ASM Sci. J., Special Issue 6, 2019 for SKSM26, 193-199

Mathematical Analysis for a System of Nonlinear Ordinary Differential Equations Related to Ethanol Production

Ahmad Izul Fakhruddin Azimi* and Norazaliza Mohd Jamil

Fakulti Sains &Teknologi Industri, Universiti Malaysia Pahang, Lebuhraya Tun Razak, 26300 Gambang, Kuantan, Pahang, Malaysia

The fermentation process is a crucial stage in transforming substrate to ethanol. Ethanol is obtained by fermenting the substrate using microbial such as yeasts or bacteria. This process can be explained in a system of nonlinear Ordinary Differential Equations (ODEs) mathematical model. The broad understanding of the model can improve the prediction of ethanol production yield. In this paper, the stability analysis is done to investigate the stability of the proposed model and followed by the investigation of its parameter behaviour towards the model.

Keywords: mathematical modelling; fermentation; ethanol

I. INTRODUCTION

The most known of ethanol production can be found nowadays are using fermentation and synthetic process. The origin resources of synthetic ethanol are from the by-product of petroleum meanwhile the natural resources for fermentation ethanol is by the substrate. Because of the limited resource and the environmental concerns, the production of ethanol using fermentation has increased in the market and has grabbed much attention among the researcher such as Khor and Lalchand (2014). The huge number of its natural resources also one of the factors that drew the attention to ethanol production by fermentation. Ethanol production using fermentation is very complex to understand and expensive to operate. One of the convenient ways to experiment the ethanol production is by using the mathematical model. The understanding of the model that describes the fermentation process will increase the production yield. As mention by Almquist *et al.* (2014), the study on the kinetic model will improve the ethanol yield by learning the behaviour of microbial and the substrate consumed in the fermentation process. In order to have a deep understanding of the microbial nature and subsequently optimise the production yield, a lot of consideration must be made such as includes all the parameters and significant factors into the model.

II. LITERATURE REVIEW

Many studies have been conducted to improve the process of ethanol production using fermentation. In addition, there are also studies by Fan *et al.* (2017) embed the Pervaporation technique to remove the ethanol during the fermentation process. This technique is invented because of the ethanol itself could inhibit the fermentation process. It is to believe that this technique could increase production, improve the utilization of the equipment and reduce water waste in the fermentation process. Despite the enhancement introduced in the fermentation process, there are yet many weaknesses in the system of fermentation ethanol that are difficult to be solved as the whole system. Scully & Orlygsson (2015) reviewed the thermophilic bacteria used in ethanol production. This type of microbial has an advantage among others because of its ability to produce ethanol from a range of substrates. There are many studies and methods have been conducted to understand

*Corresponding author's e-mail: ahmadizul.azimi@gmail.com

the process of ethanol production using fermentation. One of that method is studying the mathematical modelling that can describe the process. Moreover, a lot of studies need to be considered to clarify the actual situation in the fermentation process and to interpret it into the mathematical model of the system. Phisalaphong *et al.* (2006) have introduced a mathematical model that includes the inhibition effect into their model. This model considers not only the inhibition effect of the substrate and the product in microbial growth but also in product formation. In order to understand the inhibition effect in the mathematical model, the model present by Phisalaphong *et al.* (2006) is investigated using mathematical analysis in the next section.

III. MATHEMATICAL MODEL

The model is based on three state variables, namely microbial, product (ethanol in our case) and substrate. The differential equations describing the conservation of state variables are listed in equations (1) to (3).

The variables and parameters used in this mathematical model are as follows:

$X(t)$	is the concentration of microbial
$P(t)$	is the concentration of ethanol
$S(t)$	is the concentration of substrate
$\mu_{\max}$	is the maximum specific rate for microbial growth
$v_{\max}$	is the maximum specific rate for ethanol production
K_{SX}	is the substrate half-saturation coefficient for microbial growth
K_{SP}	is the substrate half-saturation coefficient for ethanol production
K_{IX}	is the inhibition effect on high concentrations of substrate in microbial growth
K_{IP}	is the inhibition effect on high concentrations of substrate in ethanol production
$P_{X,\max}$	is the inhibition effect on high concentrations of product in microbial growth
$P_{P,\max}$	is the inhibition effect on high concentrations of product in ethanol production
K_d	is the microbial death rate
m	is the maintenance of the microbial

