Applying Mathematical Analysis in Biosciences

M. HADJIGEORGIOU and V. GEKAS

School of Geotechnical Sciences and Environment, Department of Agriculture and Food Science,
Cyprus University of Technology (CUT), Limassol, 3600, CYPRUS

md.hadjigeorgiou@edu.cut.ac.cy
vassilis.gekas@cut.ac.cy

Abstract: Mathematical Modeling in the Biosciences (Food Engineering and Bioengineering) could be enhanced and at the same time facilitated by introducing the method of dimensionless analysis which is widely applied in other branches in Engineering for example in Fluid Dynamics and Chemical Engineering. In the present work dimensionless diagrams have been produced aiming at easily solving Time-Temperature relationship problems and Michaelis-Menten kinetics problems, as well as, bioreactor mass balances, in Biosciences. Also the dimensionless diagram concerning the Balling equation which predicts the alcohol content of the beer has been produced and is presented.

Key-words: Dimensionless numbers, dimensionless Michaels-Menten diagram, Temperature time relationship in blanching and sterilization, mass balances, bioreactor design, Balling equation

1 Introduction

The categories of mathematical modeling in Biosciences have been reviewed elsewhere [1]. A first distinction is between deterministic and non-deterministic modeling. The late models are a requirement especially for the Biosciences due to the degree of uncertainty in this field [2]. A second classification of models depends on the degree of empiricism which also is the case with many bio-applications. According to this criterion the models classify as

1. Rigorous mathematical models
2. Phenomenological models
3. Semi-empirical models
4. Empirical models

Concerning the uncertainty, the approaches include Monte Carlo procedures [2], Weibul modelling, Voronoi Tesselation and others. Recently a new idea of a Botzmann equation universal approach has is to be presented in another paper in the current WSEAS Conference. [3]

2 The Problem

The aim of this work is at helping the practical Food and Biological materials Scientist and Technologist to solve a family of problems than a particular problem each time. This can be obtained by dimensionless analysis, which is applied in nearby fields but not in the Biosciences, yet. This paper is based on the Diploma Thesis of Maria Hadjigeorgiou at the department of Agriculture and Food Science of the CUT University [4]

3 Tools and Methods

3.1. Principles of Dimensionless Analysis.

Dimensionless analysis is an output of the dimensional analysis which is applied to find the units of measurement of the various physical quantities. It is known that the interest of the Scientist about the dimensions of any physical quantity arises from the fact of the homogeneity of the equations of Physics and consequently of Engineering. This homogeneity implies that additive or equating terms in any fundamental equation have the same units. Then by dividing two of any of those terms with each other the resulting quantity is dimensionless. The dimensionless approach has been applied firstly by Chemical Engineers one century ago or so. The idea was given by the homogeneity of terms in the difficult to solve analytically Transport equation. An example is the Reynolds number. Another example in the frame of this work is the dimensionless time in the mass balance equation for the batch and also PFR reactor:

$t^* = t. Vmax/Km$

in the equation

$Vmax. t=X[So]-Km. \ln(1-X)$ {1}

where the units for example are:

[t]=min, [Vmax] = mM/min, and [Km]=mM

Applying dimensional analysis leads to a dimensionless t* [t*]=1

3.2 Mathematical tools

Sheets of the usual Excel, Windows®, tool have been used for the preparation of the produced diagrams.

.4 Applications of Dimensionless Analysis

4.1 Time-temperature diagram

In conservation unit operations such as pasteurization and sterilization a common problem is the relationship between the temperature of the process and the time required to pasteurize or sterilize the food product. A well known finding is that when temperature varies linearly the time required changes ligarithmically, or in other words when the time is linear the temperatures changes exponentially.
We further generalize the solution of this problem by defining the dimensionless time as

$$t^* = t/Fo,$$

where t the actual time and Fo the F value connected to a characteristic time, Z.
Then we define Θ* the dimensionless temperature,

$$\Theta^*= (\Theta-\Theta o)/Z$$

i.e. as the temperature Θ connected to the actual time t minus the initial temperature Θo (the characteristic temperature connected to the Fo value). divided by Z. Z is the heating temperature needed to increase the value D one order of magnitude whereas D is the heating time at a given temperature in order to reduce the microbial population by one log. [5]

