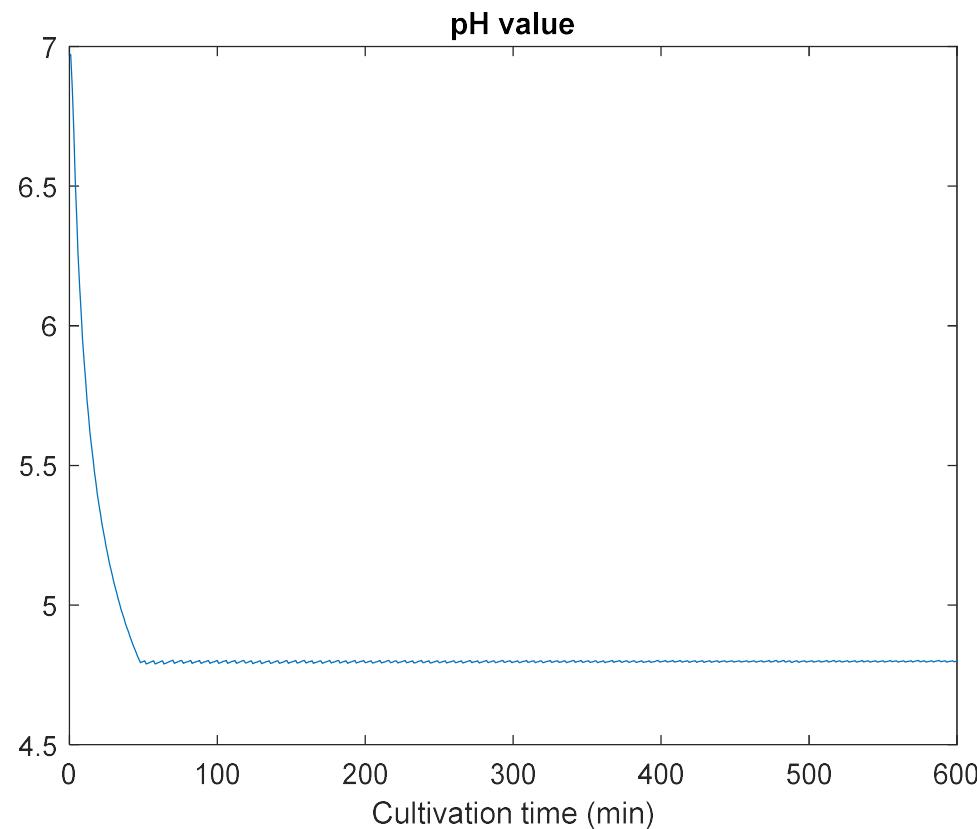
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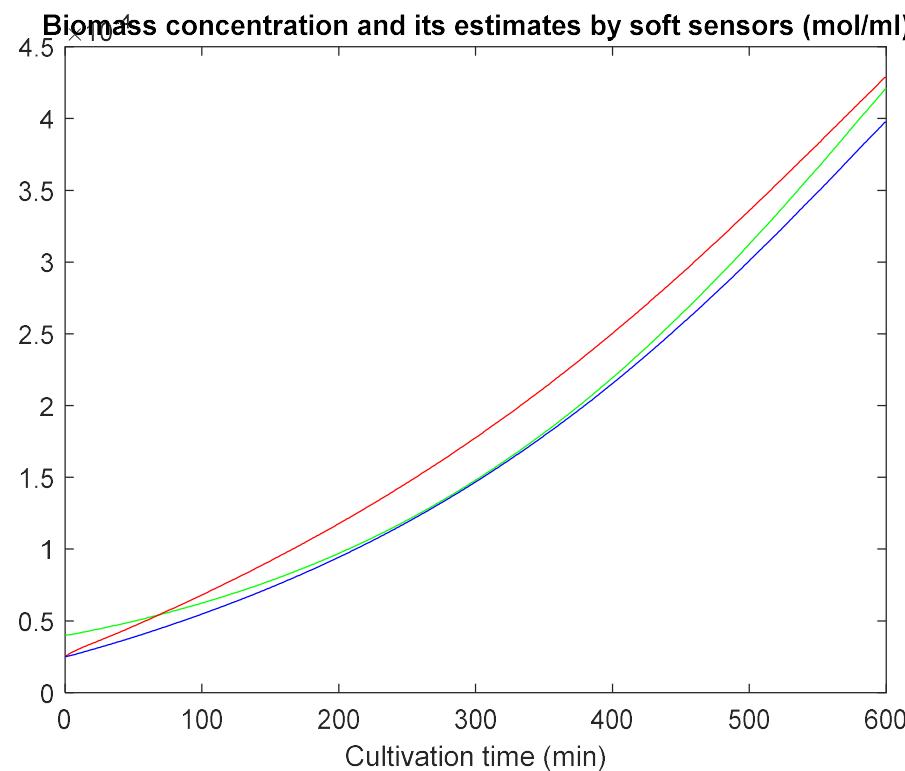
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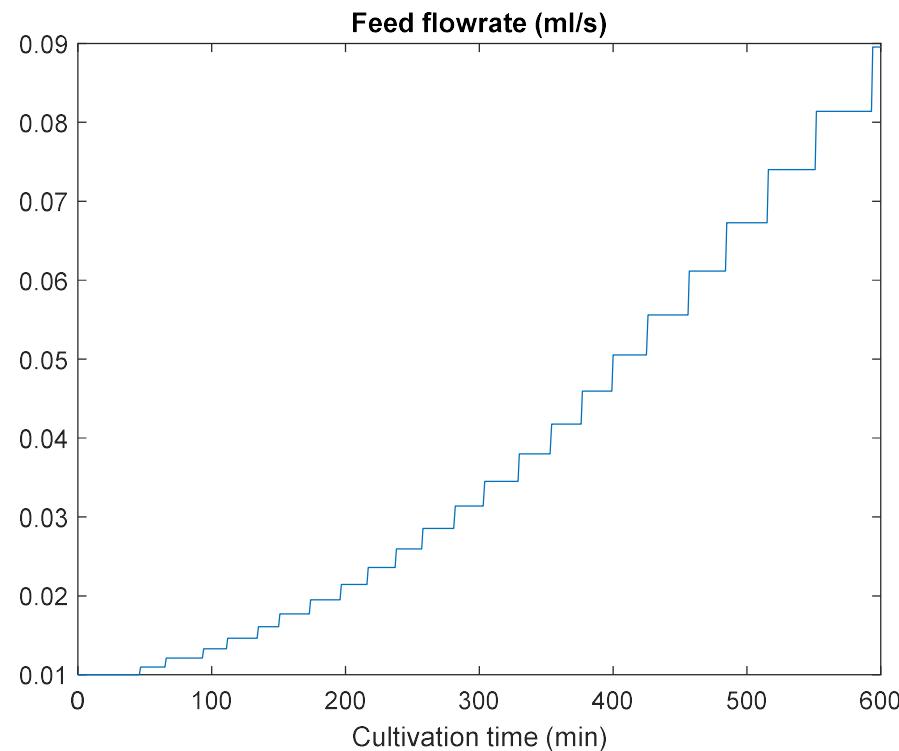
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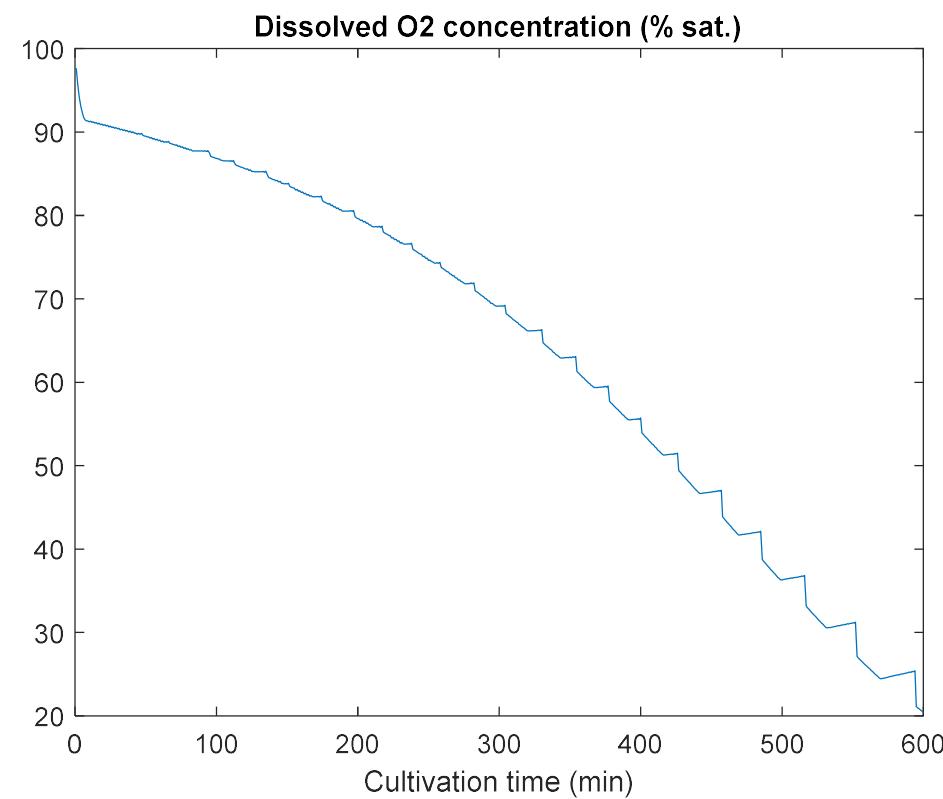
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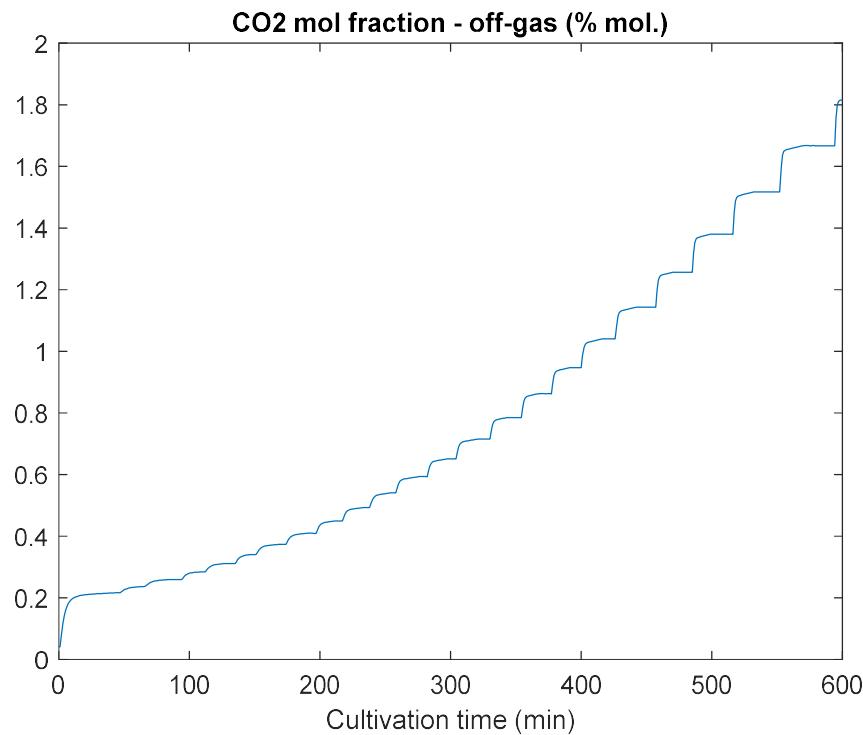
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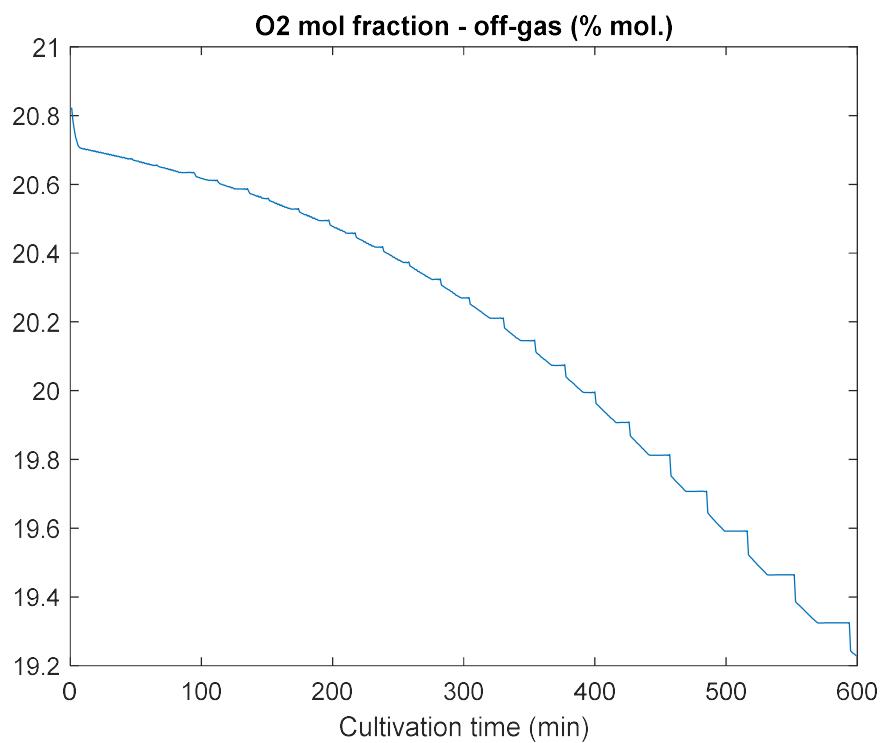
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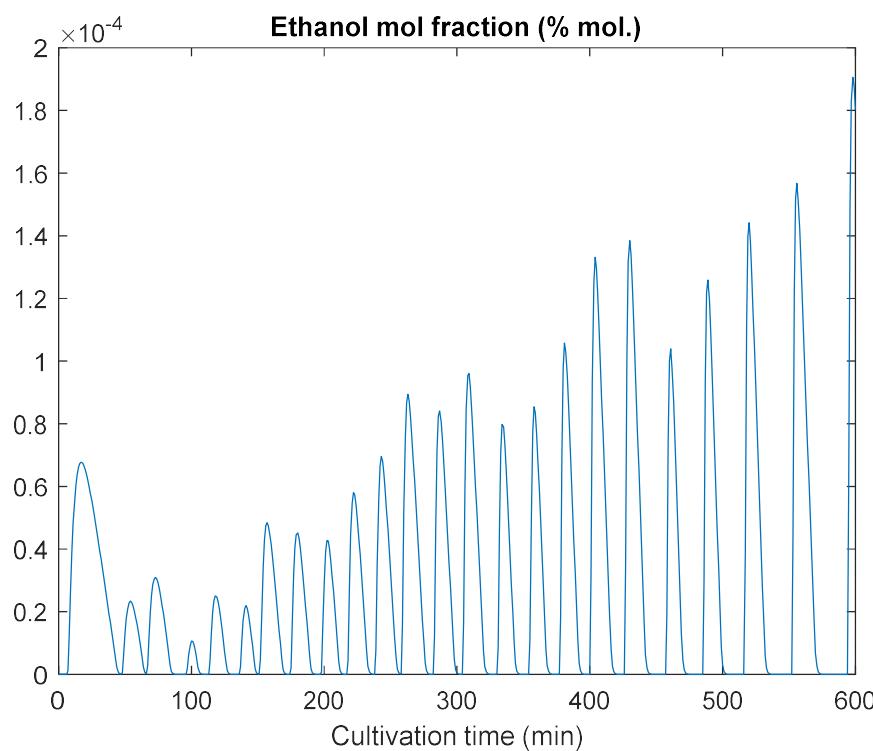
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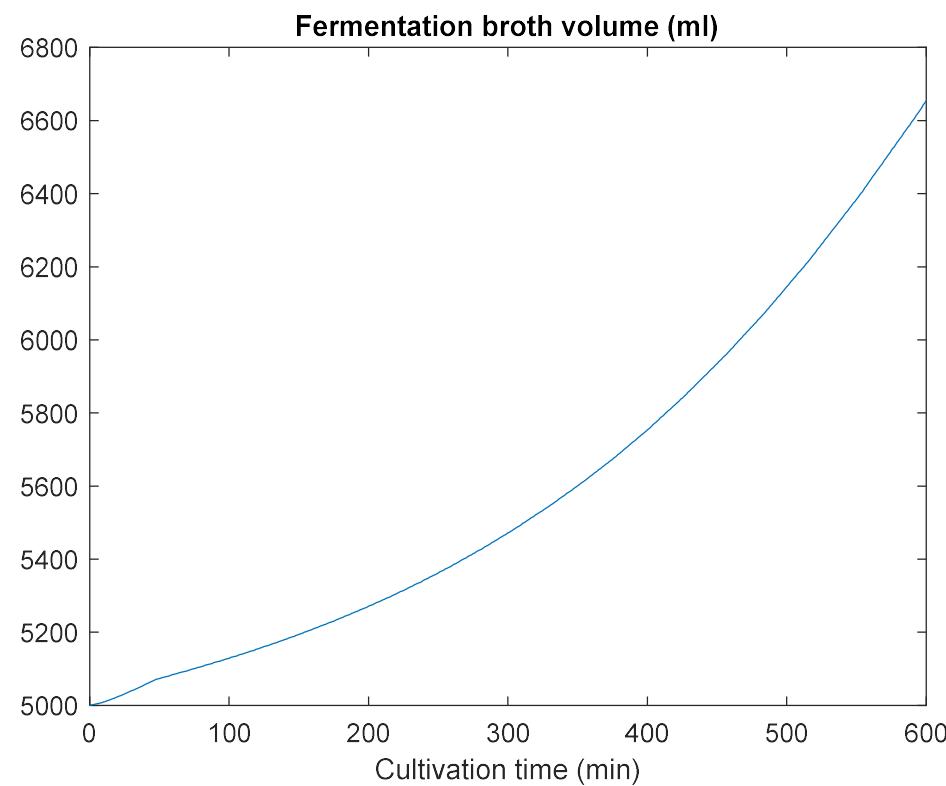
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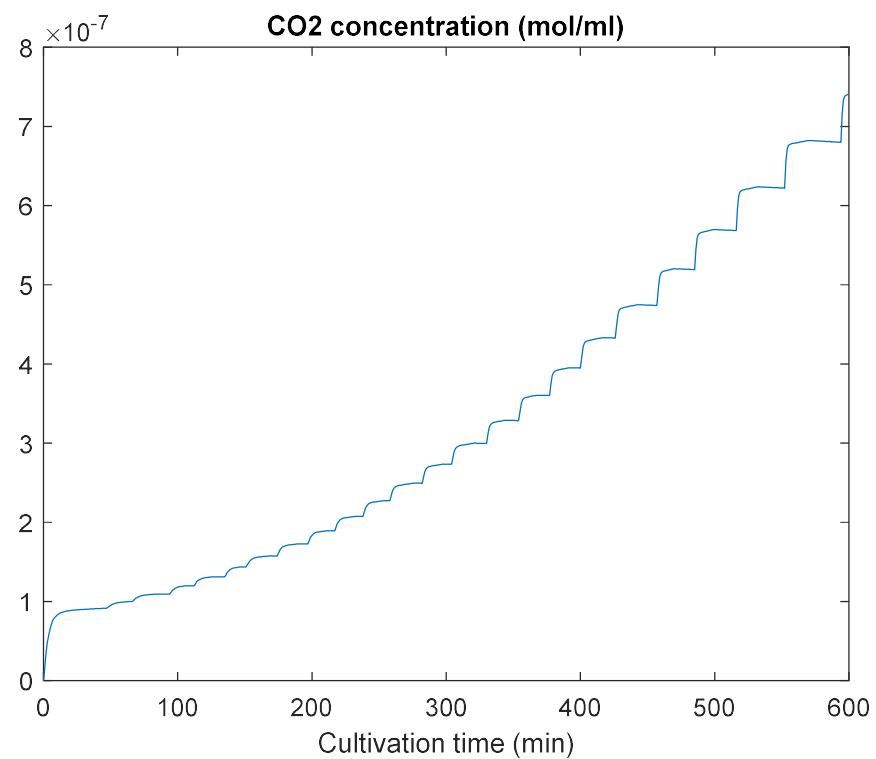
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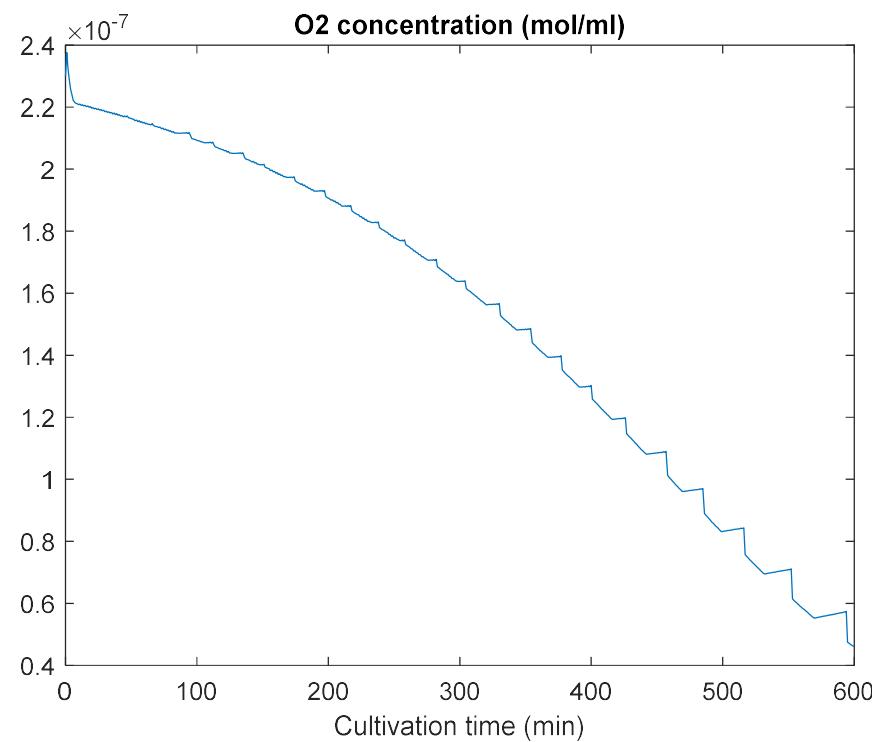
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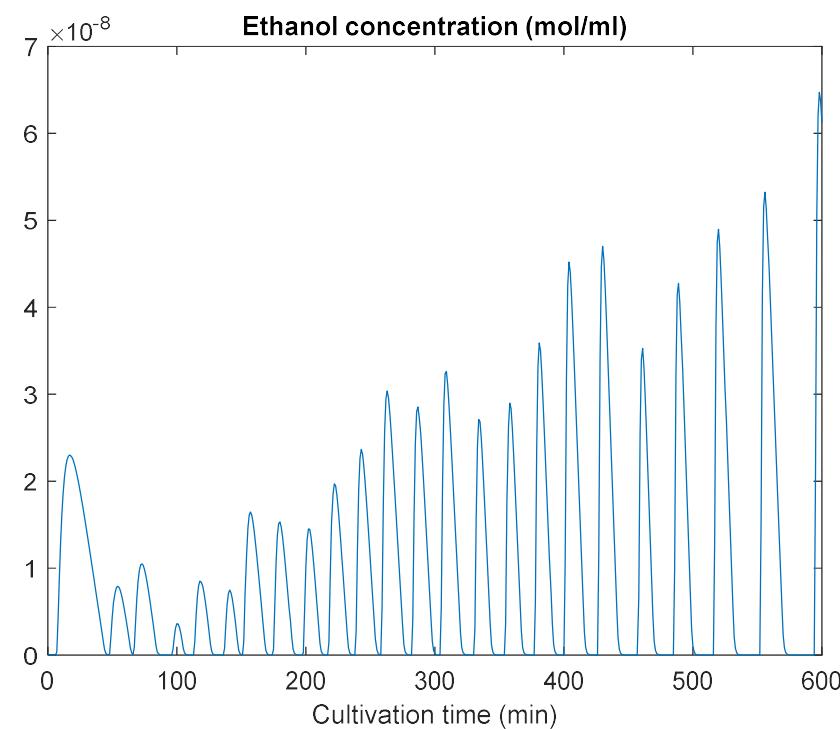
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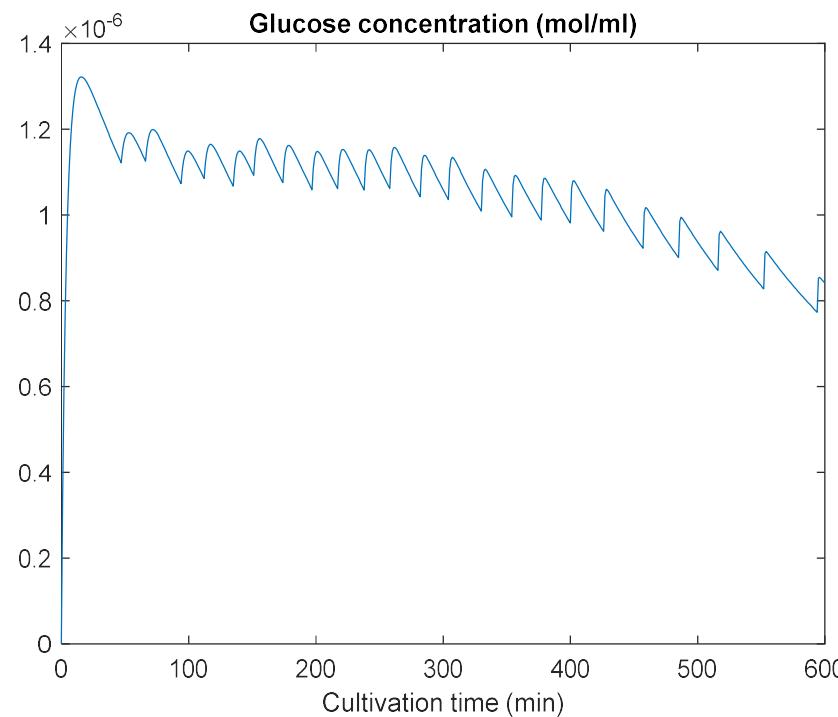