Mathematical Model 1:

$$\frac{dX(t)}{dt}=\left(\mu_{\max}\frac{S(t)}{K_{SX}+S(t)+S(t)^2/K_{IX}}\right)\left(1-\frac{P(t)}{P_{X,\max}}\right)X(t)-K_dX(t) \quad (1)$$

$$\frac{dP(t)}{dt}=\left(v_{\max}\frac{S(t)}{K_{SP}+S(t)+S(t)^2/K_{IP}}\right)\left(1-\frac{P(t)}{P_{P,\max}}\right)X(t) \quad (2)$$

$$\frac{dS(t)}{dt}=-\frac{dX(t)}{dt}-\frac{dP(t)}{dt}-mX(t) \quad (3)$$

A. Non-Dimensional Model

In this section, we describe how to modify the mathematical Model 1 into a non-dimensional model. Using the following transformations,

$$X=x(K_{IX}),\ P=p\left(\frac{v_{\max}K_{IP}}{K_d}\right),\ S=s(K_{IX}),\ t=\tau\left(\frac{1}{K_d}\right)$$

the previous Model 1 can be written in a non-dimensional form as follows.

Mathematical Model 2:

$$\frac{dx}{d\tau}=(1-\lambda p)\sigma\frac{sx}{\alpha+s+s^2}-x \quad (4)$$

$$\frac{dp}{d\tau}=(1-\kappa p)\frac{sx}{\gamma+\beta s+s^2} \quad (5)$$

$$\begin{aligned}\frac{ds}{d\tau}&=(\lambda p-1)\sigma\frac{sx}{\alpha+s+s^2}\\&+(\kappa p-1)\phi\frac{sx}{\gamma+\beta s+s^2}+(1-\rho)x\end{aligned} \quad (6)$$

where

$$\sigma=\frac{\mu_{\max}}{K_d}\quad \alpha=\frac{K_{SX}}{K_{IX}}\quad \beta=\frac{K_{IP}}{K_{IX}}\quad \lambda=\frac{v_{\max}K_{IP}}{K_dP_{X,\max}}$$

$$\phi=\frac{v_{\max}K_{IP}}{K_dK_{IX}}\quad \rho=\frac{m}{K_d}\quad \gamma=\frac{K_{SP}K_{IP}}{K_{IX}{}^2}\quad \kappa=\frac{v_{\max}K_{IP}}{K_dP_{P,\max}}$$

Those constants are described as follow:

σ is the ratio of maximum specific microbial growth to its death rate

α is the ratio of substrate half-saturation coefficient for microbial growth to its inhibitory effect

β is the ratio of substrate inhibitory effect between ethanol production and microbial growth

λ is the ratio of maximum specific ethanol production and its substrate inhibitory effect to microbial death rate and its product inhibitory effect

ϕ is the ratio of maximum specific ethanol production and its substrate inhibitory effect to microbial death rate and its product inhibitory effect

ρ is the ratio of microbial maintenance coefficient to its death rate

γ is the ratio of substrate half-saturation coefficient for ethanol production and its substrate inhibitory effect towards the product inhibitory effect in microbial growth.

κ is the ratio of maximum specific ethanol production and its substrate inhibitory effect towards microbial death rate and the product inhibitory effect in ethanol production.

Model 2 is analysed in terms of the stability and the behaviour of its parameters toward the model. There are several parameters that can be investigated.

B. Stability Analysis

The stability of Model 2 is determined by the eigenvalues of the Jacobian matrix at an equilibrium solution $\left(x^*, p^*, s^*\right)$. By setting each equation of Model 2 to zero leads to the equilibrium solutions of the model. MATLAB has been used in finding the equilibrium point. The result shows that the model has 2 equilibrium point which is $(0,0,0)$ and $(0,1/\kappa,0)$ and the Jacobian for each point is calculated as follows:

at $(0,0,0)$

$$J(0,0,0)=\begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 0 \\ 1-\rho & 0 & 0 \end{pmatrix}$$

and at $(0,1/\kappa,0)$

$$J\left(0,\frac{1}{\kappa},0\right)=\begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 0 \\ 1-\rho & 0 & 0 \end{pmatrix}$$

