Homework 2

Modeling Exponential Growth and Substrate Utilization

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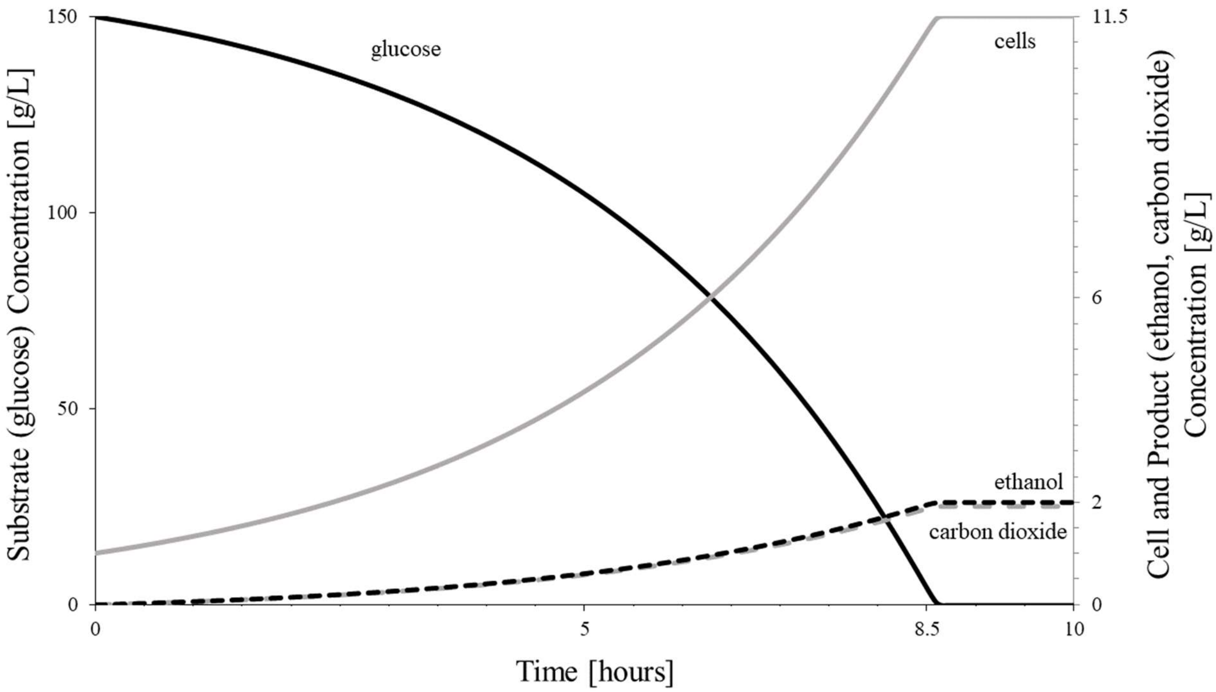

Figure 1: Cell, Ethanol, Carbon Dioxide, and Glucose Concentration [g/L] vs. Time [hours]

Derevation of Theoretical Yield of Ethanol Differential Equations

The theoretical yield of product can be derived from the continuity equation (Equation 1).

$$In - Out + Generation - Consumption = Accumulation \qquad [1]$$

As the process is assumed to be performed within a batch reactor, the in and out terms can be assumed to be zero. Additionally, as the ethanol is a product, it can be assumed that it is not consumed; thus, the consumption term can also be assumed to be zero. The continuity equation can now be simplified to Equation 2.

$$Generation = Accumulation \qquad [2]$$

From Maiorella et al., 1983, the generation term is a function of the cell concentration, as the cells are what produce the ethanol, the ethanol productivity of the cells, and the ethanol production to cell growth ratio, as well as the bleed-to-feed ratio and the dilution rate. The bleed-to-feed ratio is assumed to be 1 for the purpose of this situation and, again, as this is assumed to be a batch reaction, there is no dilution rate to consider. As such, the theoretical yield is seen in Equation 3.

$$vXY_{X/P} = \frac{dP1}{dt} \qquad [3]$$

In Equation 3, P1 represents the ethanol concentration in grams per liter, v is the ethanol productivity, in grams of ethanol per grams of cells per hour, X is the concentration of cells in grams per liter, and $Y_{X/P}$ is the ratio of ethanol production to cell growth with units of change in grams of cells per change in grams of ethanol. The ethanol productivity is calculated with Equation 4.