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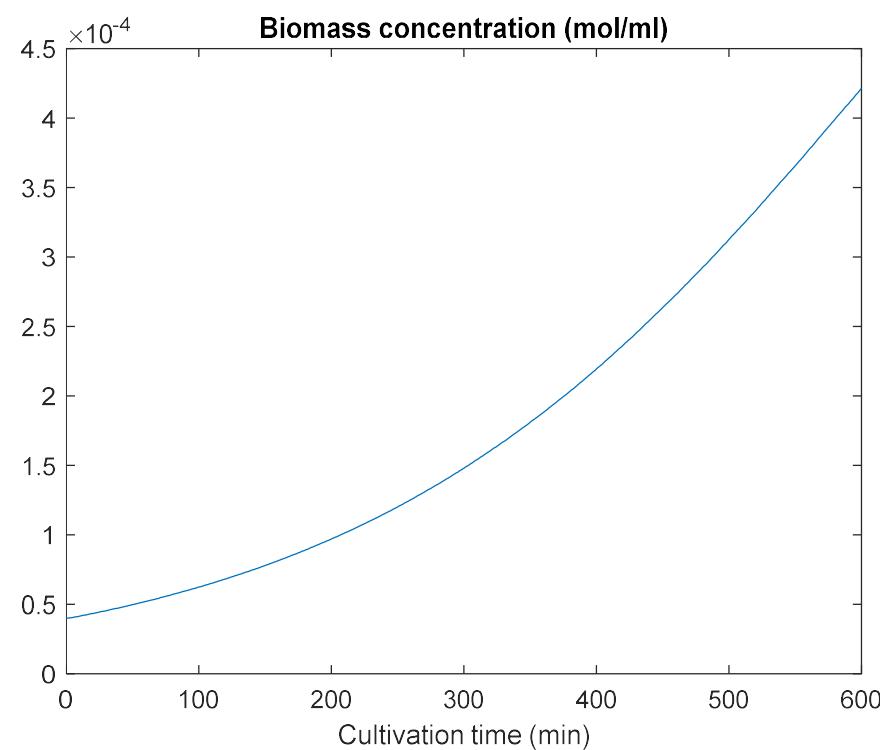
# Simulation Results for Weak Acid Weak Base and Set Point of 4.8



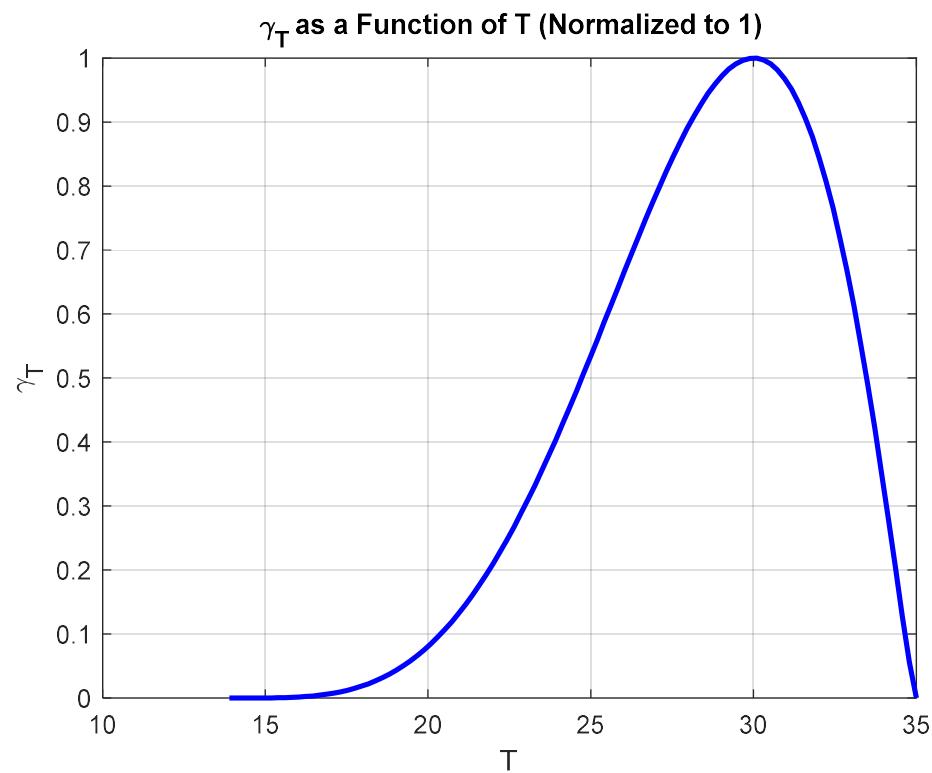
# Simulation Results for Weak Acid Weak Base and Set Point of 4.8



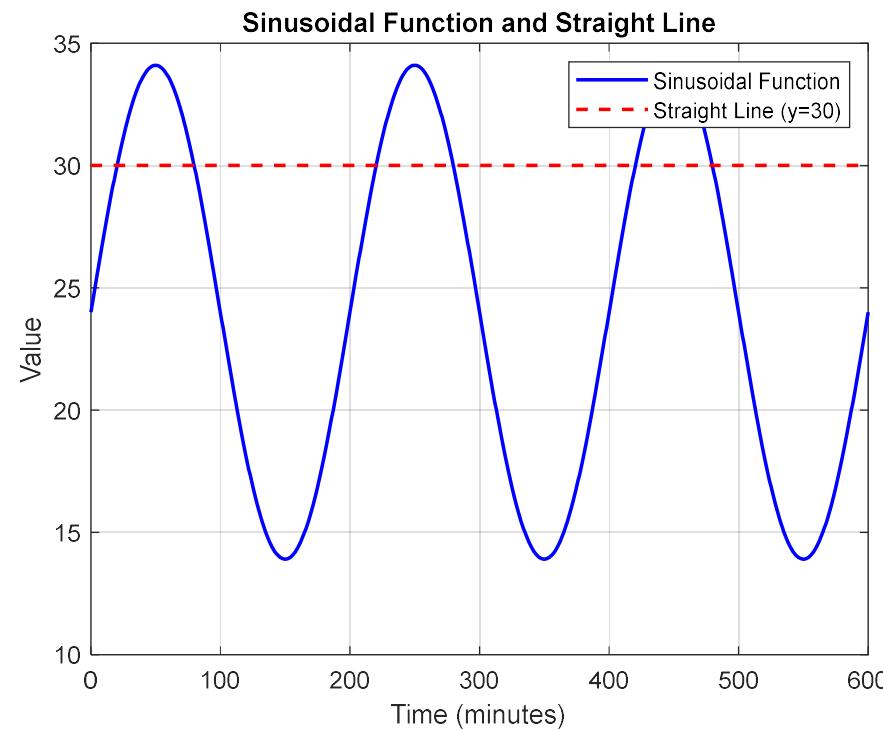
# Simulation Results for Weak Acid Weak Base and Set Point of 4.8



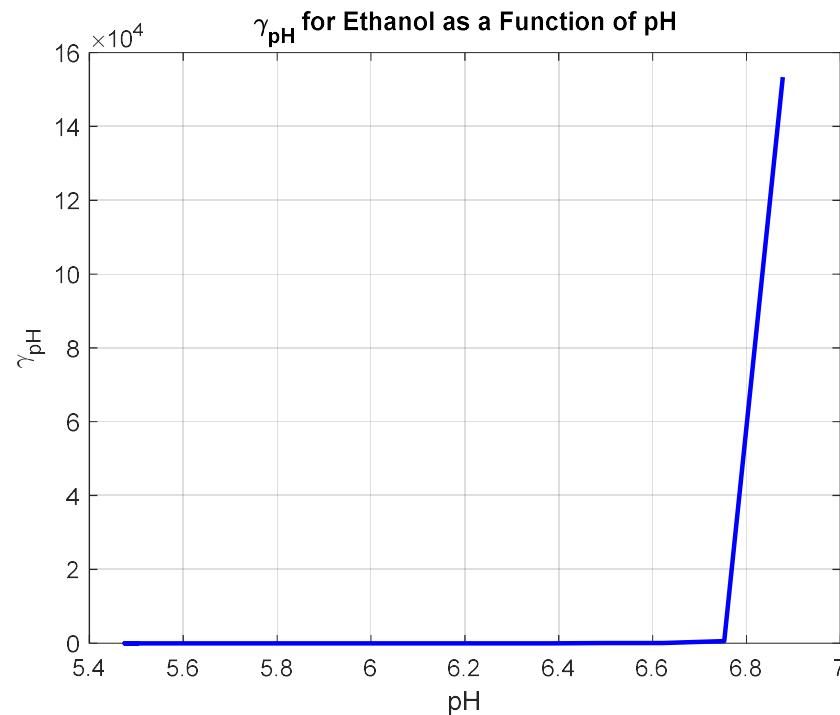
# Simulation Results for Weak Acid Weak Base and Set Point of 5.5 with Steady State Value of 5.4977



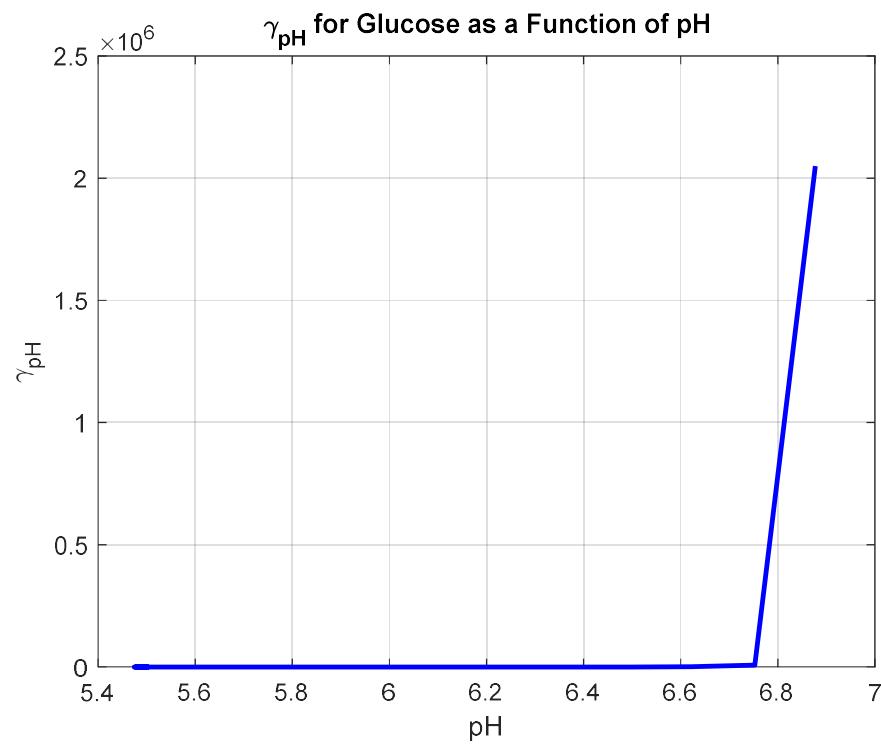
# Simulation Results for Weak Acid Weak Base and Set Point of 5.5



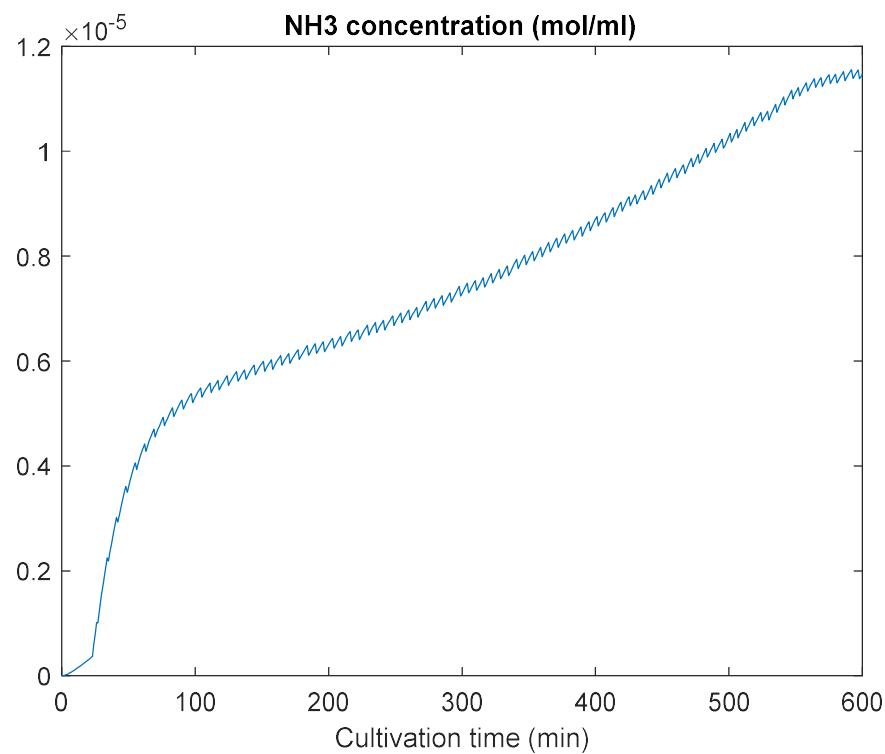
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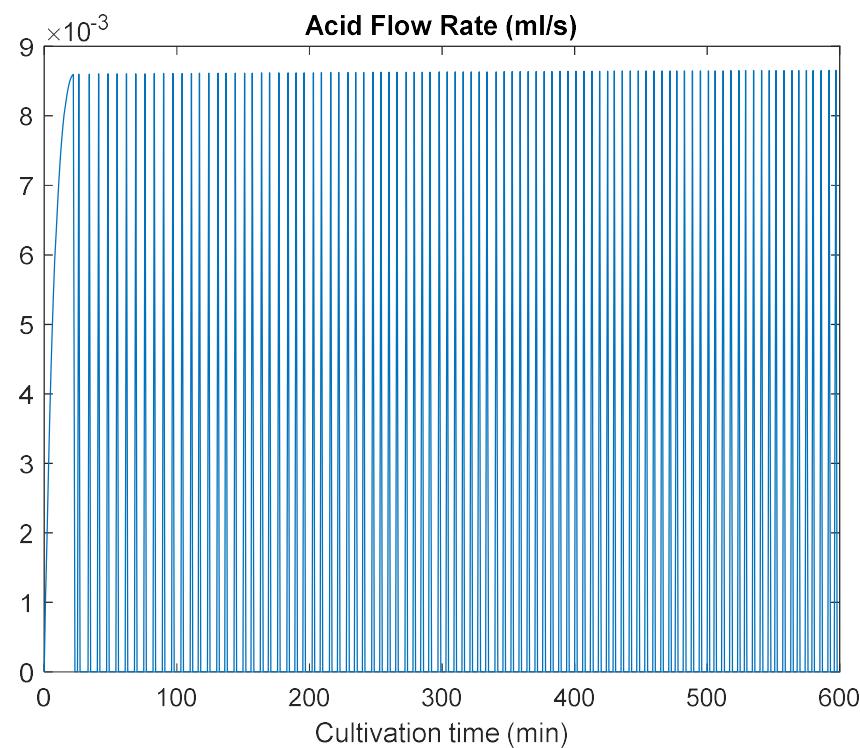
# Simulation Results for Weak Acid Weak Base and Set Point of 5.5



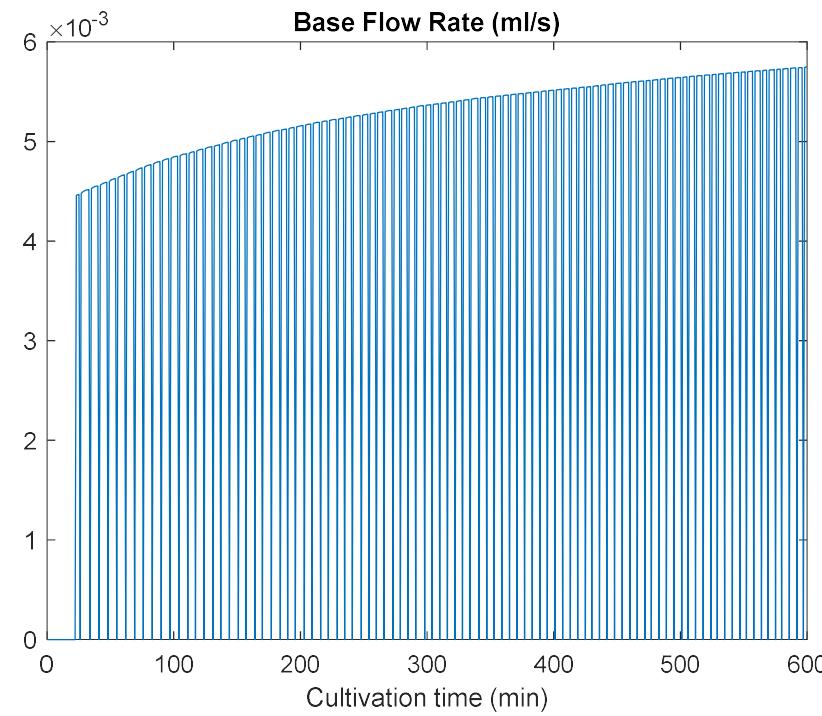
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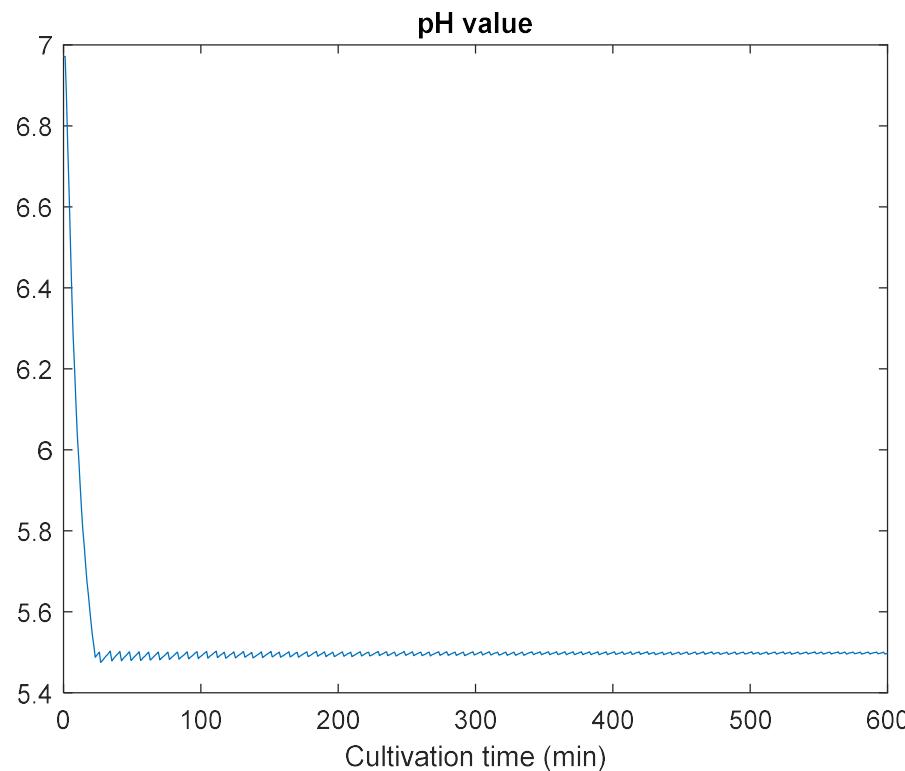
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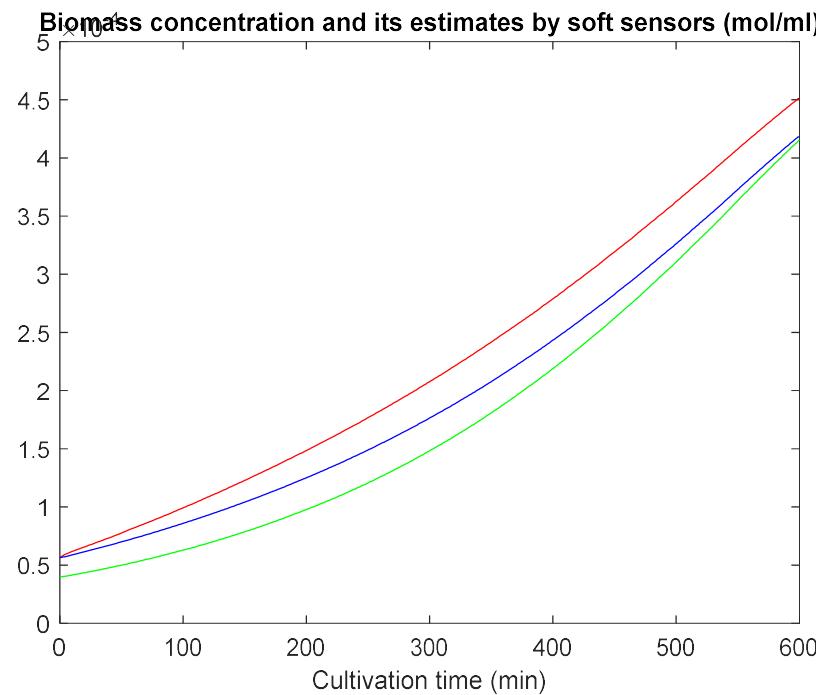
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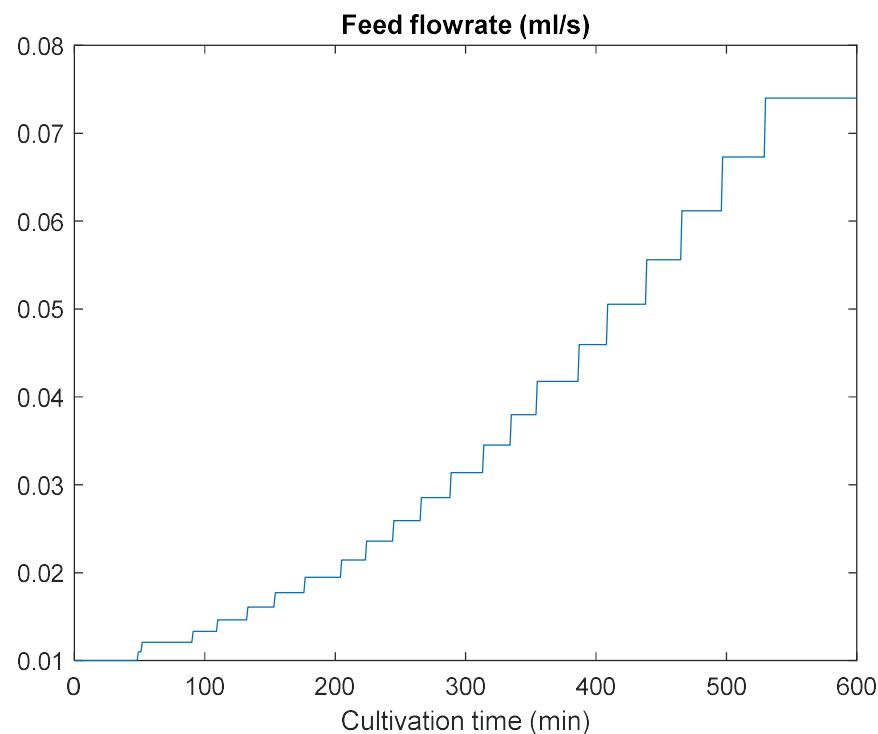