The calculation $\det|J-\lambda I|=0$ is done once because of both points have the same value of the matrix J.

$$\det\begin{vmatrix} -1-\lambda & 0 & 0 \\ 0 & -\lambda & 0 \\ 1-\rho & 0 & -\lambda \end{vmatrix}=0$$

$$(-1-\lambda)\left(\lambda^2\right)=0$$

Then $\lambda=-1,\quad \lambda=0$

And the eigenvector

for $\lambda=-1$,

$$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 1-\rho & 0 & 1 \end{pmatrix}\begin{pmatrix} x \\ p \\ s \end{pmatrix}=\begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

$p=0 \quad , (1-\rho)x+s=0$

$p=0 \quad$, let $x=1$

$$e_1=\begin{pmatrix} 1 \\ 0 \\ \rho-1 \end{pmatrix}$$

for $\lambda=0$,

$$\begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 0 \\ 1-\rho & 0 & 0 \end{pmatrix}\begin{pmatrix} x \\ p \\ s \end{pmatrix}=\begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

$(1-\rho)x=0$

$x=0$

$$e_2 \ \& \ e_3=\begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}$$

As stated in Brandon J & Wiggins S. (1991), the eigenvalue zero real part is indicating this model have centre manifold at both equilibrium point. Meanwhile, the eigenvalue with the negative real part represents the decay manifold as shown in Figure 1. Hence this model is stable.

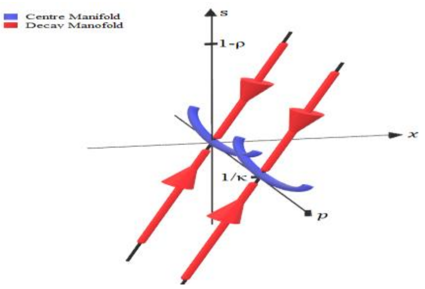


Figure 1. Phase Portrait of Model 2

C. Parameters Behaviour

Model 2 is a nonlinear system of the ODE which is complicated to solve analytically. Some assumption has to be made to ease the analysis and also to understand the behaviour of the parameters in the model. Equation 4 and Equation 5 can be solved by assuming

$z=\dfrac{s}{\alpha+s+s^2}$ and $m=\dfrac{sx}{\gamma+\beta s+s^2}$. Equation 4 is solved as follows:

$$\frac{dx}{d\tau}=\left[\sigma z(1-\lambda p)-1\right]x$$

$$\int\frac{1}{x}dx=\int\left[\sigma z(1-\lambda p)-1\right]d\tau$$

$$x(\tau)=x_o e^{\left[\sigma z(1-\lambda p)-1\right]\tau}$$

while for Equation 5:

$$\frac{dp}{d\tau}=(1-\kappa p)m$$

$$\int\frac{1}{(1-\kappa p)}dp=\int m\,d\tau$$

$$p(\tau)=\frac{1-(1-\kappa p_o)e^{-\kappa\tau m}}{\kappa} \quad (7)$$

then the solution for Equation 4 is:

$$x(\tau)=x_o e^{\left[\sigma z\left(1-\lambda\left\{\frac{1-(1-\kappa p_o)e^{-\kappa\tau m}}{\kappa}\right\}\right)-1\right]\tau} \quad (8)$$

The parameter x_o and p_o is the initial value for the concentration of microbial and the concentration of ethanol respectively.

The investigation of the parameters behaviour toward Model 2 is done by using Equation 7 and Equation 8. Figure 2 shows the investigation of parameter κ towards ethanol production. In this analysis, a graph of concentration of ethanol versus time is plotted with the different value of κ which is 10, 20, 30 and 40. This experiment shows that the parameter κ is the inhibiting effect of ethanol production. This is proven by the reduced amount of time for each ethanol concentration goes to zero when the value of κ increased.

The analysis of parameter m is conducted by setting the value of the parameter $\kappa=10$ and the initial concentration of ethanol, p_o is 10. As shown in Figure 3, this investigation is to experiment with the different value of the parameter m in ethanol production. The experiment value of m are 0.0001, 0.0002, 0.0003 and 0.0004. Based on the pattern shown in Figure 3, the parameter m also provides the inhibition in ethanol production as the increasing of its value resulting in the lower amount of time for each ethanol concentration goes to zero.