$$v = v_{max}\left[\frac{S}{K_S + S}\right][1 - \frac{P1}{P1_{max}}]^n \quad [4]$$

The maximum ethanol productivity is represented by v_{max} which has a value of 1.15 grams of ethanol per grams of cells per hour. S represents the concentration of glucose in the reactor, in grams per liter, and is calculated with Equation 5. K_S is 0.315 grams of glucose per liter and represents the concentration of glucose at which the ethanol productivity is half of the maximum productivity. P1 represents the concentration of ethanol in the reactor in grams per liter which is calculated with Equation 3 and $P1_{max}$ is the maximum concentration the of ethanol for the reactor, which has a value of 87.5 grams per liter. The sensitivity coefficient is represented by n, a unitless factor with a value of 0.36. The cell concentration in Equation 3 is calculated with Equation 6.

$$\frac{dS}{dt} = -\frac{1}{Y_{X/S}}\frac{dX}{dt} \quad [5]$$

In Equation 5, $Y_{X/S}$ is the ratio of cell mass change to glucose consumption and has a value of 0.07 change in grams of cells per change in grams of glucose.

$$\frac{dX}{dt} = Ev \cdot X \quad [6]$$

In Equation 6, E represents the efficiency of cell mass production, which has a value of 0.249 grams of cells per grams of ethanol. Again, the ethanol production, v, is calculated with Equation 4. From Equation 3, $Y_{X/P}$ can be calculated by dividing $Y_{X/S}$ by $Y_{P/S}$, which has a value of 0.434 change in grams of ethanol per change in grams of glucose, such that $Y_{X/P}$ has units of change in grams of cells per change in grams of ethanol.

Model Results

From Figure 1, the maximum ethanol concentration is about 2 grams per liter, the maximum cell concentration is 11.5 grams per liter, and about 2 grams per liter of carbon dioxide was generated. The cells took about 8.5 hours to consume the initial glucose. The code used to produce Figure 1 can be seen in Figure 4.

Sensitivity Analysis

Ethanol Sensitivity Factor

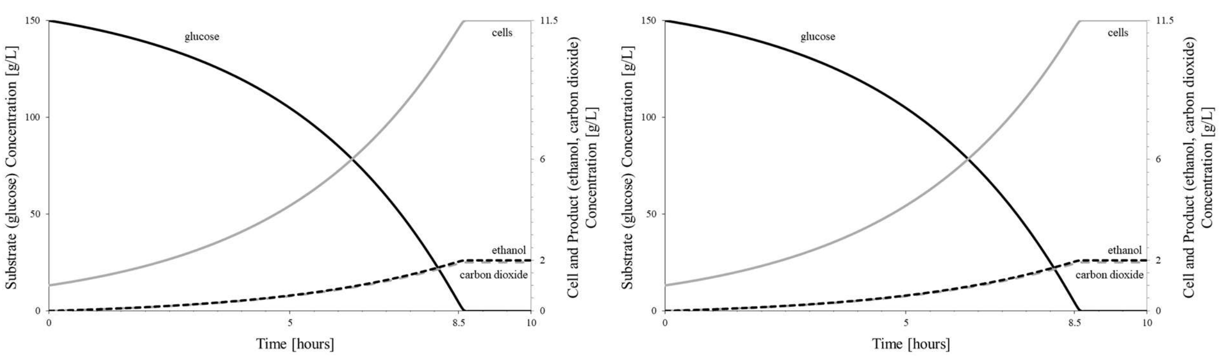

Figure 2: Cell, Ethanol, Carbon Dioxide, and Glucose Concentration [g/L] vs. Time [hours] when (left) n is double the original value (0.72) and (right) half the original value (0.18).

As shown in Figure 2, a change in the sensitivity to ethanol, n, has no effect on the time to utilize the glucose, the final ethanol or cell concentration. The results are not different because when the differential equations are solved, the v equations cancel each other out in the equation for the product concentrations.