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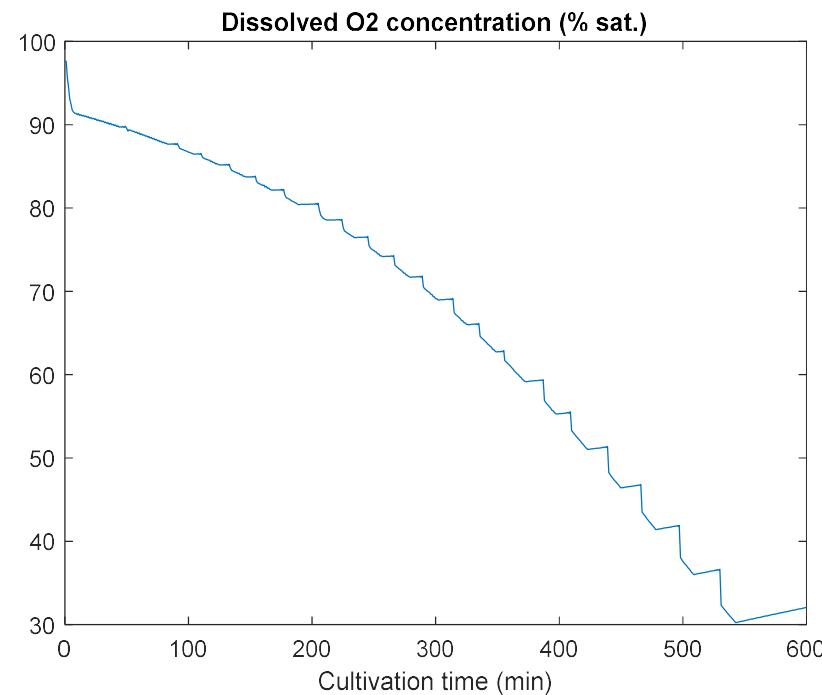
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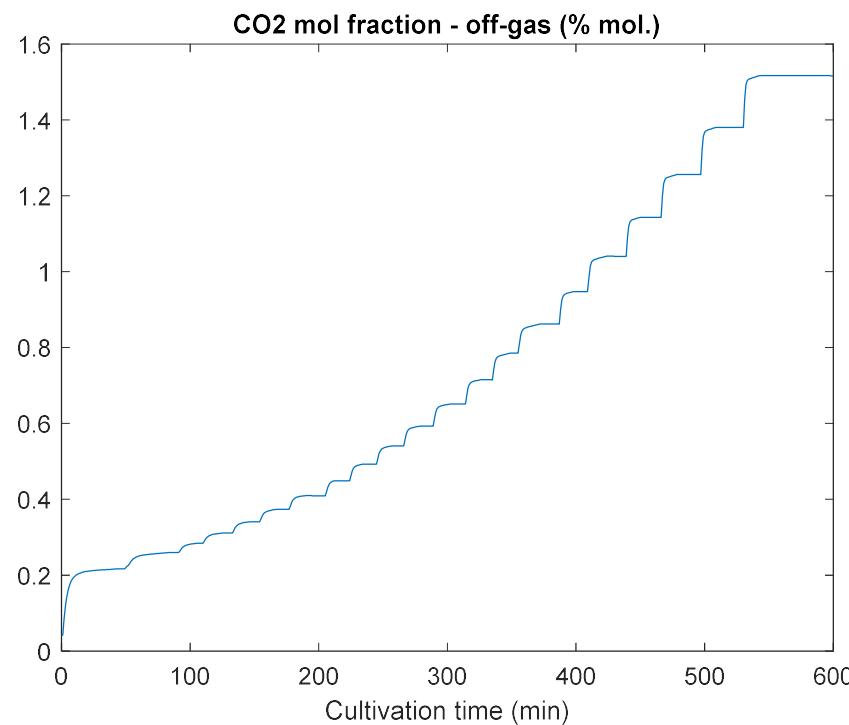
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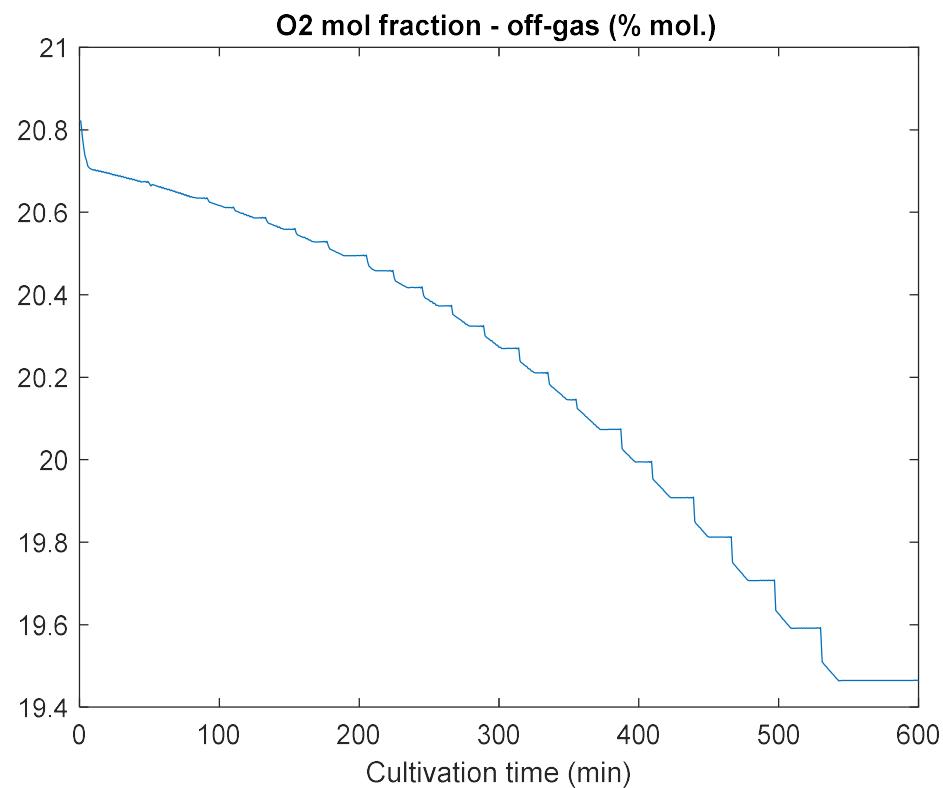
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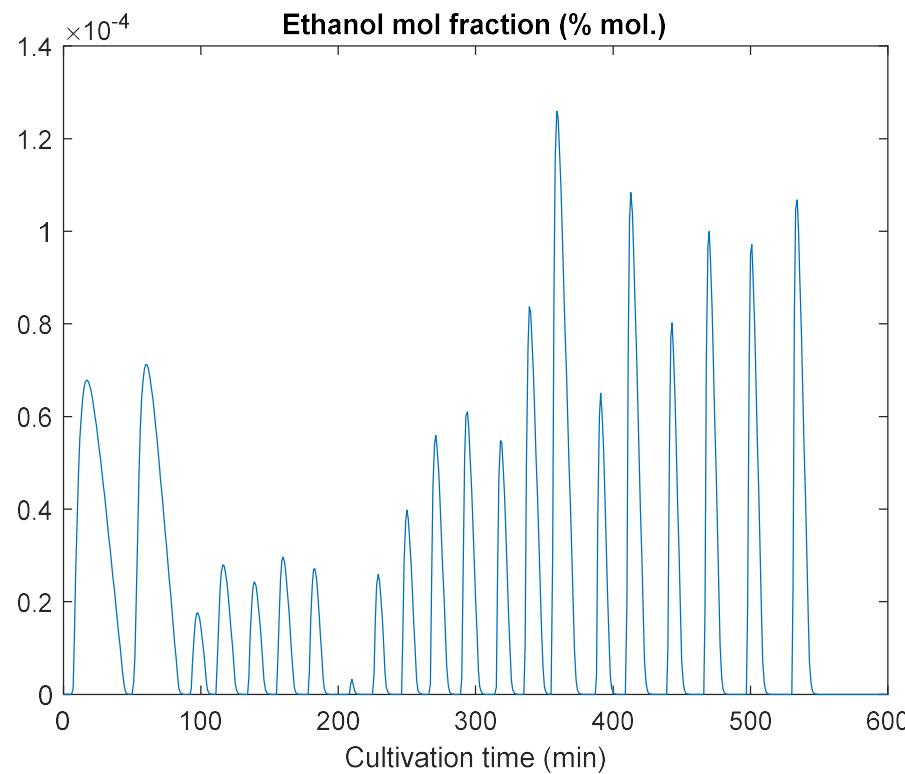
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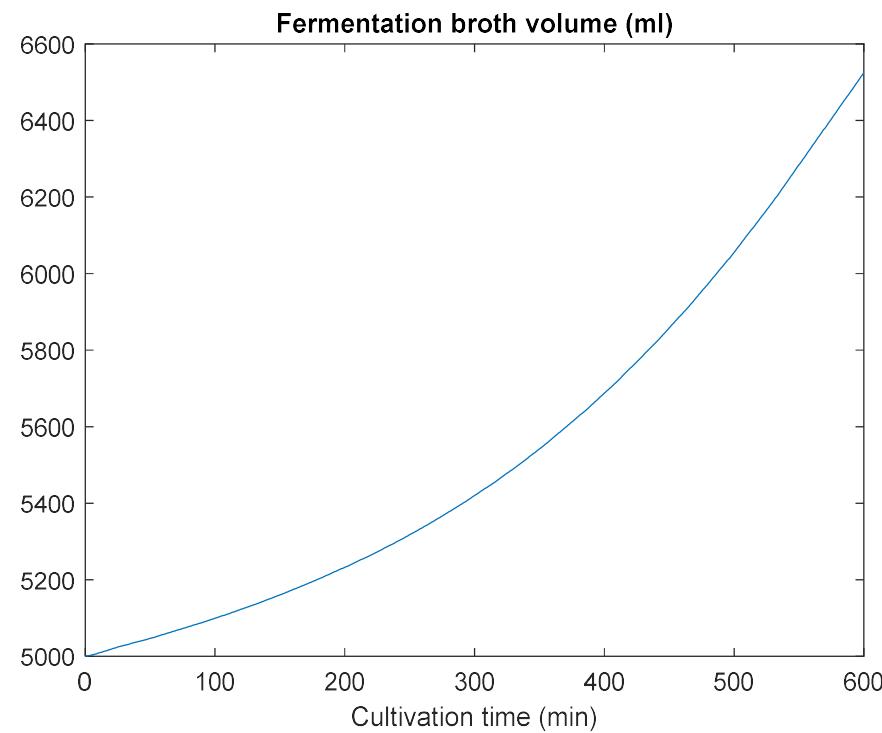
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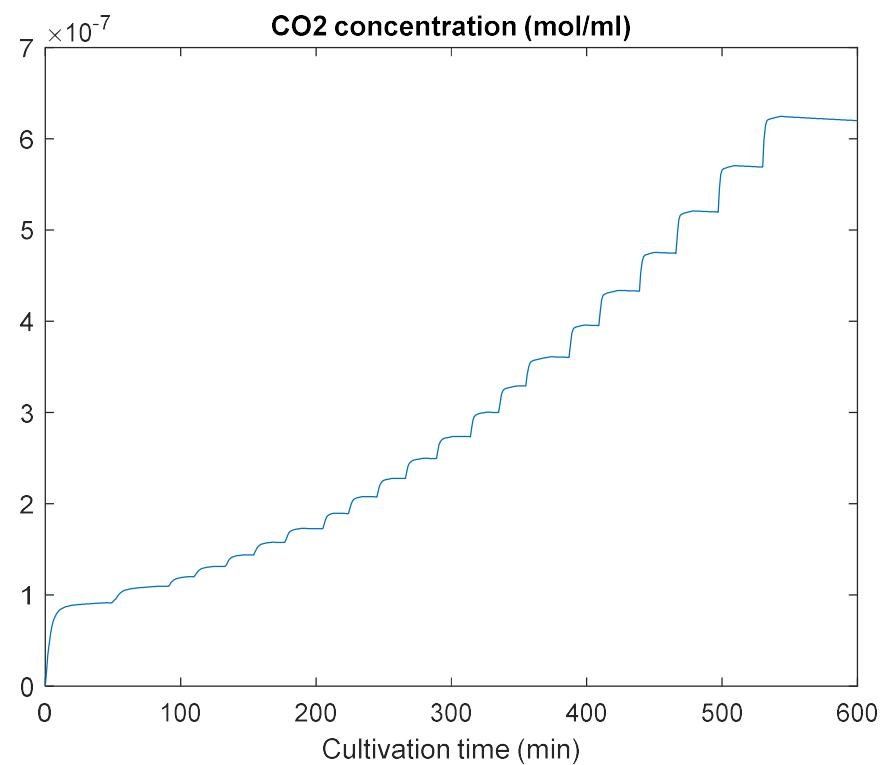
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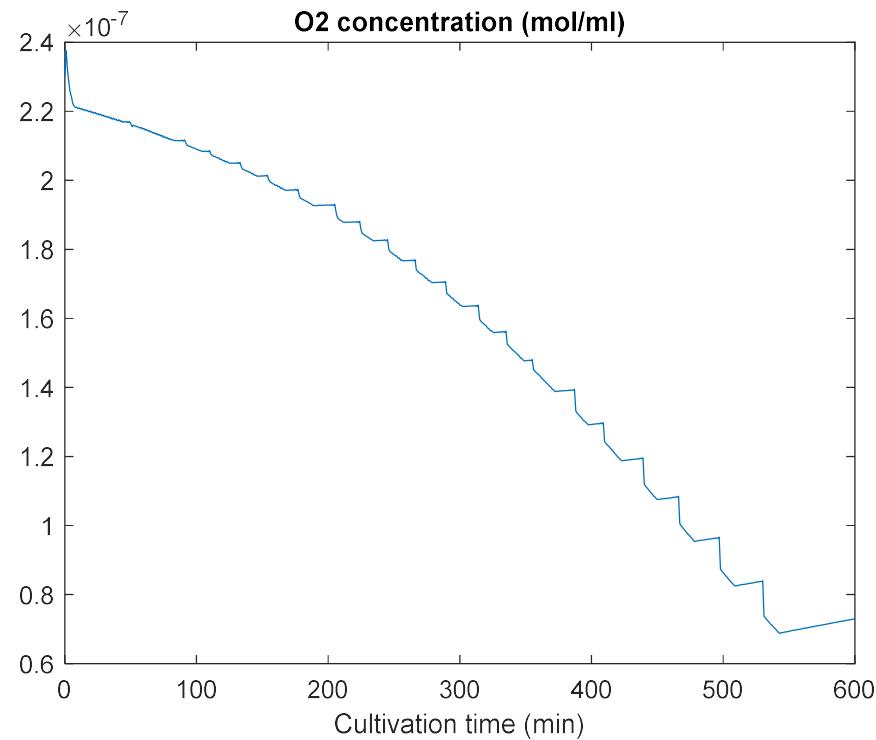
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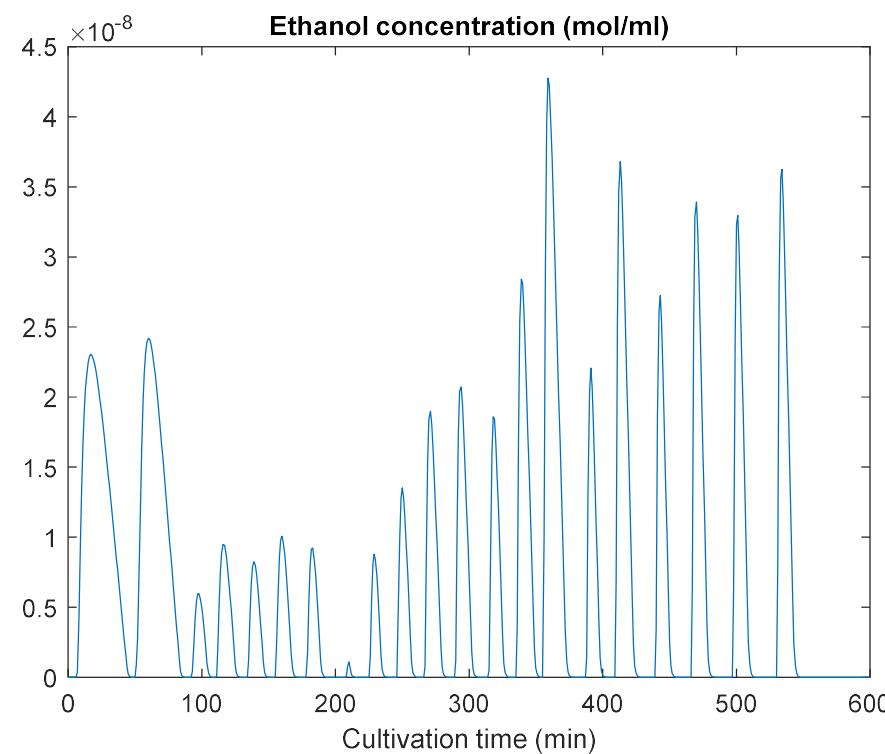
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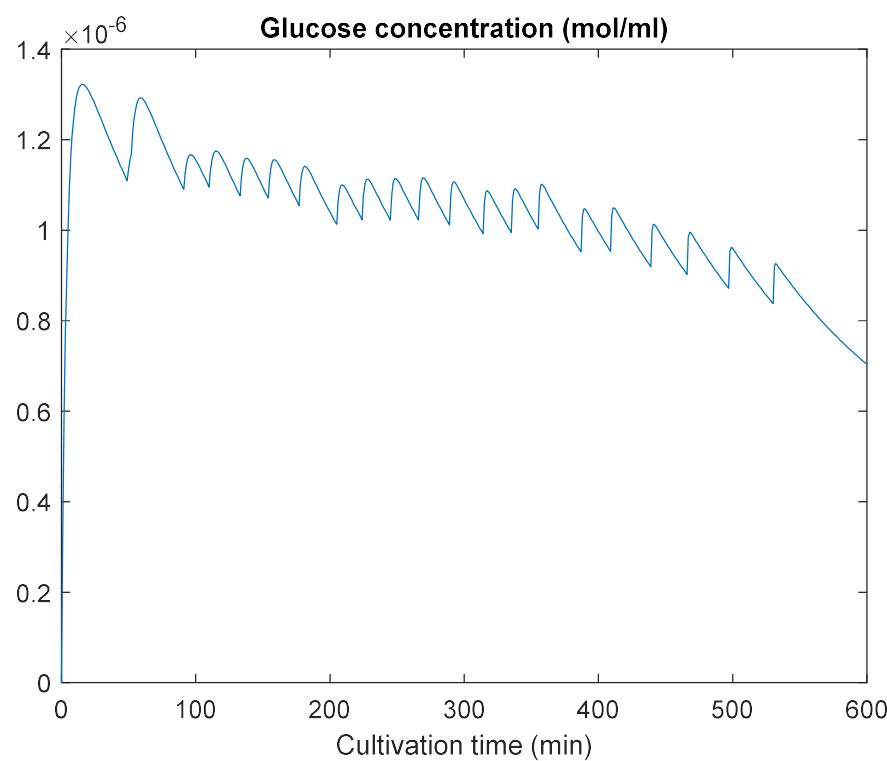
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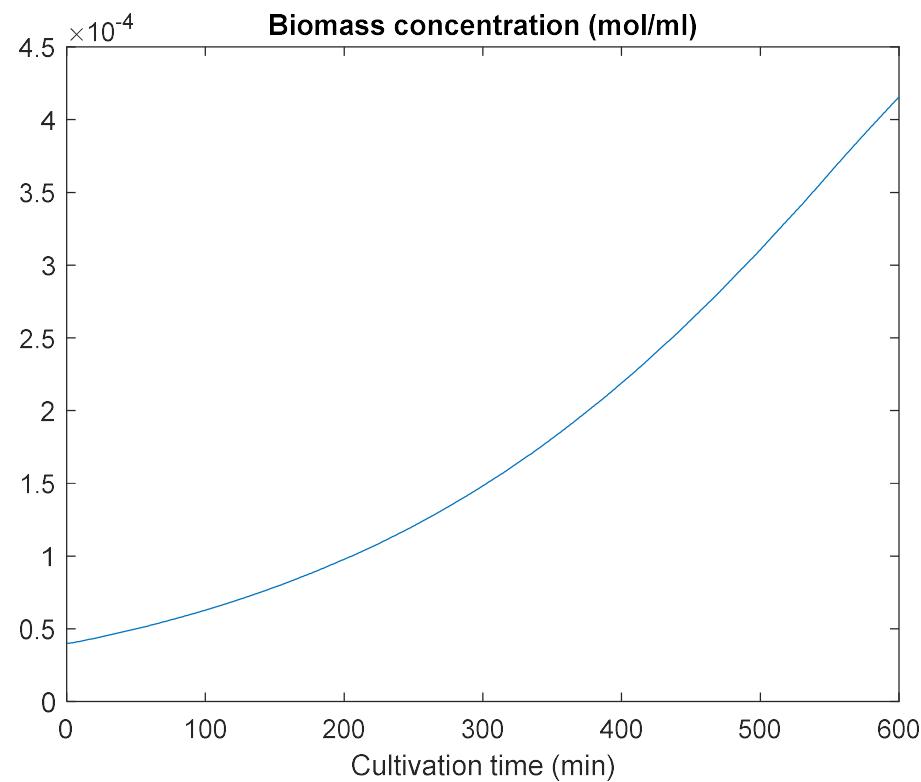
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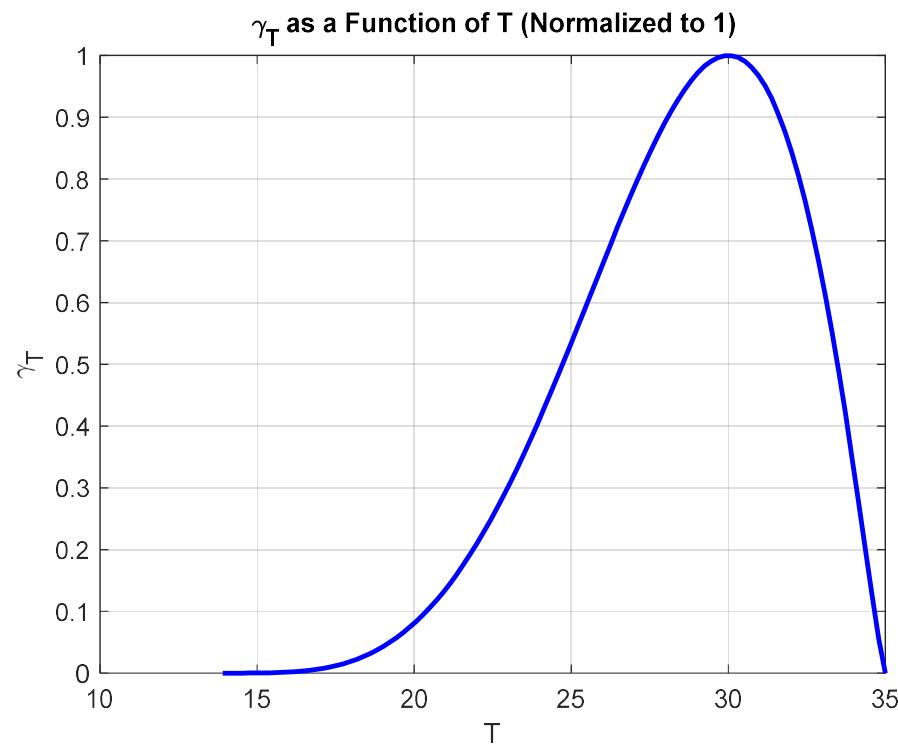