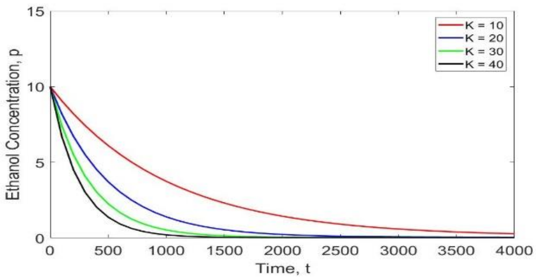


Figure 2. The change of ethanol production towards κ with $p_o=10$ and $m=0.0001$

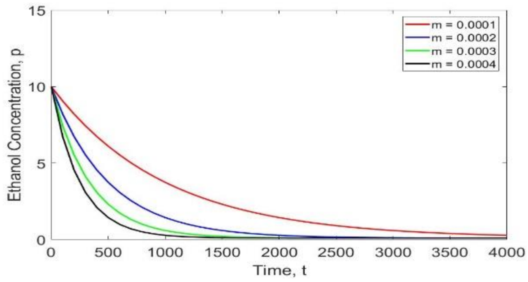
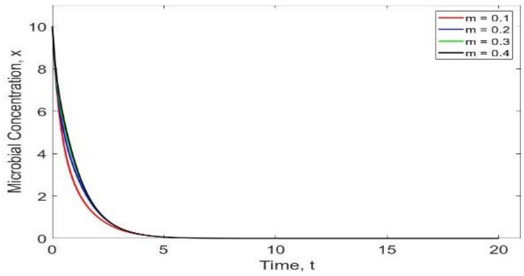
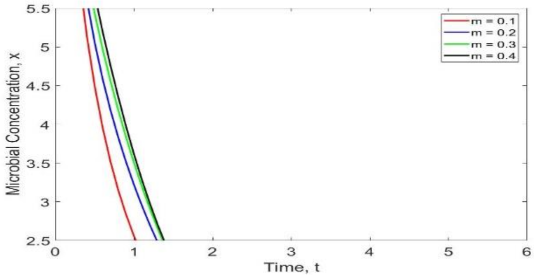


Figure 3. The change of ethanol production towards m with $p_o=10$ and $\kappa=10$

Equation 8 is related to microbial growth that will contribute to the production of ethanol in fermentation. This equation has five parameters (m, κ, λ, σ and z) and it is important to understand their role in microbial growth. The study is conducted as same as in ethanol production for the parameter m but the values are increased in order to observe the change of Equation 8. The analyse values of m are 0.1, 0.2, 0.3 and 0.4. Figure 4 illustrates the reduction of microbial concentration against time. The parameter m shows the contrary result in this equation compares with Equation 7. Figure 4(b) shows that the lowest value of m (the red line) is the first to reach the microbial concentration at 2.5 compare with others. It also indicates that the small value of m will inhibitsmicrobial growth.



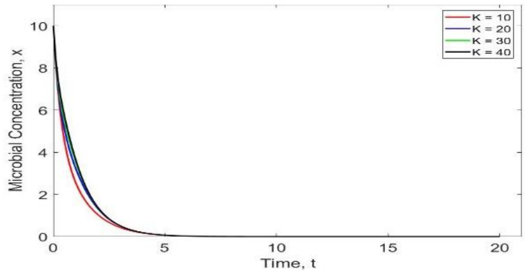
(a)



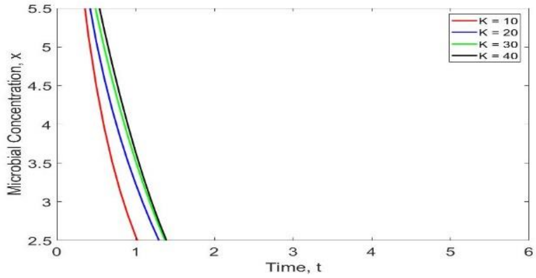
(b)

Figure 4. The effect of the parameter m to microbial growth with $x_o = 10$, $\lambda = 10$, $\kappa = 10$, $\sigma = 0.1$ and $z = 0.1$. (a) The overall system of microbial growth; (b) Time difference for the concentration of microbial, x = 2.5

The second parameter to analysed in Equation 8 is parameter κ. The parameter κ is analysed using the same value as in Equation 7. However, this parameter also produces the same form of result with the parameter m for Equation 8 and it contradicts with the result for Equation 7 as shown in Figure 5. The microbial concentration is reduced to 2.5 at the time, $\tau = 1$ when $\kappa = 10$ (the lowest among the other value) while the others need time greater than 1. This indicates that the smallest value of κ will increases the inhibition effect in microbial growth.