Maximum Specific Ethanol Production Rate

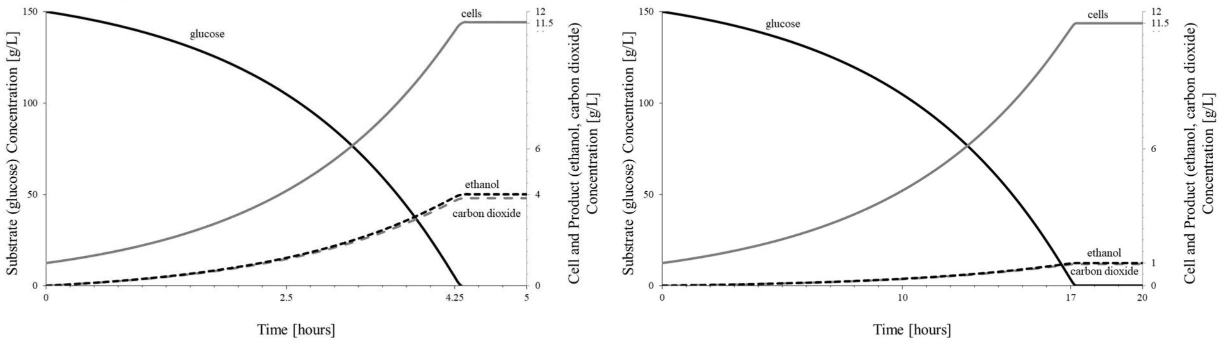

Figure 3: Cell, Ethanol, Carbon Dioxide, and Glucose Concentration [g/L] vs. Time [hours] when (left) v_m is double the original value (2.30) and (right) half the original value (0.575).

Figure 3 shows that when v_m is doubled, the time to consume all of the glucose is halved and the final ethanol and carbon dioxide concentrations are doubled, and when v_m is halved, the time to consume all of the glucose is doubled and the final ethanol and carbon dioxide concentrations are halved.

Cell Yield

Figure 3 shows that v_m does not affect the final cell yield if it is increased or decreased.

```
Sub constants()
    'Enter the values for the step size and the number of equations here.
    stepSize = 0.05
    numEq = 4

    '*******************************************
    ReDim I(numEq), O(numEq)        ' Just leave this line alone.  It dimensions the
                                    ' input and output arrays
    '*******************************************

    ' Enter the initial conditions
    startTime = 0                 'Time value at which the intial conditions are known
    O(1) = 1                      'O(1) = X = cell concentration [g/L]
    O(2) = 150                    'O(2) = S = substrate concentration [g/L]
    O(3) = 0                      'O(3) = P1 = ethanol concentration [g/L]
    O(4) = 0                      'O(4) = P2 = carbon dioxide concentration [g/L]

    'Enter the time at which you would like the simulation to end
    stopTime = 24

End Sub

Function inputs(eqnNumber As Integer, timeValue As Variant, outputs() As Variant)
    '*******************************************
    Dim j As Integer                  'Just leave this code alone.
                                      '
    For j = 1 To numEq                '
        O(j) = outputs(j)             '
    Next j                            '

    t = timeValue                     't is the time
    '*******************************************

    'Enter the constants here
    Pi = 3.14
    Ks = 0.315                        '[g / L]
    Pmax = 87.5                       '[g / L]
    vm = 1.15                         '[g ethanol / g cells / hour]
    E = 0.249                         '[g cells / g ethanol]
    Yxs = 0.07                        '[delta g cells / delta g glucose]
    Yps = 0.434                       '[delta g ethanol / delta g glucose]
    n = 0.36                          '[--]
    Yxp1 = Yxs / Yps                  '[delta g cells / delta g ethanol]
    Yxp2 = Yxs / Yps * 46 / 44        '[delta g cells / delta g carbon dioxide],
                                      '   fermentation produces 46 g of ethanol
                                      '   for every 2 44 g carbon dioxide

    'Constraints
    If O(1) <= 0 Then O(1) = 0
    If O(2) <= 0 Then O(2) = 0
    If O(3) <= 0 Then O(3) = 0
    If O(4) <= 0 Then O(4) = 0
    If O(2) >= 200 Then O(2) = 200  '[g / L] due to substrate inhibition


    'Enter the input equations here
    I(1) = E * vm * ((O(2) / (Ks + O(2))) * (1 - (O(3) / Pmax)) ^ n) * O(1)    'dX/dt
    I(2) = -1 / Yxs * I(1)          'dS/dt
    I(3) = vm * ((O(2) / (Ks + O(2))) * (1 - (O(3) / Pmax)) ^ n) * I(1) * Yxp1          'dP1/dt
    I(4) = vm * ((O(2) / (Ks + O(2))) * (1 - (O(3) / Pmax)) ^ n) * I(1) * Yxp2          'dP2/dt


    '*******************************************
    inputs = I(eqnNumber)

End Function
```

Figure 4: SIMBAS Code used to create Figure 1