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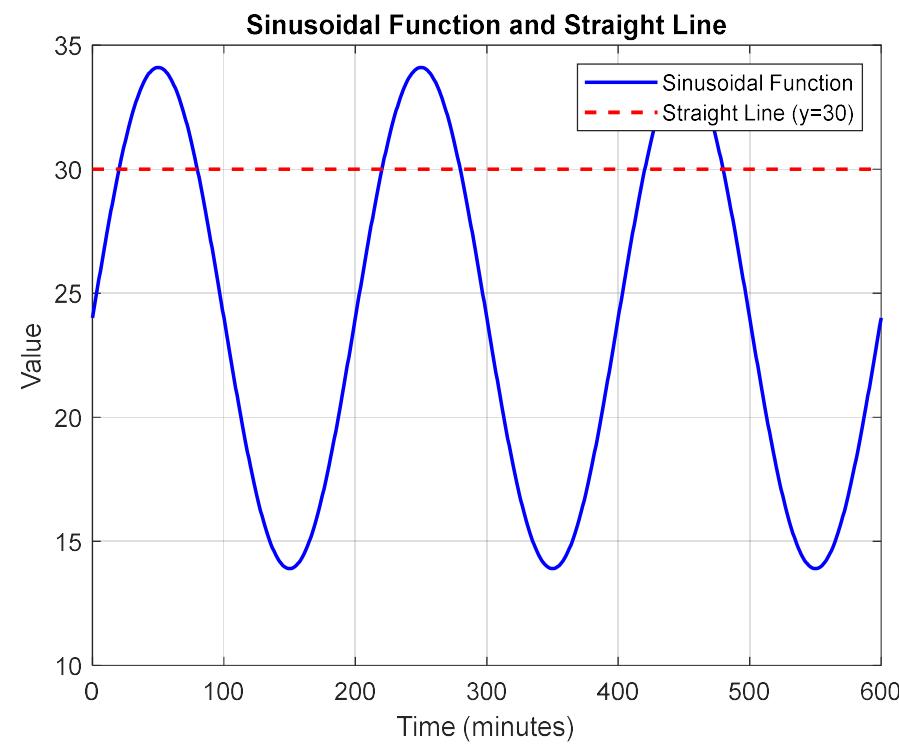
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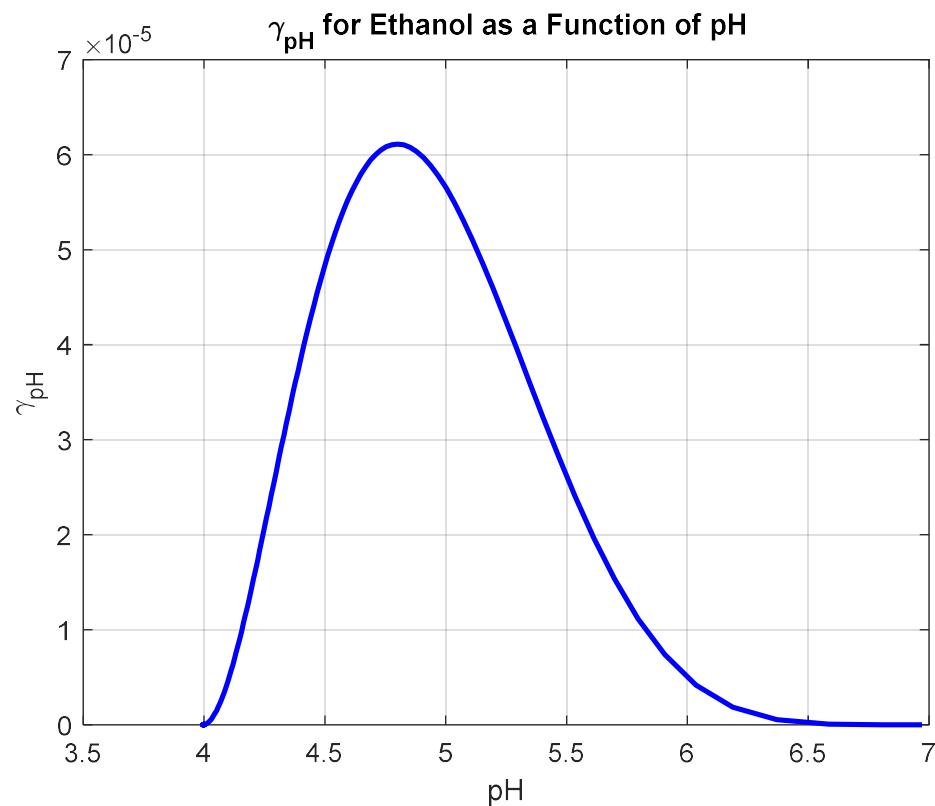
# Simulation Results for Strong Acid Strong Base and Set Point of 4 with Steady State Value of 4.0002



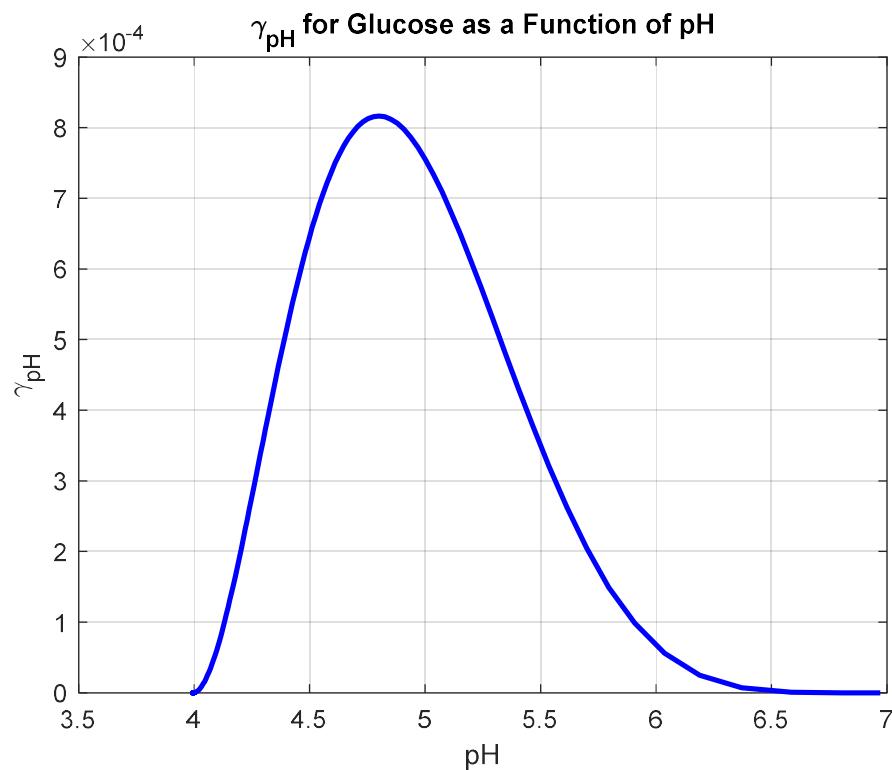
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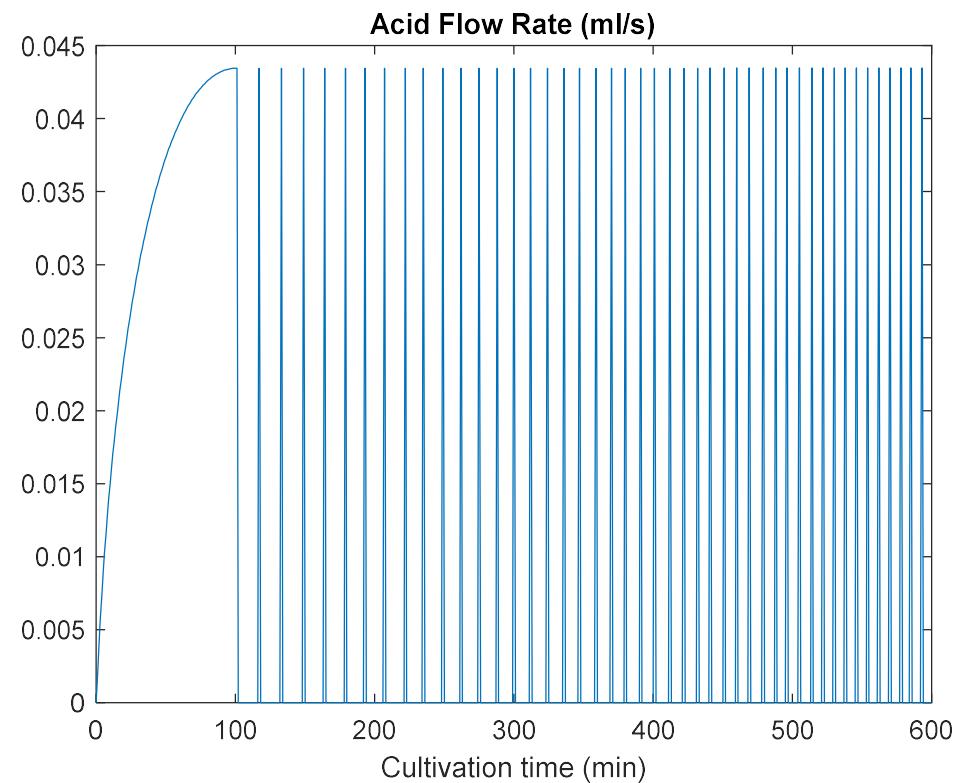
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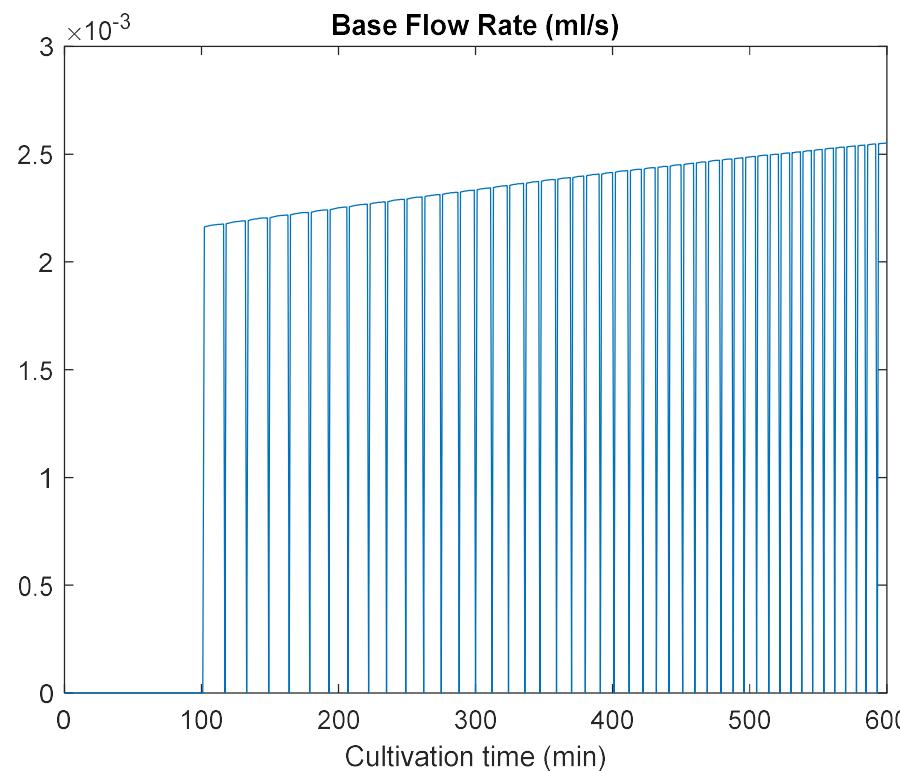
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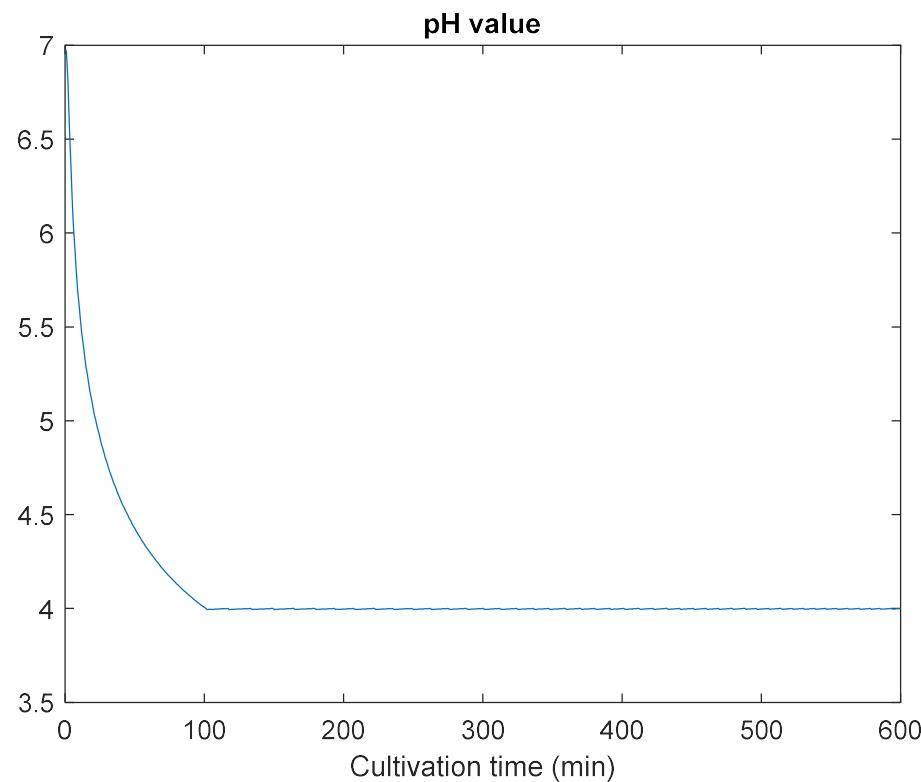
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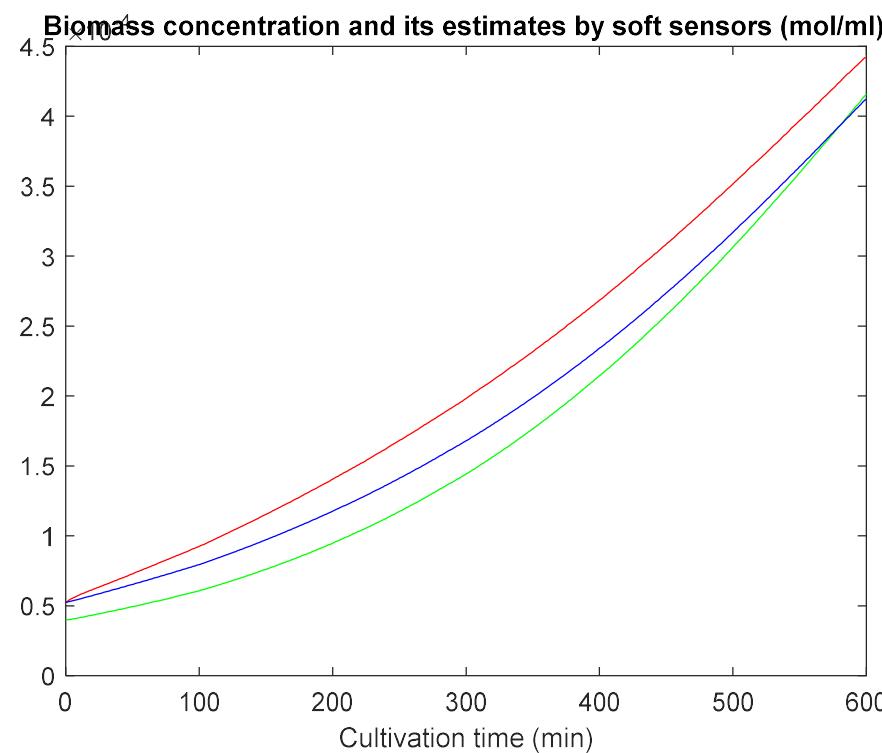
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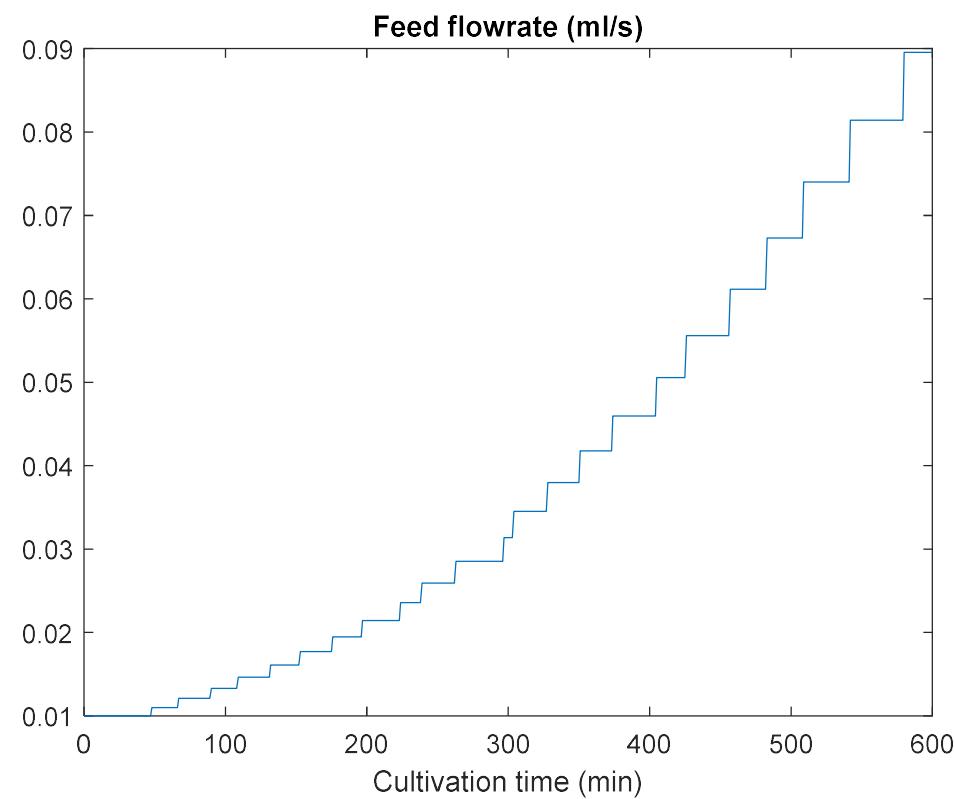
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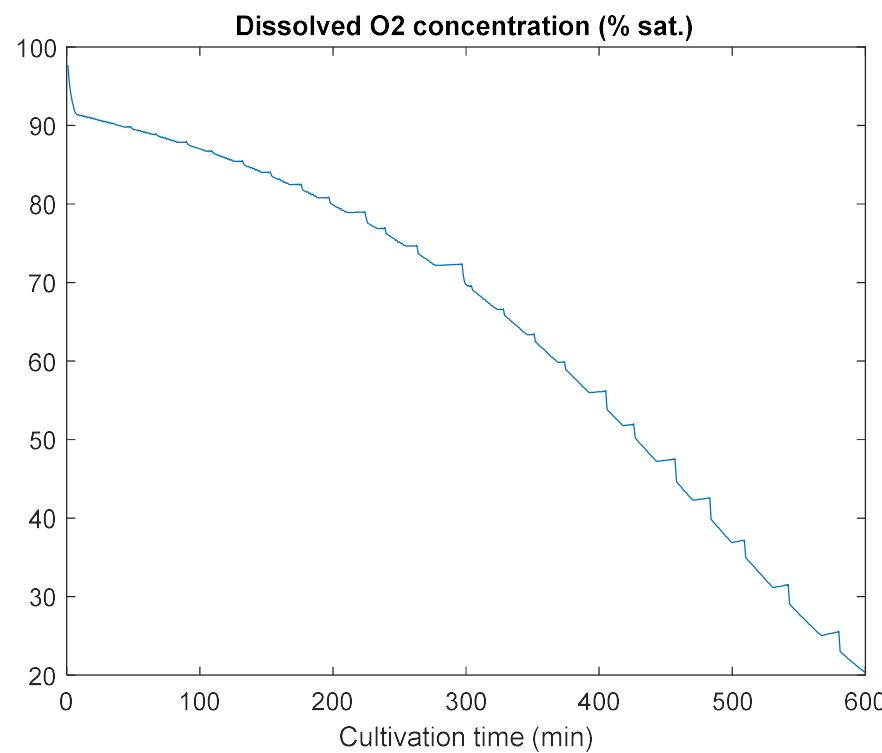
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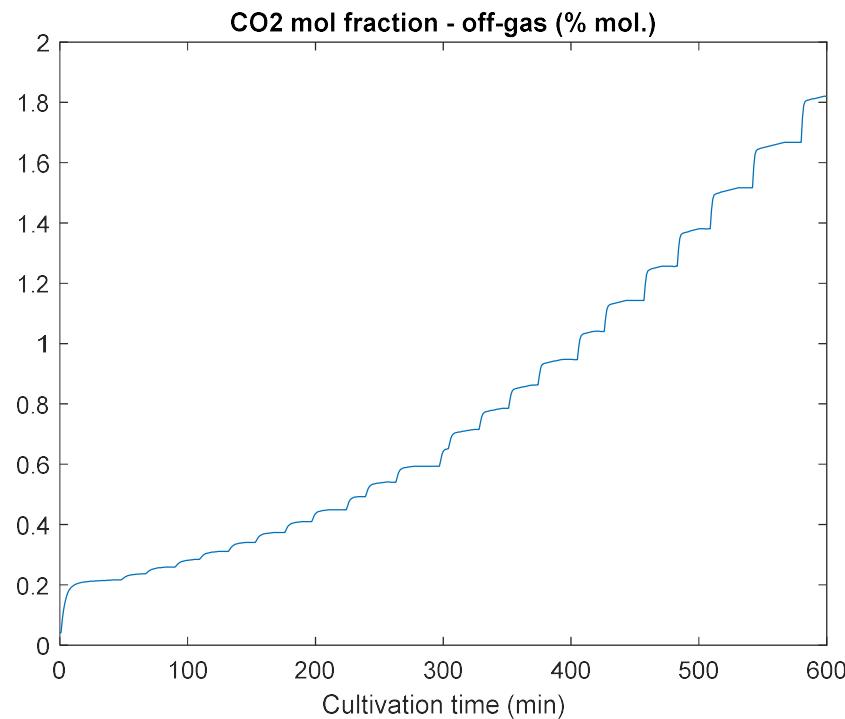
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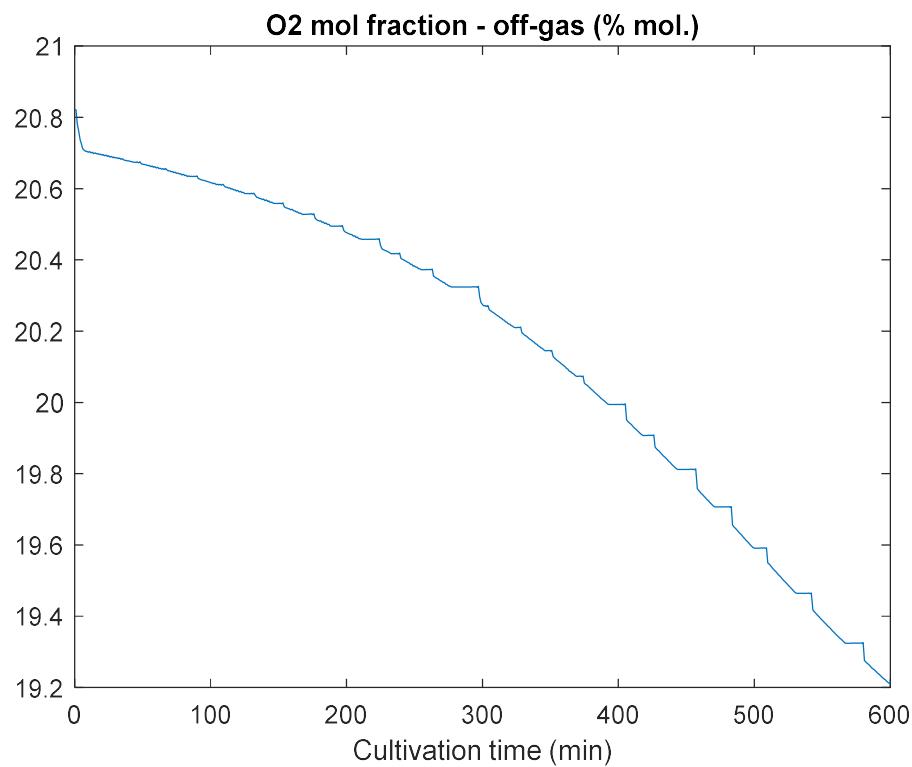