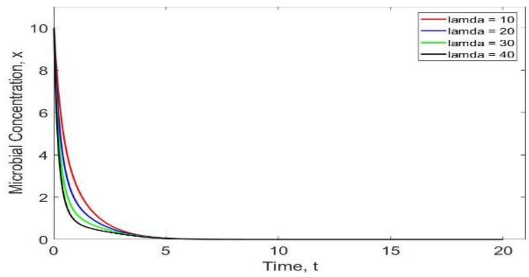
(a)



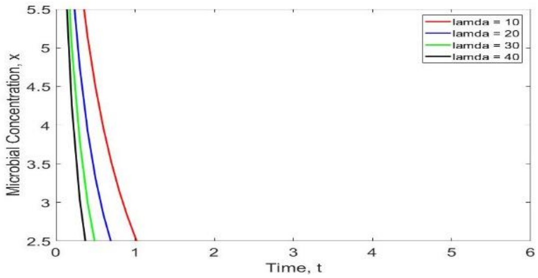
(b)

Figure 5. The effect of the parameter κ to microbial growth with $x_o = 10$, $\lambda = 10$, $m = 0.1$, $\sigma = 0.1$ and $z = 0.1$. (a) The overall system of microbial growth; (b) Time difference for the concentration of microbial, x = 2.5

The parameter λ has examined using the same concept as other parameters. The manipulative values of this parameter are 10, 20, 30 and 40 and the behaviour of it changes value is recorded in Figure 6. The figure shows that the microbial concentration is decreasing and the rate of decline increase with the increment of λ value. It implies that the inhibition effect of microbial is directly proportional to the increasing value of the parameter λ.



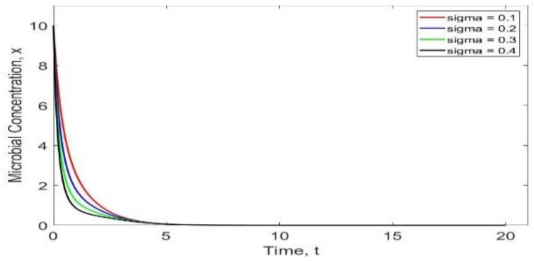
(a)



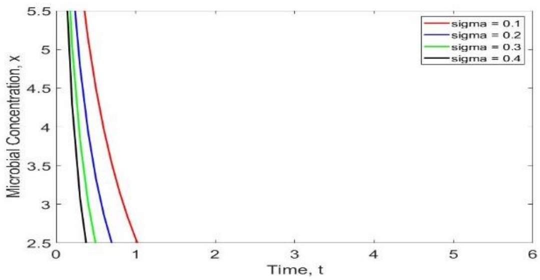
(b)

Figure 6. The effect of the parameter λ to microbial growth with $x_o = 10$, $\kappa = 10$, $m = 0.1$, $\sigma = 0.1$ and $z = 0.1$. (a) The overall system of microbial growth; (b) the Time difference for the concentration of microbial, x = 2.5

Figure 7 and Figure 8 represent the study of parameter σ and parameter z toward the microbial growth respectively. The experimented values of parameter σ and parameter z are 0.1, 0.2, 0.3 and 0.4. These two parameters give the same outcome when the study of their behaviour toward Equation 8 is conducted. Their increasing values has lessened the time for the microbial concentration reaches 2.5. It demonstrates that both parameters will increase the inhibition effect in microbial growth if their value increases.