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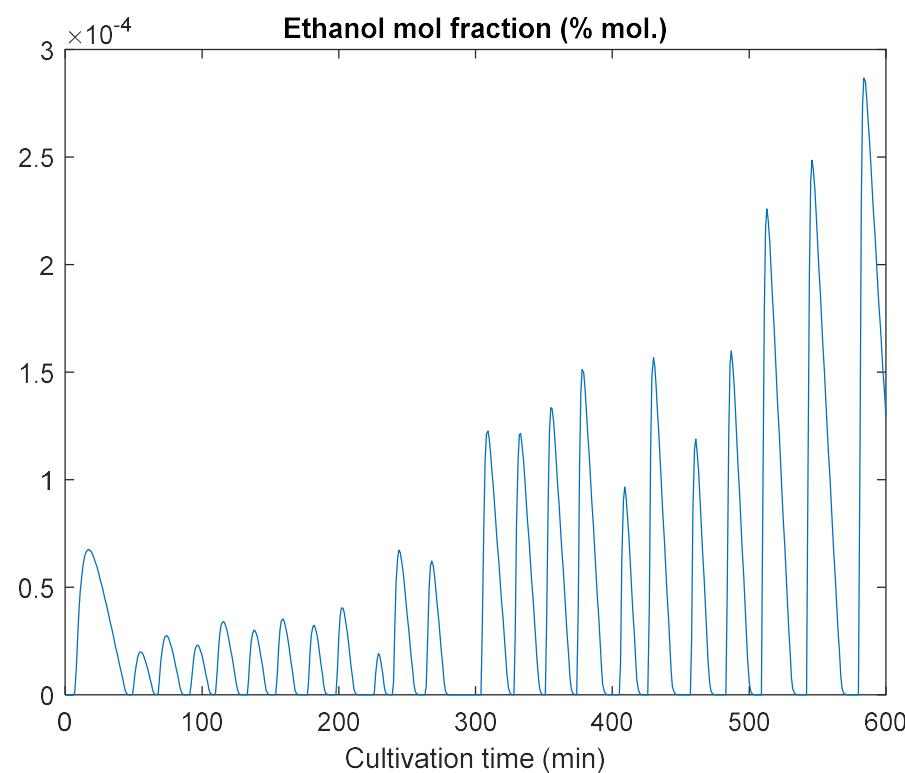
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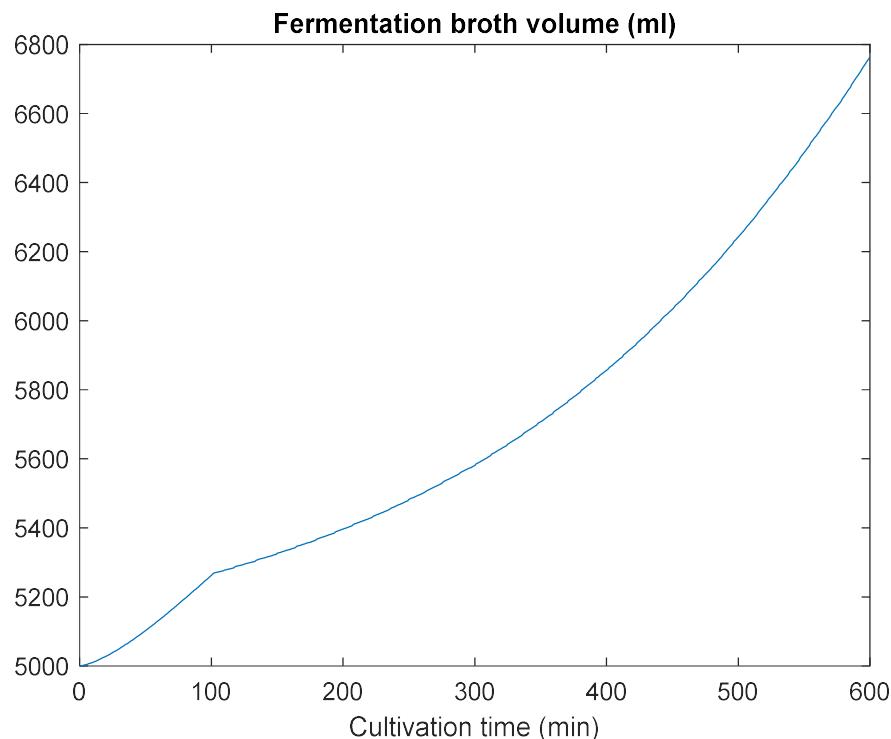
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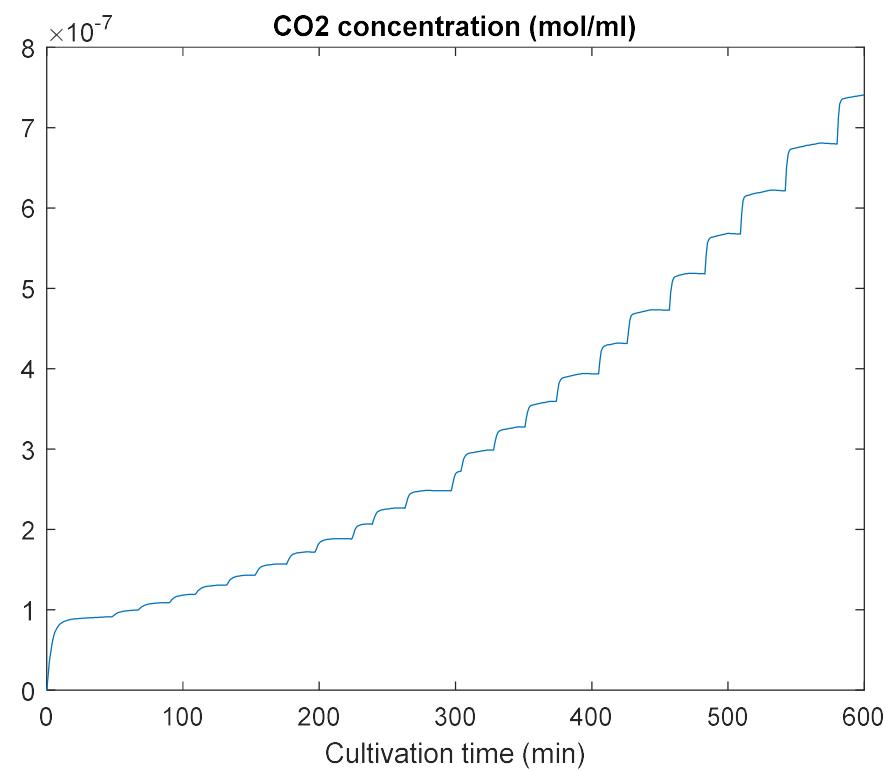
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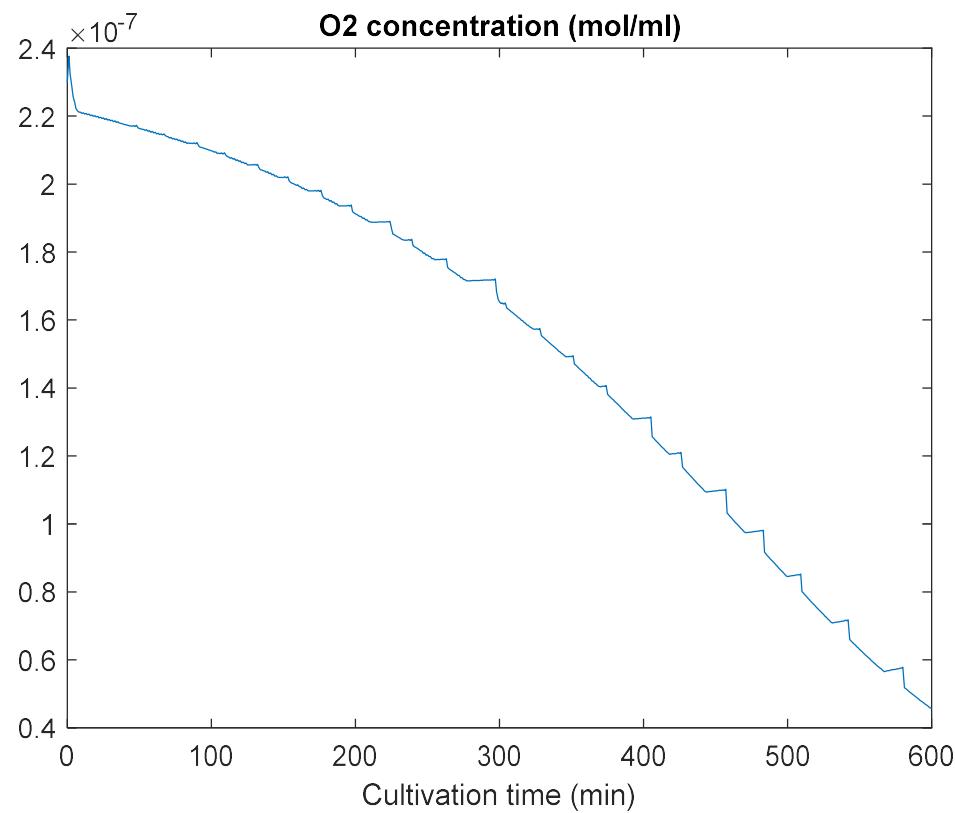
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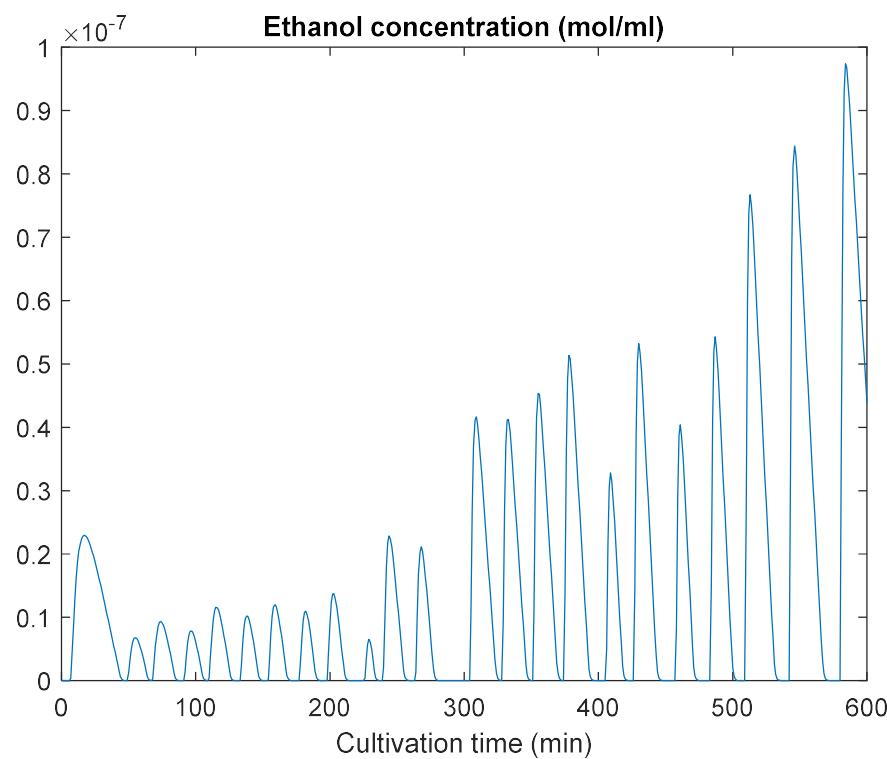
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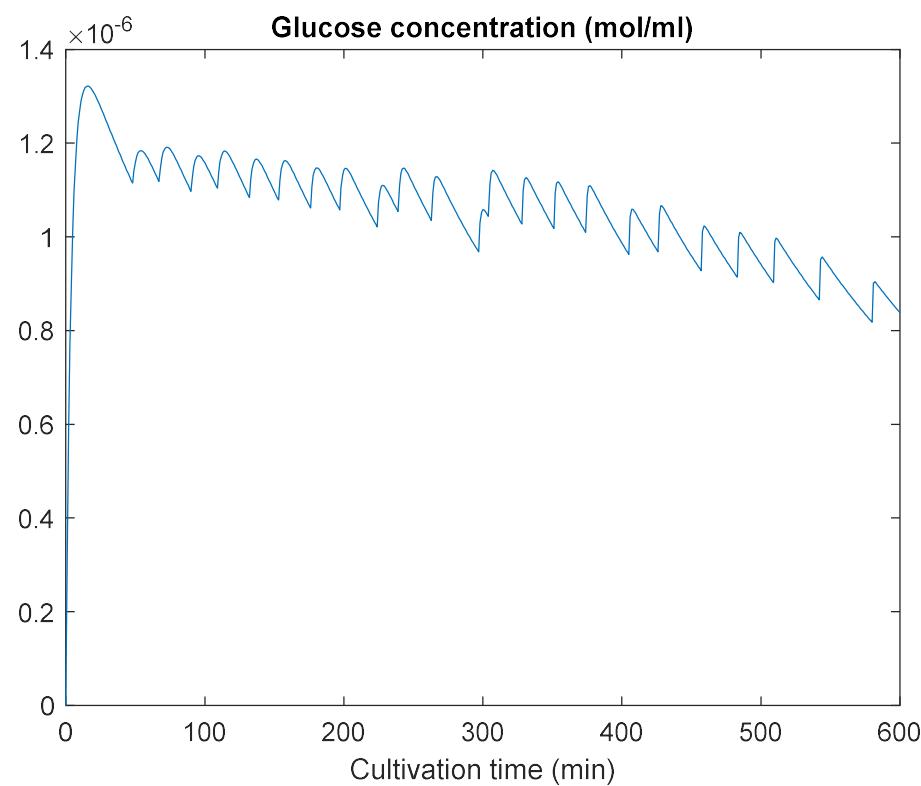
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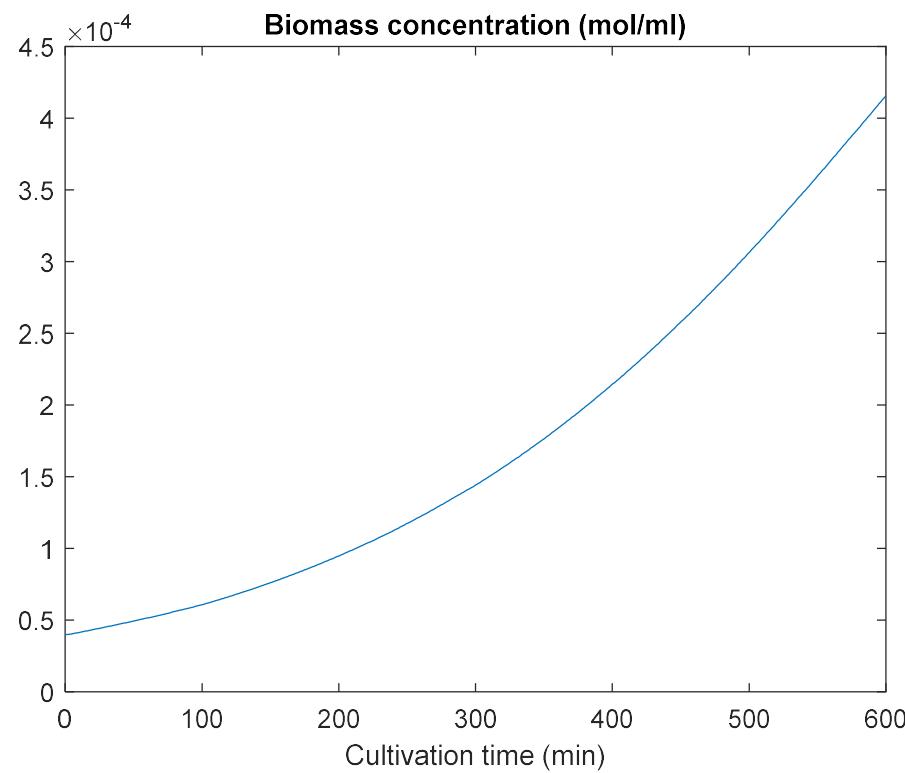
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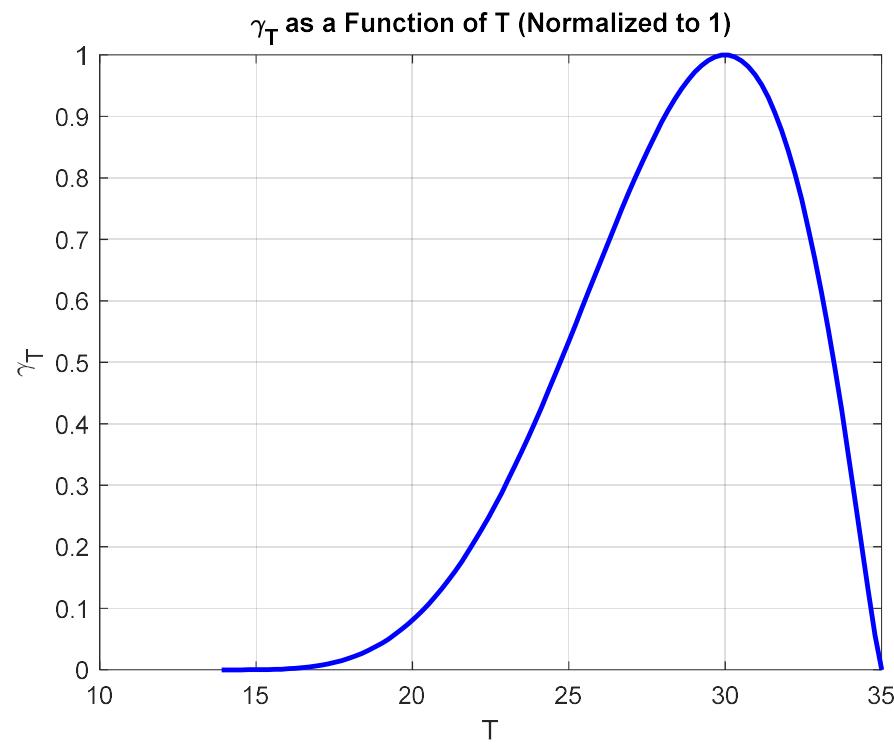
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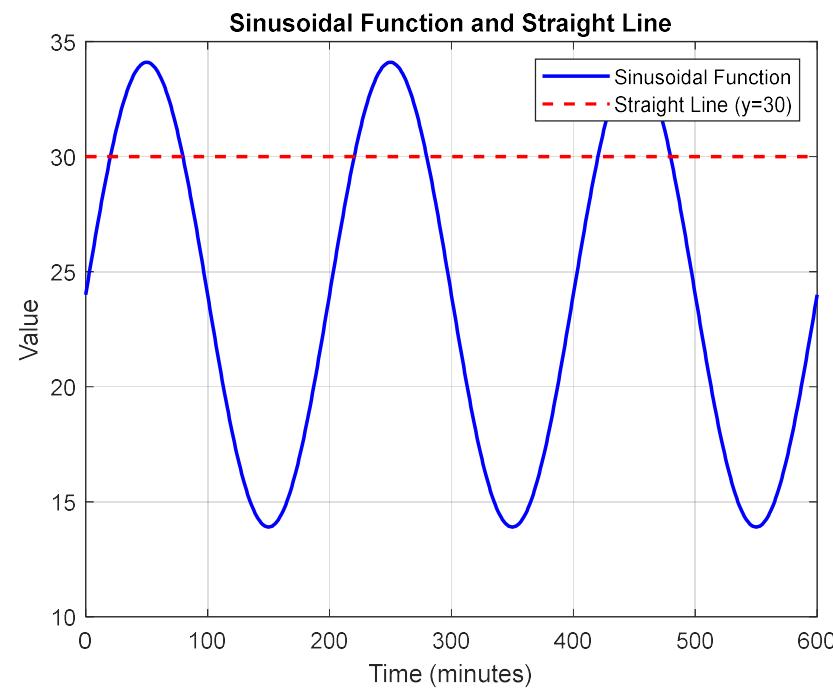
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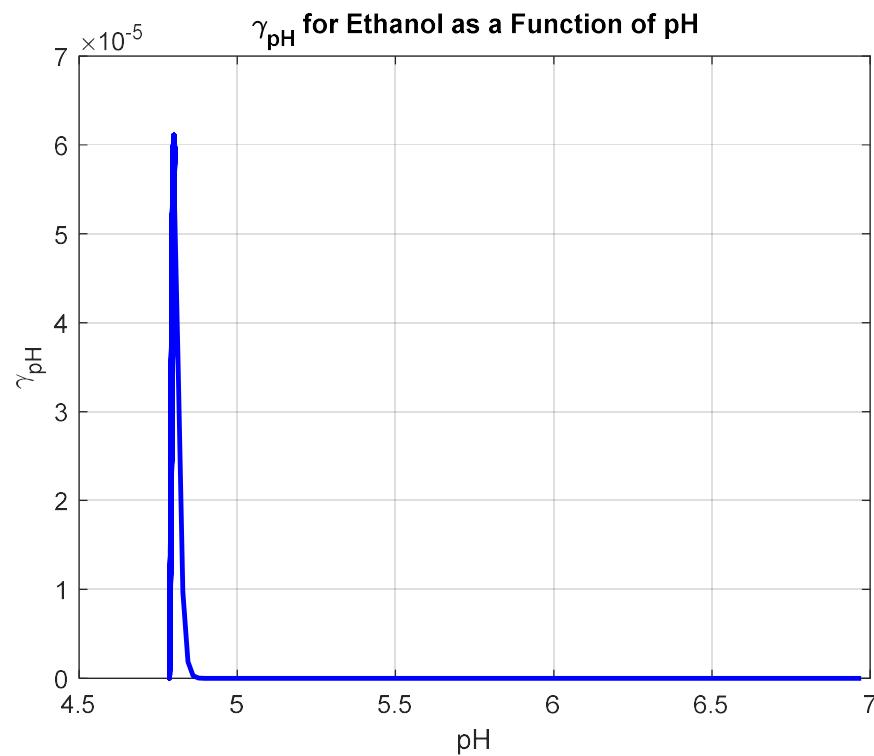
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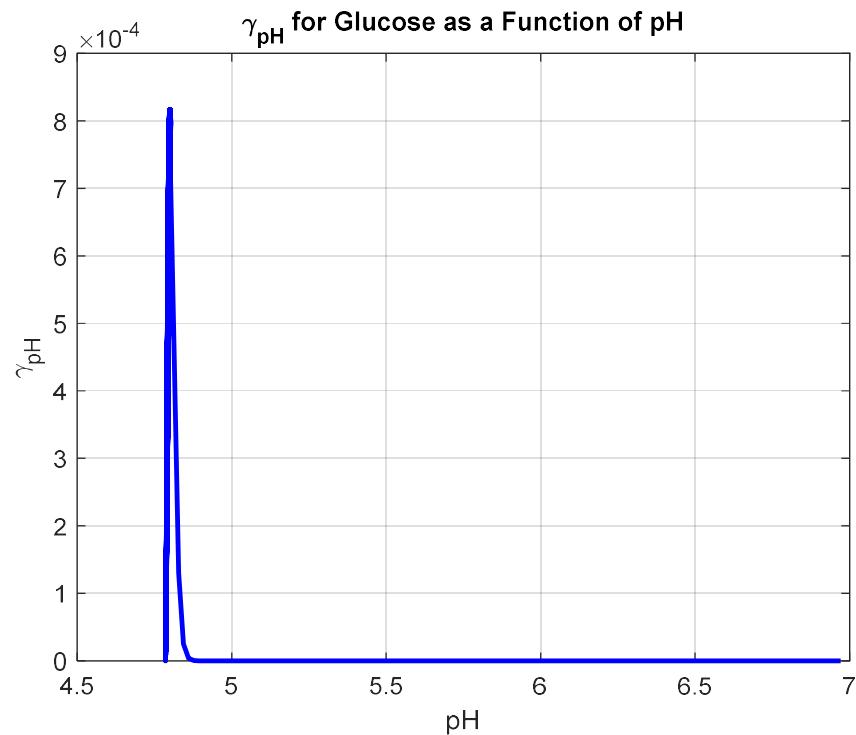
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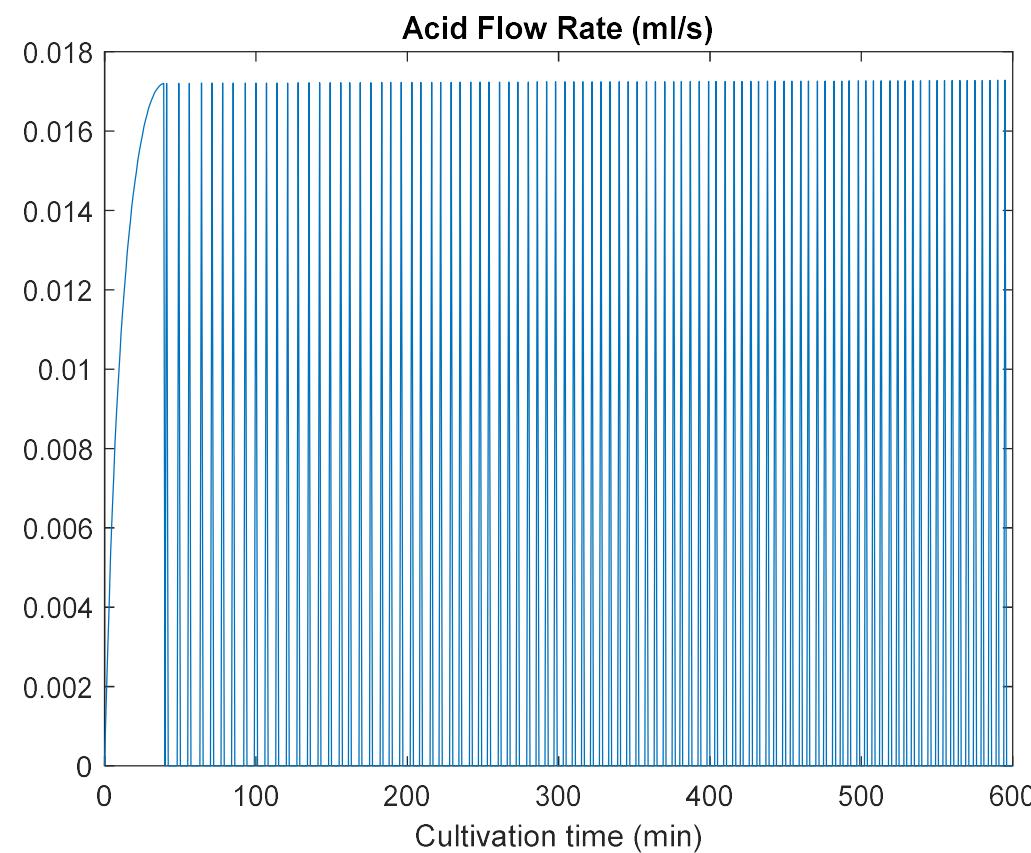
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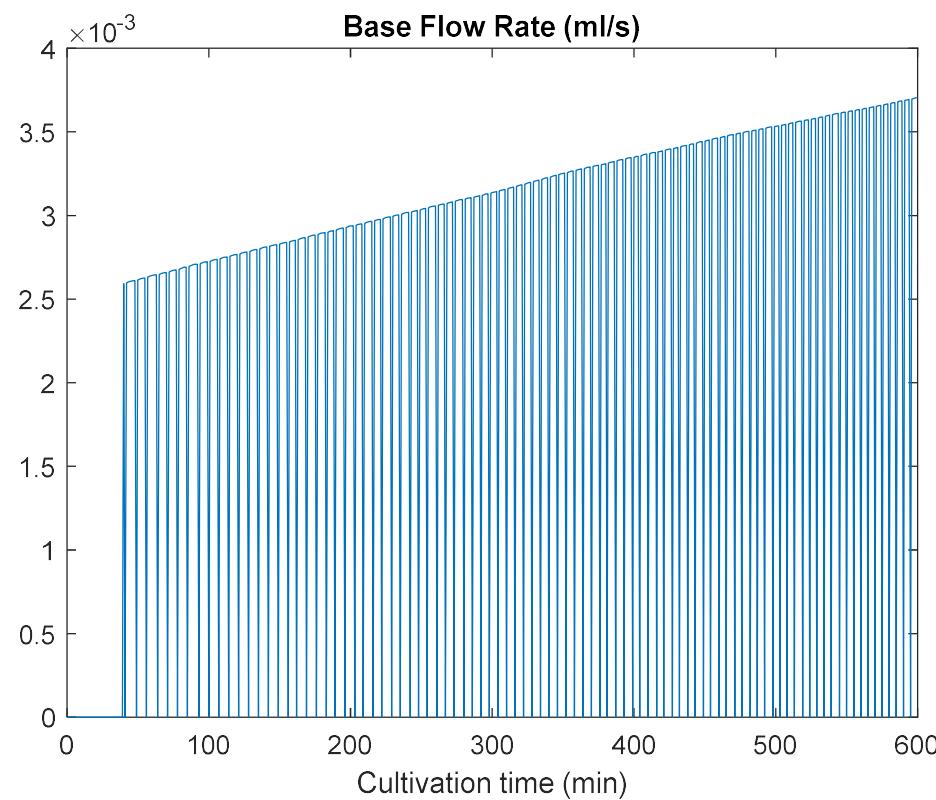
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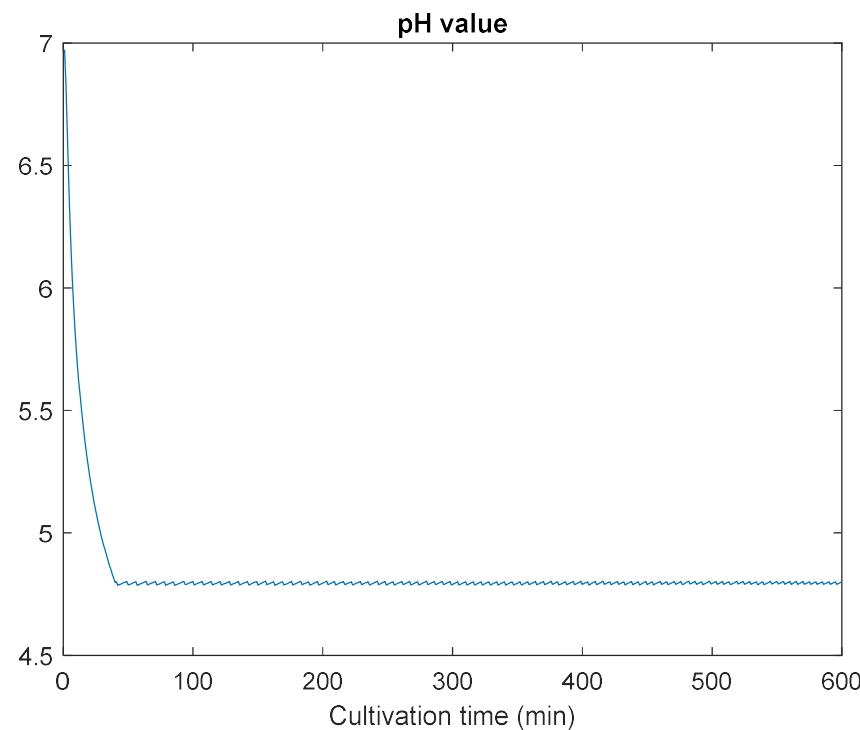
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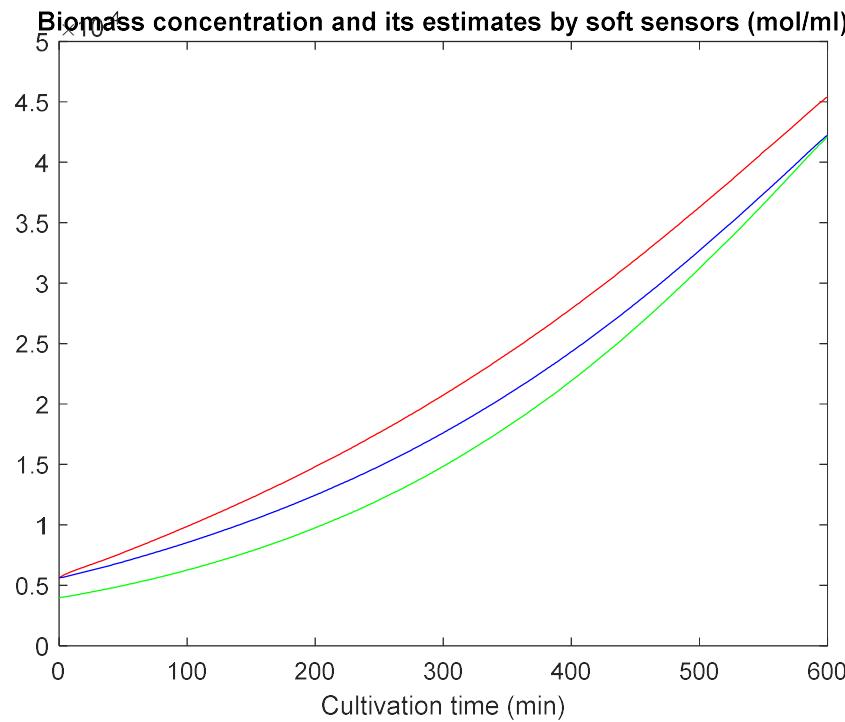
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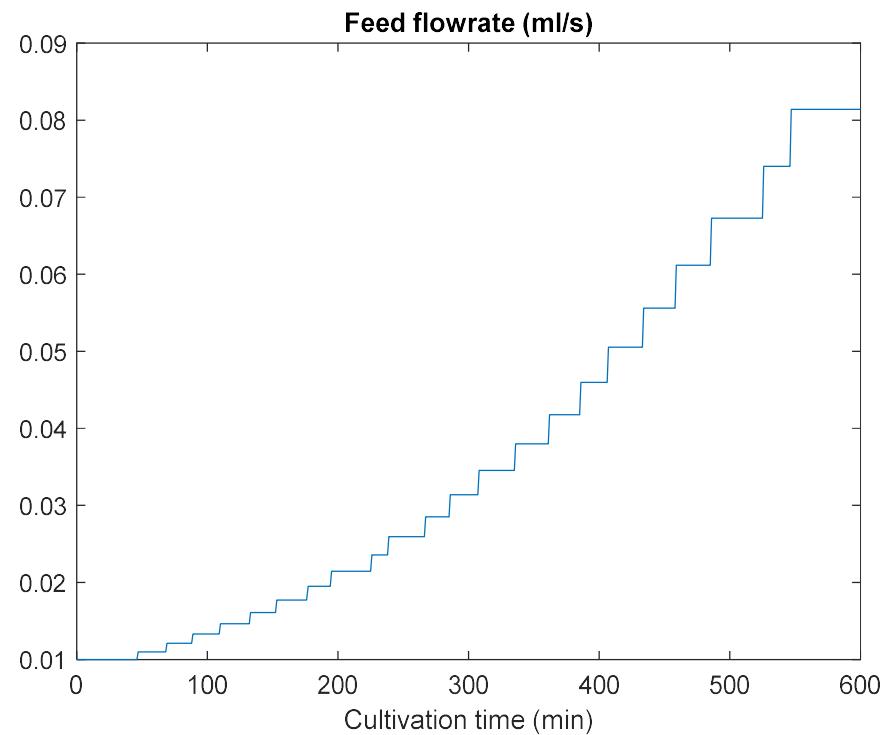
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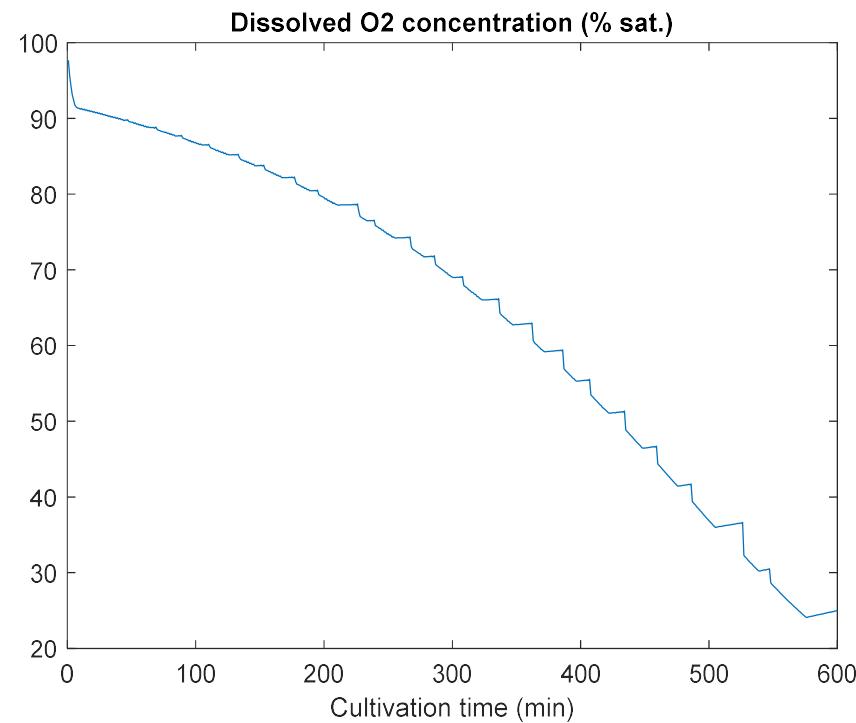
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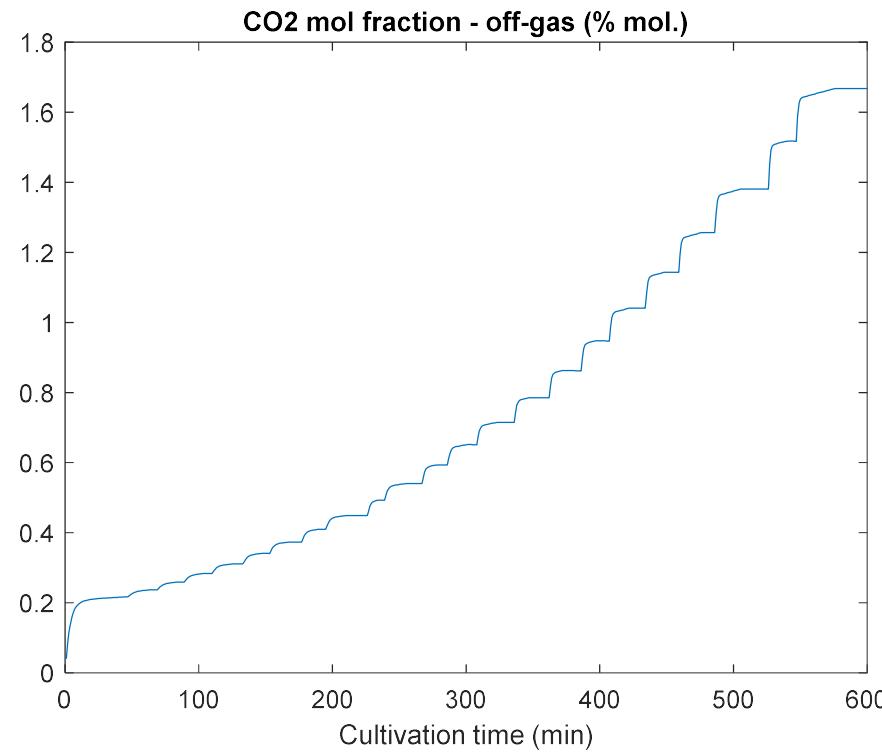
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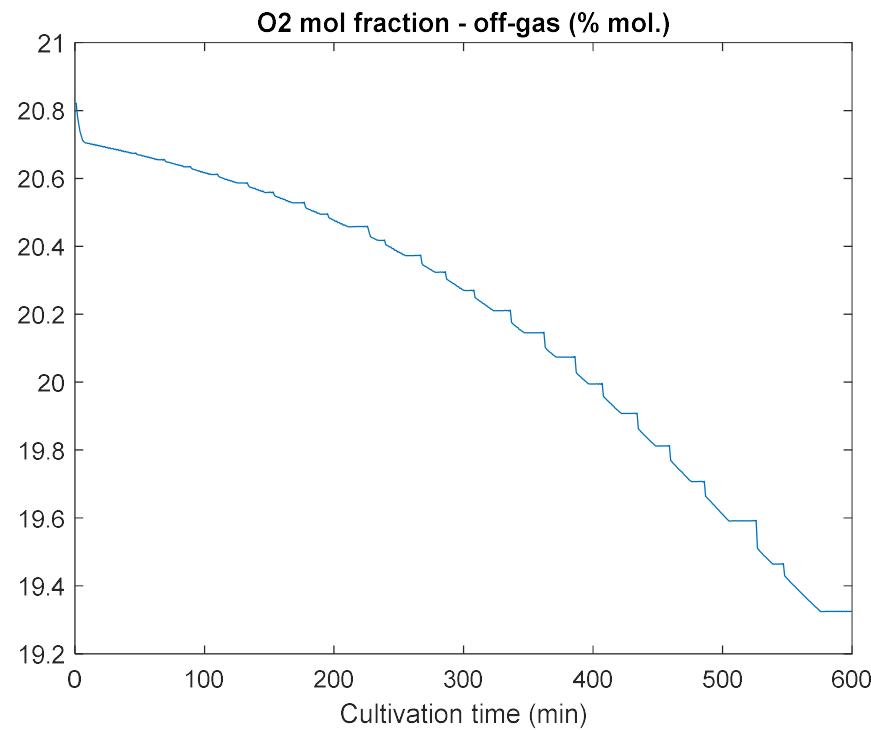
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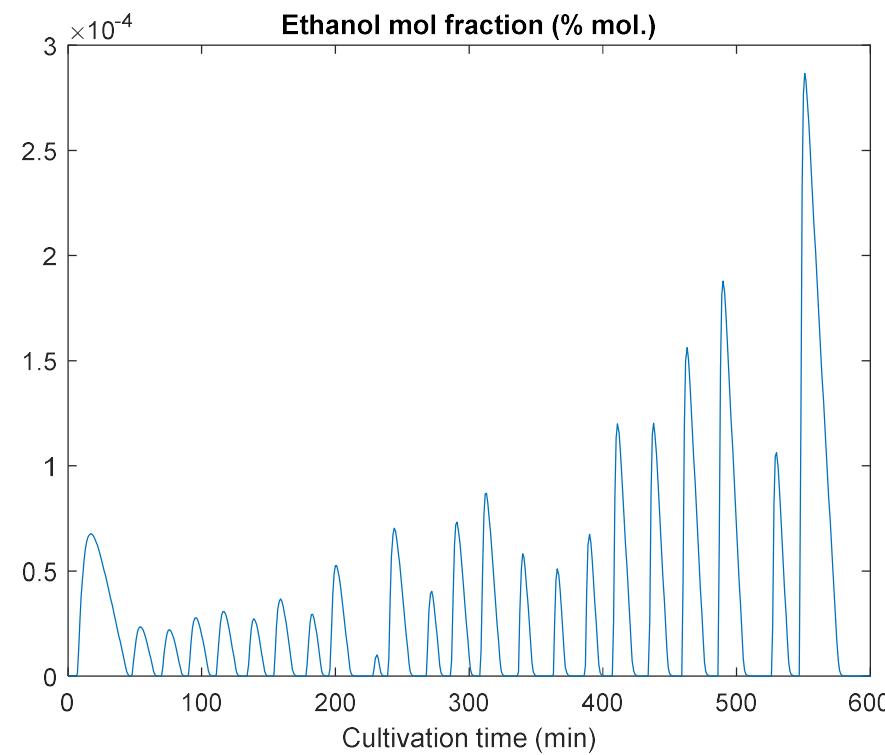
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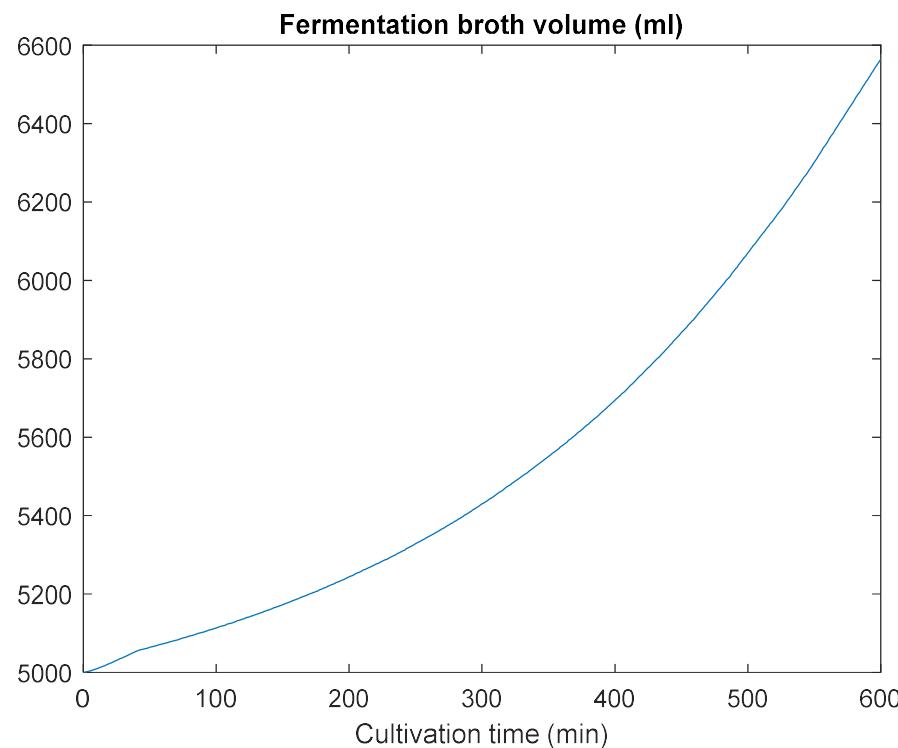
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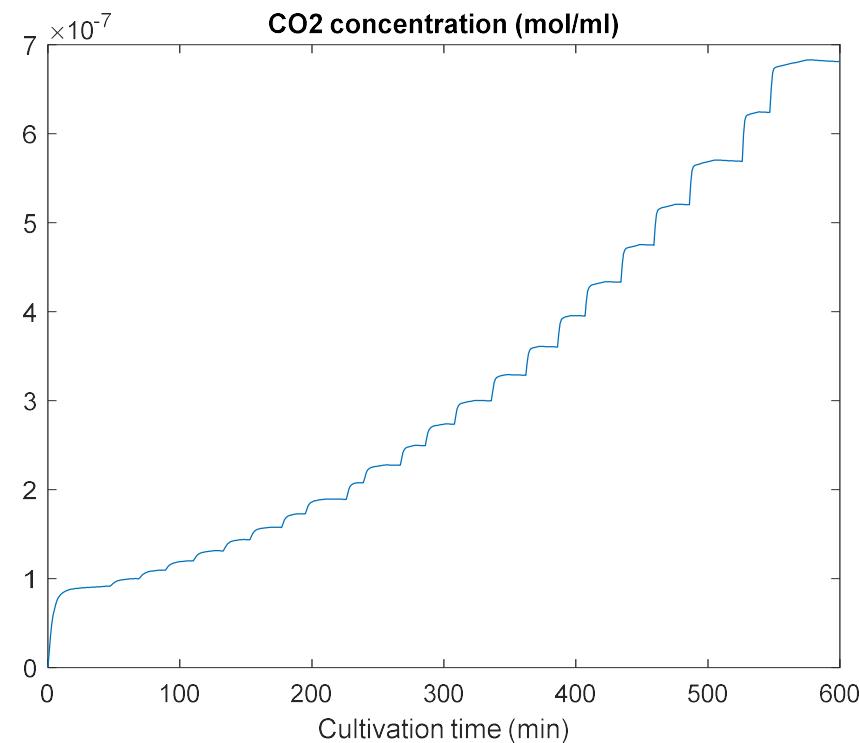
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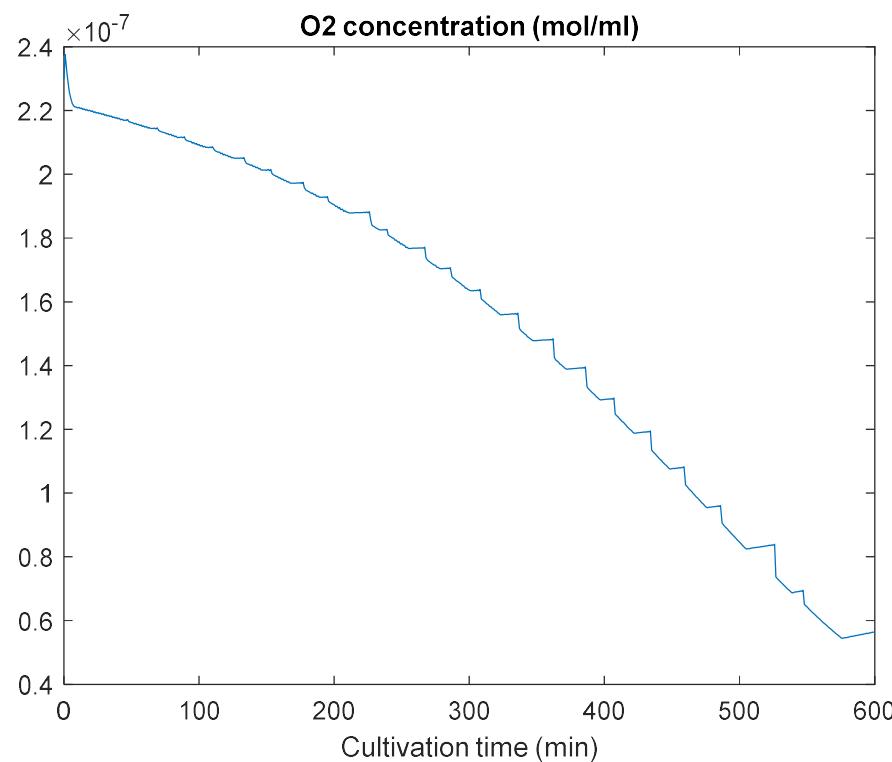
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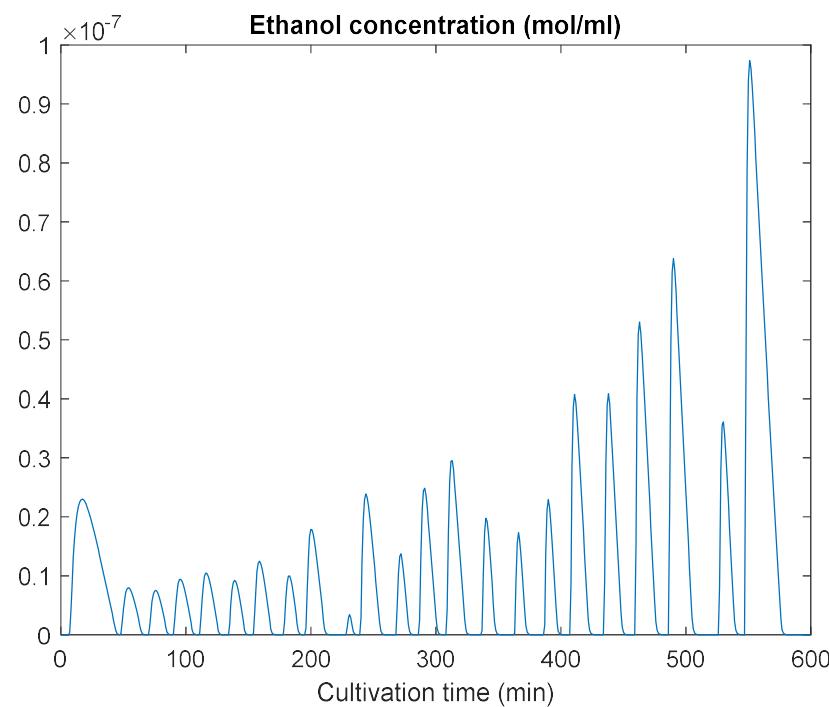