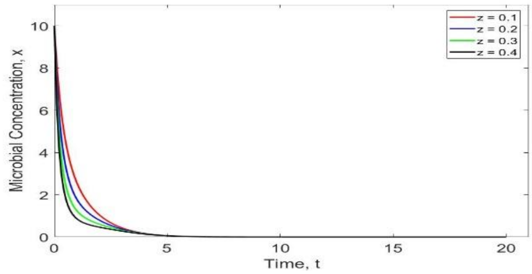


(a)

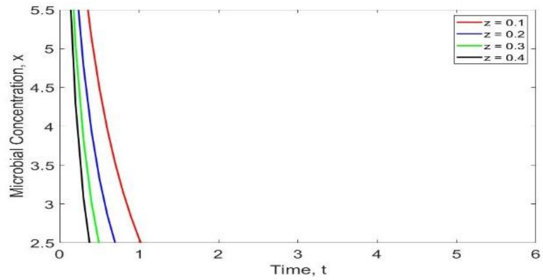


(b)

Figure 7. The effect of the parameter σ to microbial growth with $x_o = 10$, $\lambda = 10$, $m = 0.1$, $\kappa = 10$ and $z = 0.1$. (a) The overall system of microbial growth; (b) the Time difference for the concentration of microbial, x = 2.5



(a)



(b)

Figure 8. The effect of the parameter z to microbial growth with $x_o = 10$, $\lambda = 10$, $m = 0.1$, $\sigma = 0.1$ and $\kappa = 10$. (a) The overall system of microbial growth; (b) the Time difference for the concentration of microbial, x = 2.5

IV. CONCLUSIONS

The studied model presents a system of nonlinear ODEs for ethanol production using fermentation process. The broad understanding of this model could estimate the ethanol production yield precisely. The stability of Model 2 is studied in the first place and the result shows that this model is stable at two points which are at $(0,0,0)$ and $(0,1/\kappa,0)$. Five parameters such as κ, m, λ, σ and z behaviour are investigatedtoward the model. By definition, the parameter κ is defined as the ratio of inhibition effect in ethanol production to the death rate of microbial. The increasing value of the parameter κ will increase the microbial growth but reduce the ethanol production and it is consistent with the result shown in Figure 2 and Figure 5. The parameter m is evaluated in two different situations which is in small value and in ordinary value. The small value of m occurs when the great amount of substrate is used. This lead to increased substrate inhibition in ethanol production as shown in Figure 3. Meanwhile, the ordinary value of m is analysed when the substrate is not a significant factor in Figure 4. Hence the microbial growth is directly proportional to the parameter m. Figure 6 shows the increment of λ value will inhibit microbial growth. By definition, this happens because it will increase the maximum concentration of ethanol $v_{\max}$ and indirectly increase the inhibition effect to the microbial growth. The increase of parameter σ value that has a maximum concentration of microbial, $\mu_{\max}$ will increase the rate of intra relationship between the microbial and eventually cause the inhibition in microbial growth. The parameter z that related to inhibition effect in microbial growth has shown the increase in its value will accelerate the reduction of the concentration of microbial.

V. ACKNOWLEDGEMENT

The authors would like to thank RDU160116 for funding this research.

VI. REFERENCES

Almquist, J., Cvijovic, M., Hatzimanikatis, V., Nielsen, J & Jirstrand, M. (2014). Kinetic models in industrial biotechnology - Improving cell factory performance. Metabolic Engineering, 24, pp. 38–60.

Brandon, J. & Wiggins, S. (1991). Introduction to Applied Nonlinear Dynamical Systems and Chaos. The Mathematical Gazette.

Fan, S., Xiao, Z., Li, M. & Li, S. (2017). Ethanol Fermentation Coupled with Pervaporation by Energy Efficient Mechanical vapor Compression. Energy Procedia, 105, pp. 933–938.

Khor, C. S. & Lalchand, G. (2014). A review on sustainable power generation in Malaysia to 2030: Historical perspective, current assessment, and future strategies. Renewable and Sustainable Energy Reviews, 29, pp. 952–960.

Phisalaphong, M, Srirattana, N & Tanthapanichakoon, W. (2006). Mathematical modeling to investigate temperature effect on kinetic parameters of ethanol fermentation. Biochemical Engineering Journal, 28, pp.36–43.

Scully, S. M. & Orlygsson, J. (2015). Recent advances in second generation ethanol production by thermophilic bacteria. Energies, 8, pp. 1–30.