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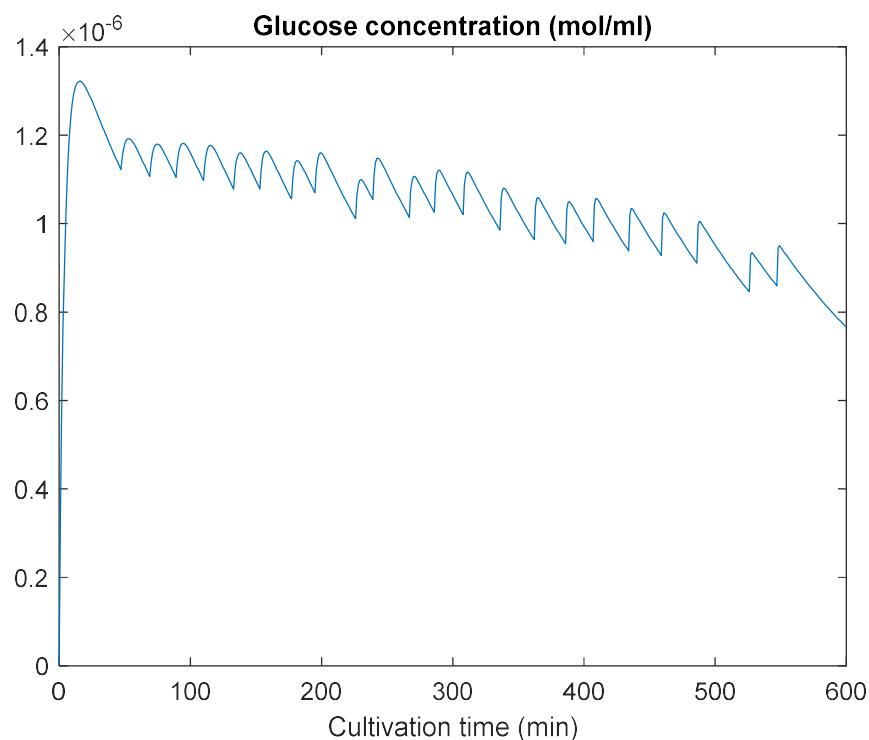
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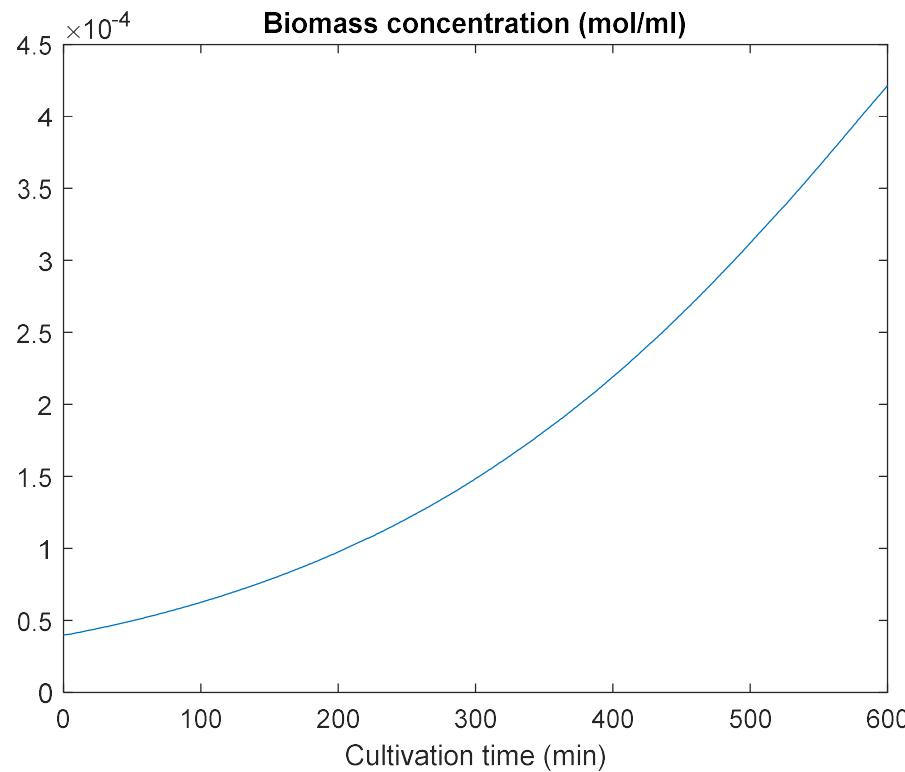
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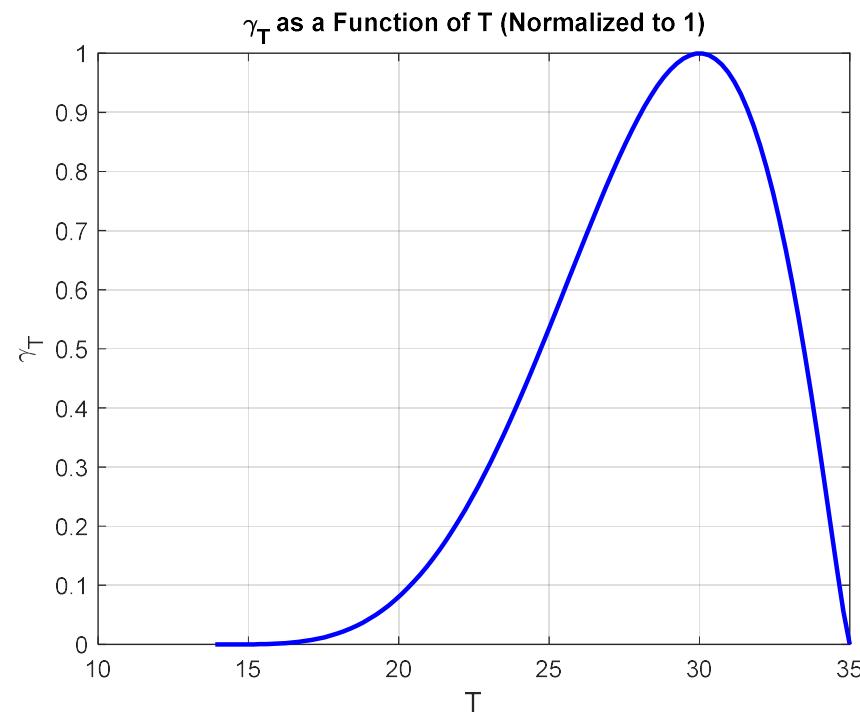
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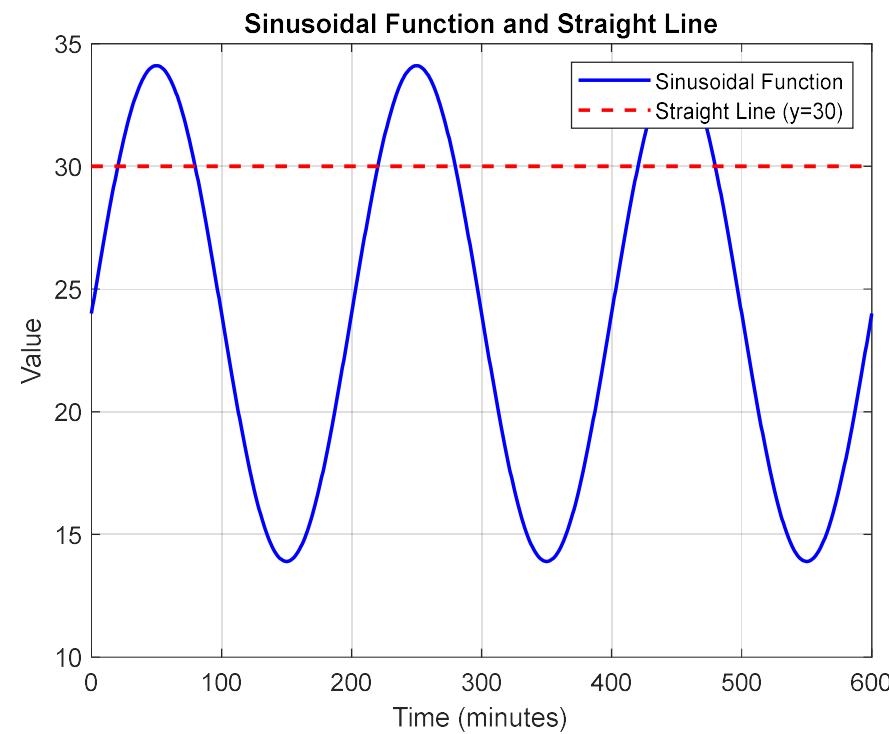
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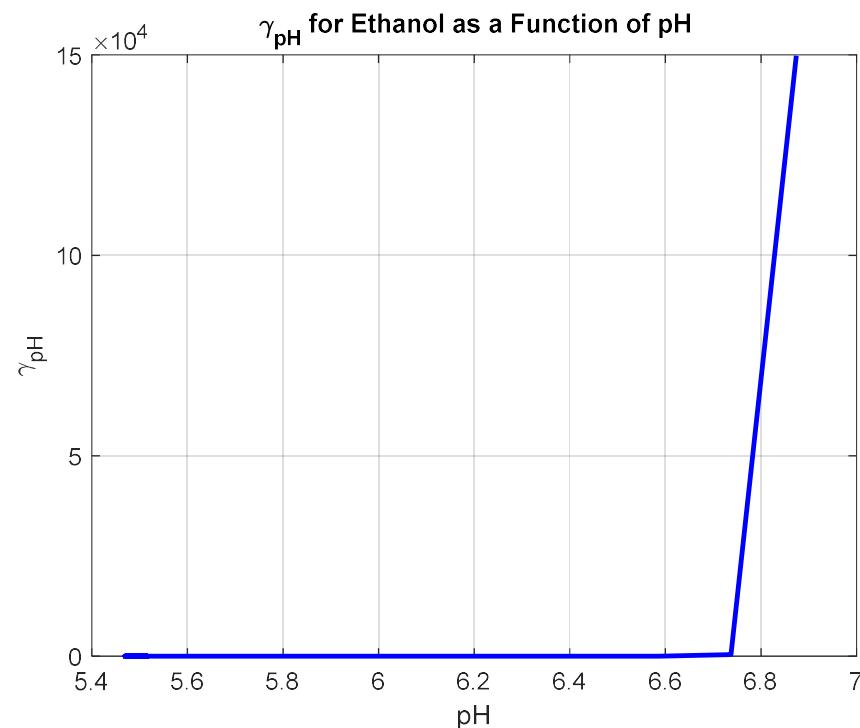
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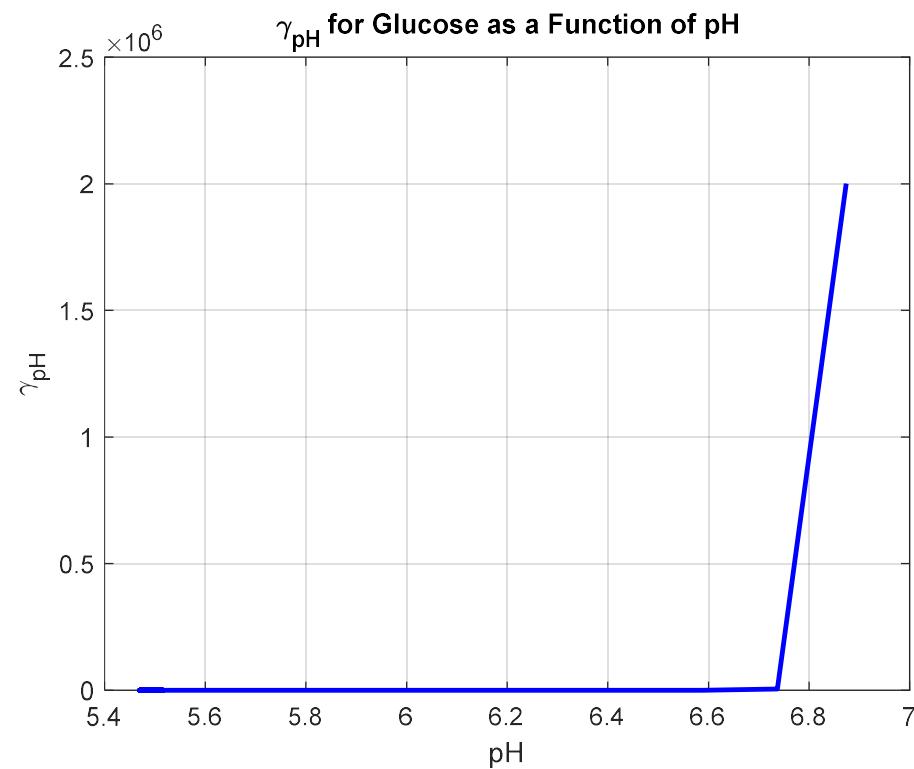
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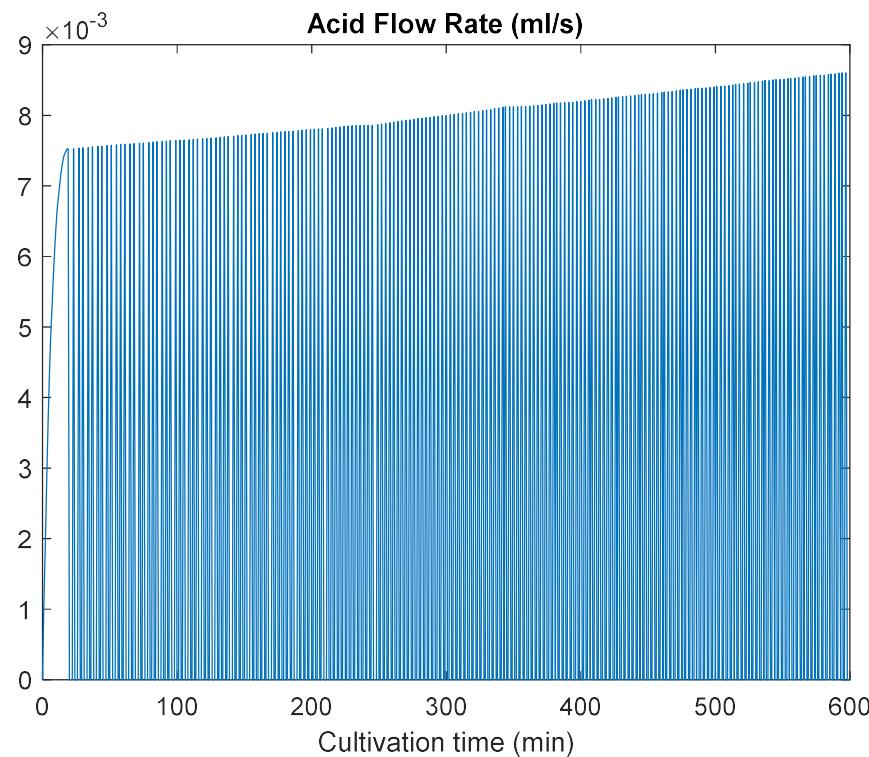
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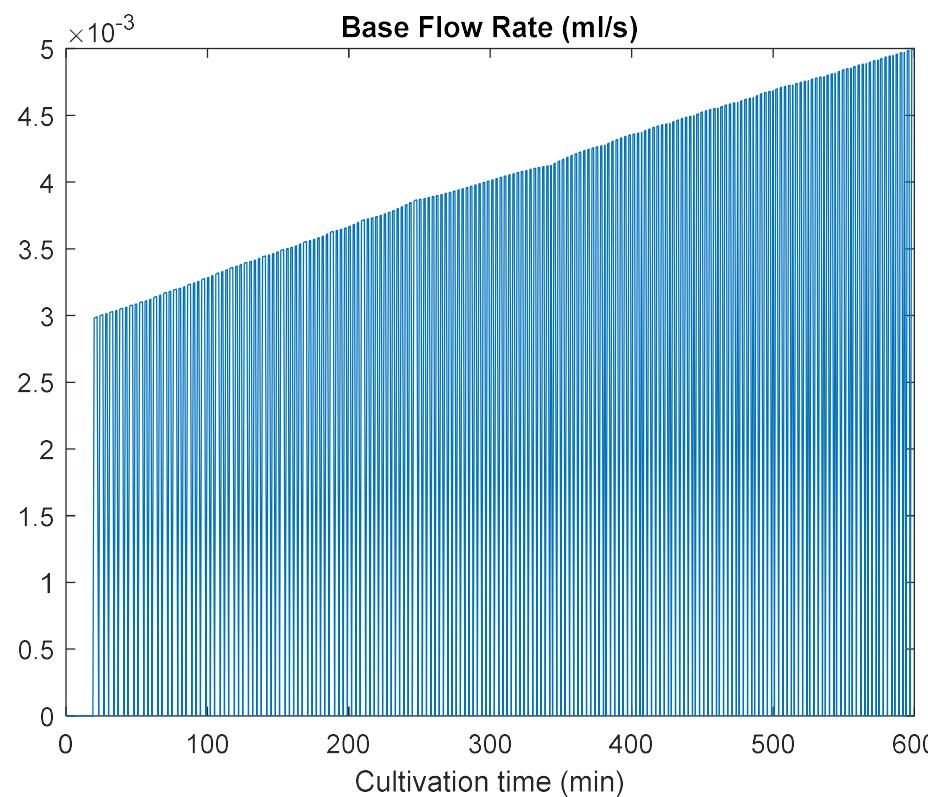
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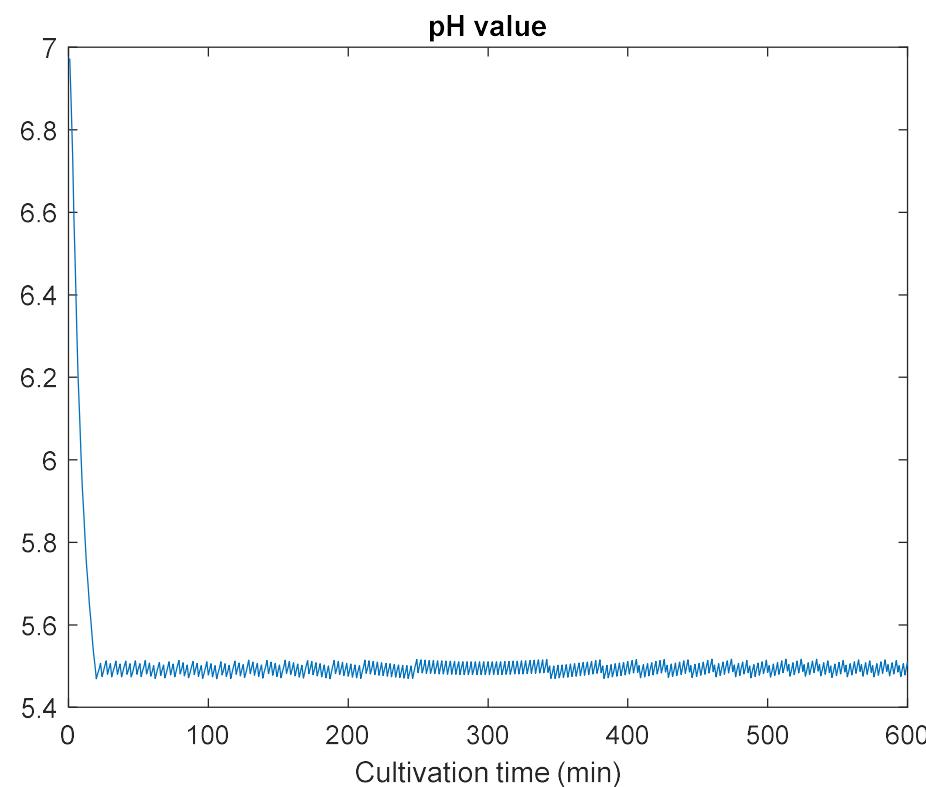
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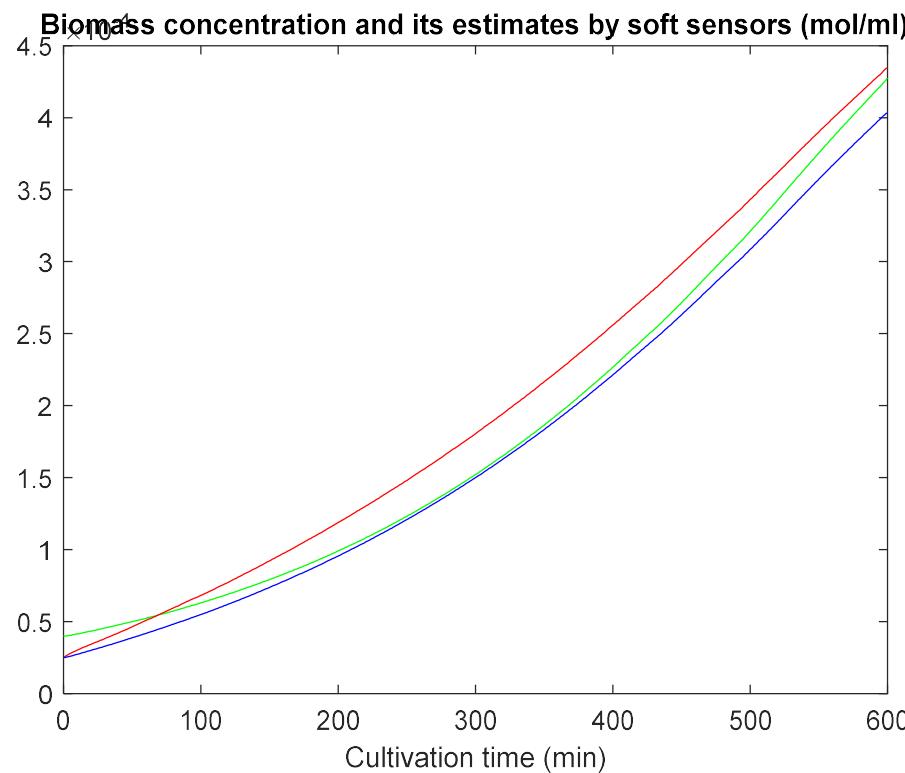
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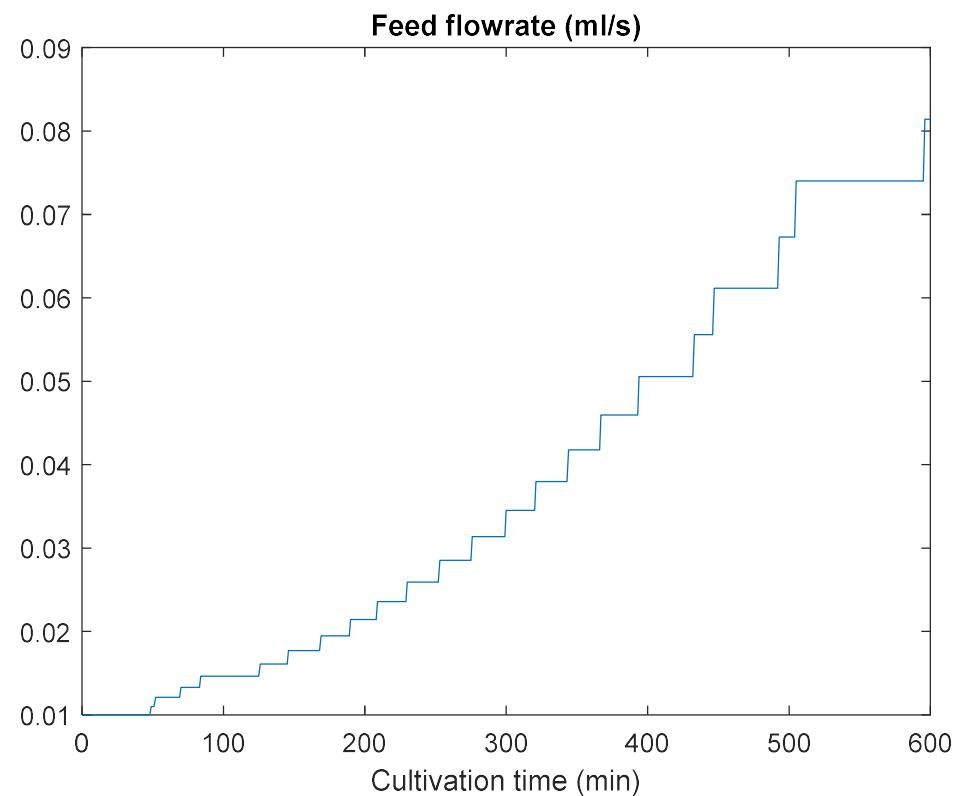
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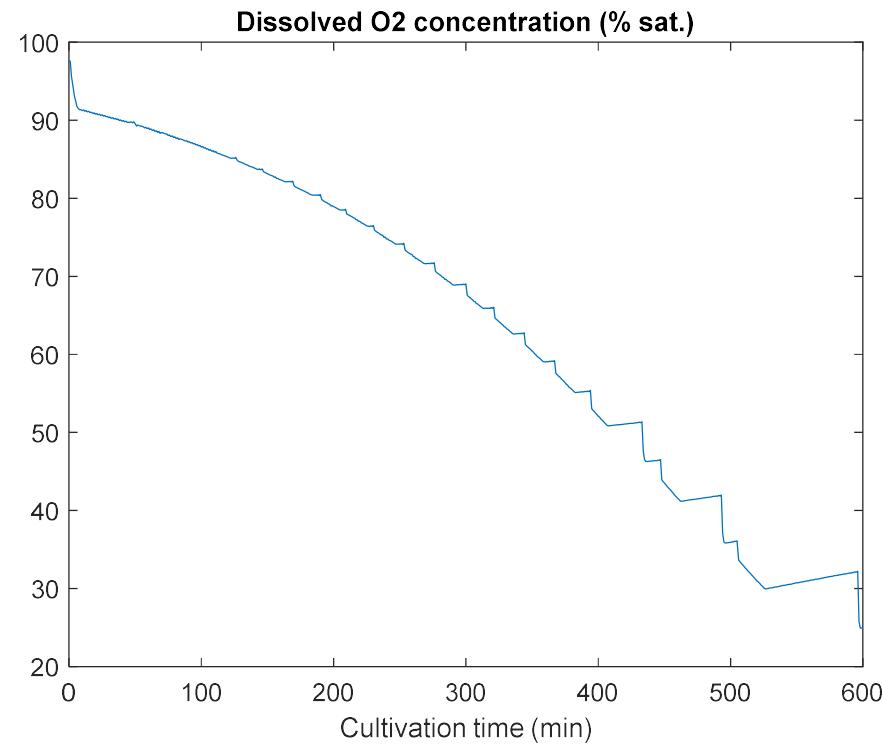
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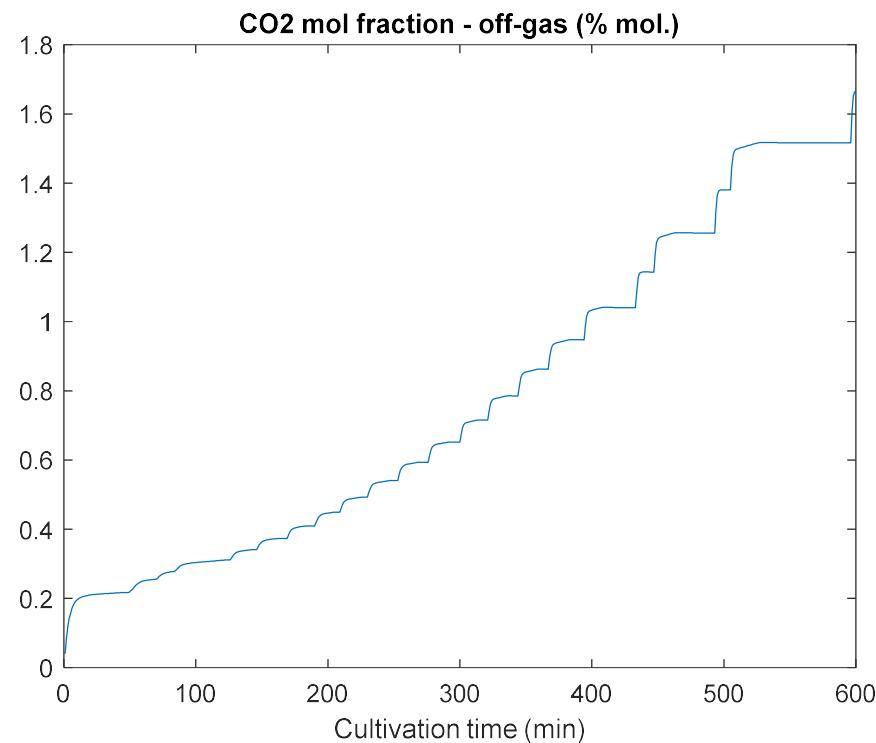
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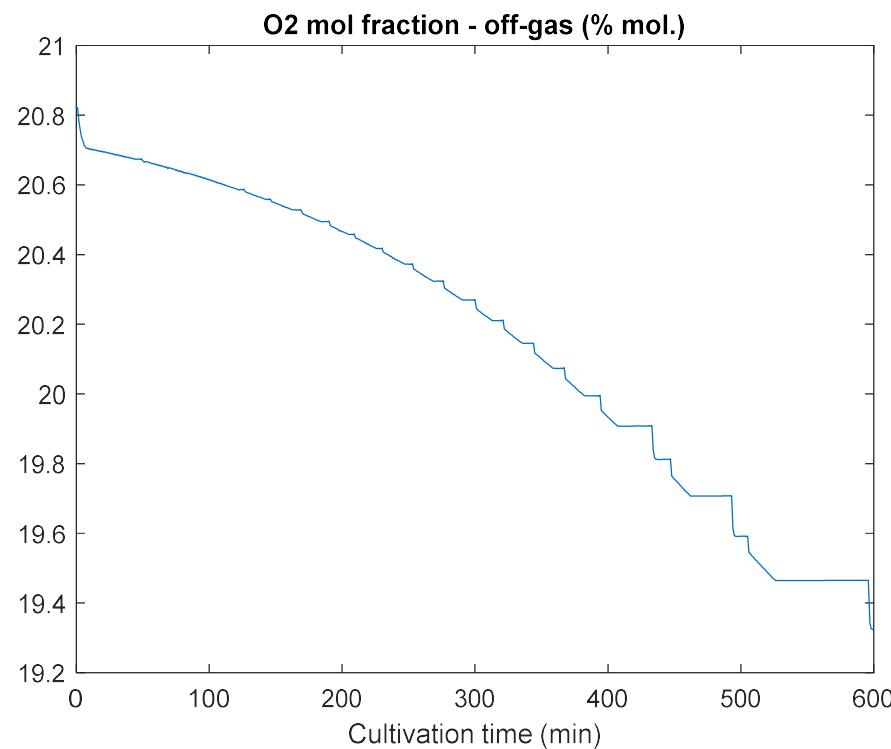
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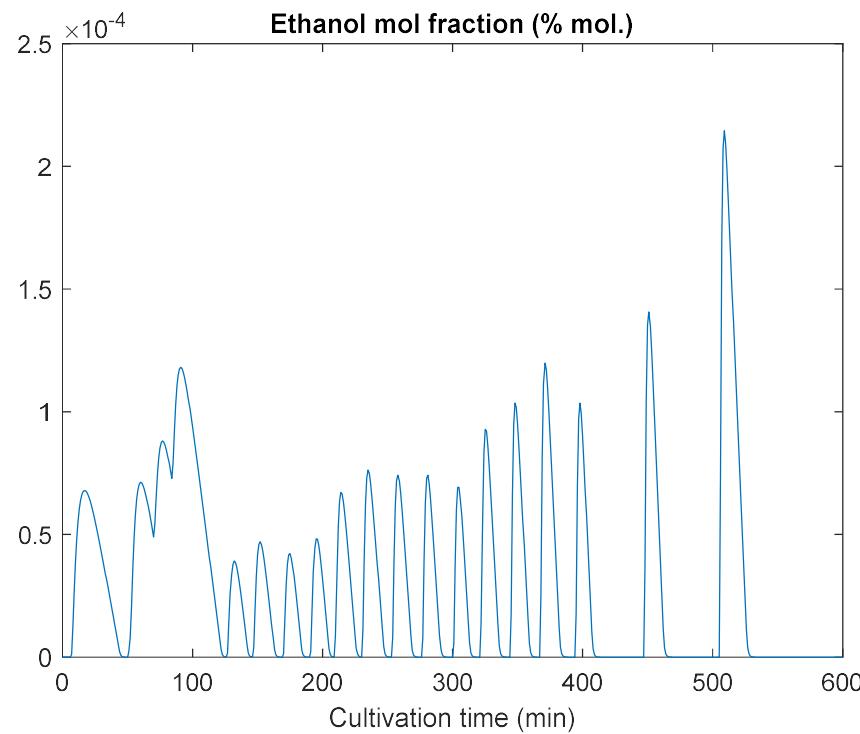
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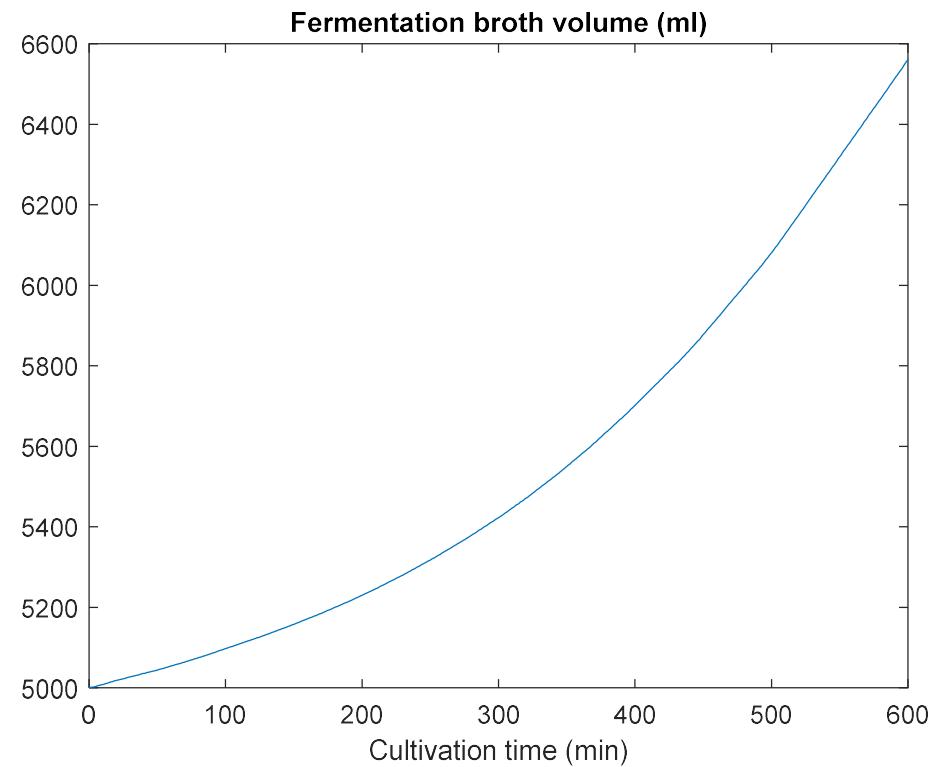
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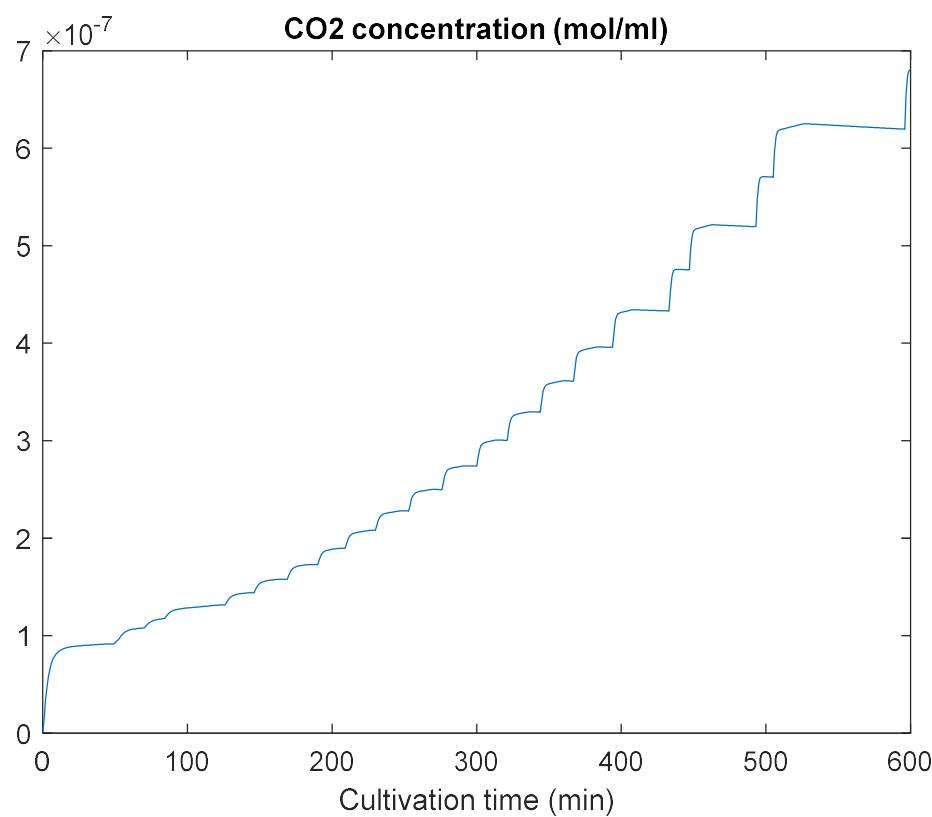
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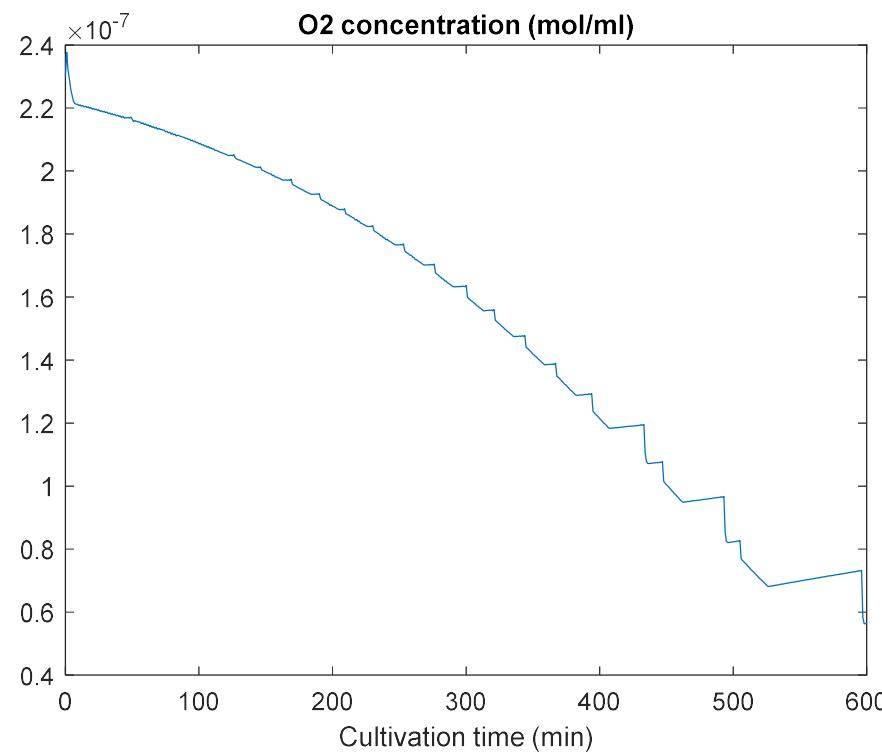
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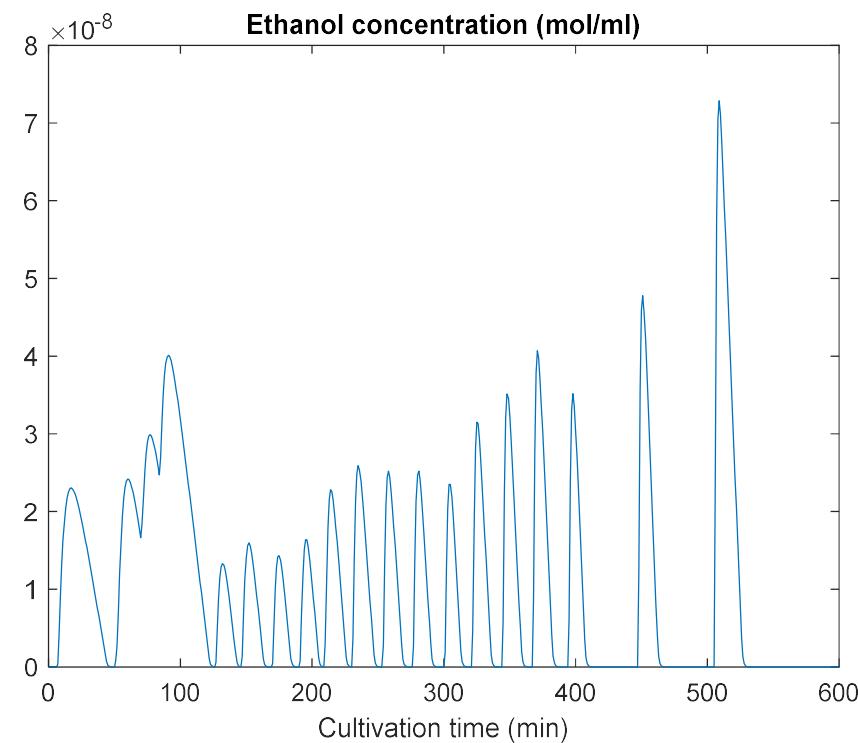
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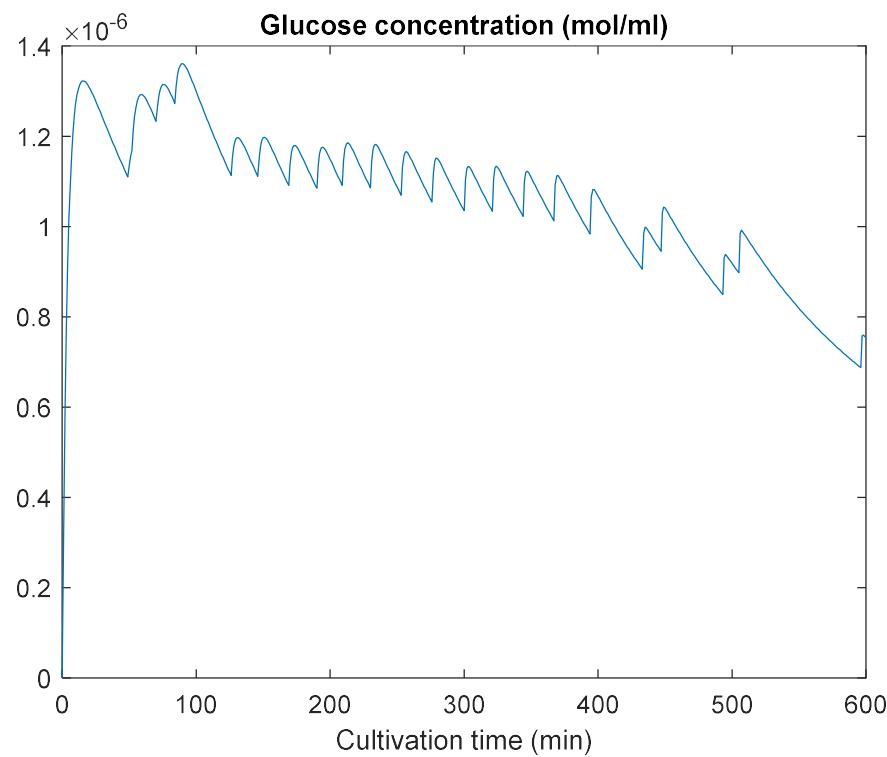
# Simulation Results for Strong Acid Strong Base and Set Point of 5.5



# Simulation Results for Strong Acid Strong Base and Set Point of 5.5



# Simulation Results for Strong Acid Strong Base and Set Point of 5.5



# Simulation Results for Strong Acid Strong Base and Set Point of 5.5