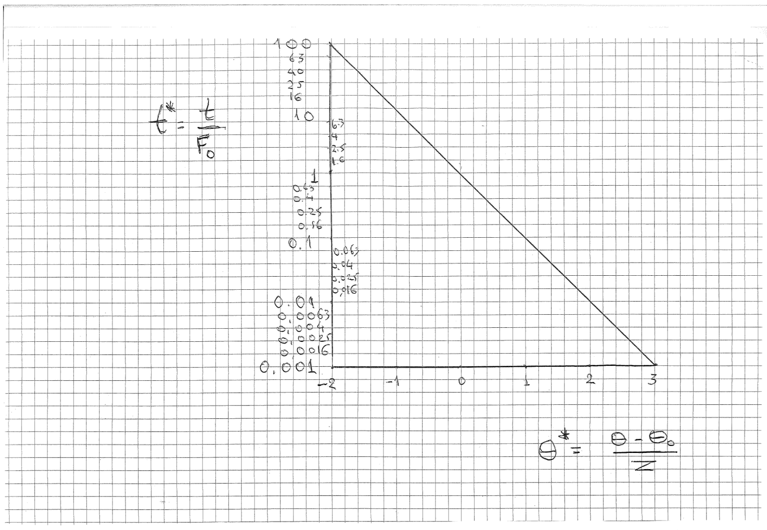


Figure 1 Dimensionless Time-Temperature diagram, t* is the dimensionless time and Θ* the dimensionless temperature, defined in the text

To be noted is that this procedure is applicable to any couple of microorganism/ food , of course the microorganisms of reference for each food are usually preferred. It is shown that the relationship lnt* vs Θ* is a linear one. This is depicted in Figure 1.

4.2 Michaelis-Menten

This equation as it is known is the following:

$\upsilon = Vmax S/ (Km+ S)$ {2}

In a linearized form the equation (the Lineweaver-Burk inversion) the equation becomes

$1/ \upsilon = 1/Vmax + Km/Vmax. 1/S$ {3}

. In this work we generalize as follows. We define the dimensionless reaction velocity

$\upsilon^* = \upsilon /Vmax$ and the dimensionless substrate concentration

$S^* = S/Km$,

then eq. {3} gives the linearized dimensionless form of the Michaelis Menten equation (Fig.2):

$1/ \upsilon^* = 1 + 1/S^*$ {4}

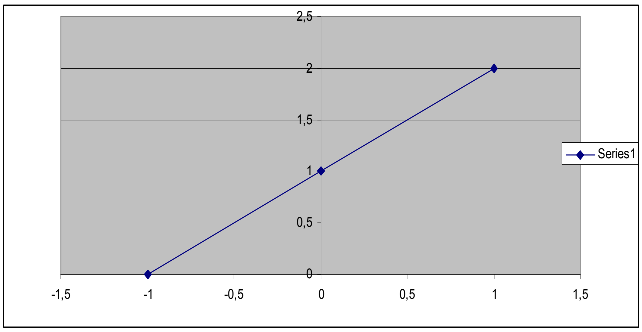


Figure 2 Linearized dimensionless Michaelis Menten diagram. In the axis of X is the invese of the dimensionless substrate concentration 1/S* and in the axis of Y is the dimensionless reaction rate 1/υ*

4.3 Balling diagram

The Balling equation gives the concentration of alcohol, Aw, in g/100g of produced beer, in terms of the Plato values , the initial, P, value of the wort and the final n value, that is the remaining carbohydrate concentration in the beer.

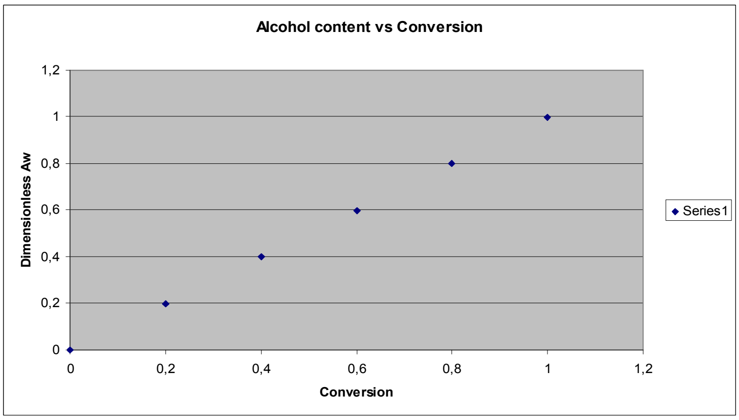


Figure 3 Dimensionless Balling diagram

The Balling equation has the following form

$$A_w = \frac{(P-n)}{(2.0665 - 1.0665P/100)}$$

where the symbols have the meaning given above.

Knowing that the Conversion, X, is by definition X= (P-n)/P and therefore dimensionless, we define the dimensionless alcohol concentration , as

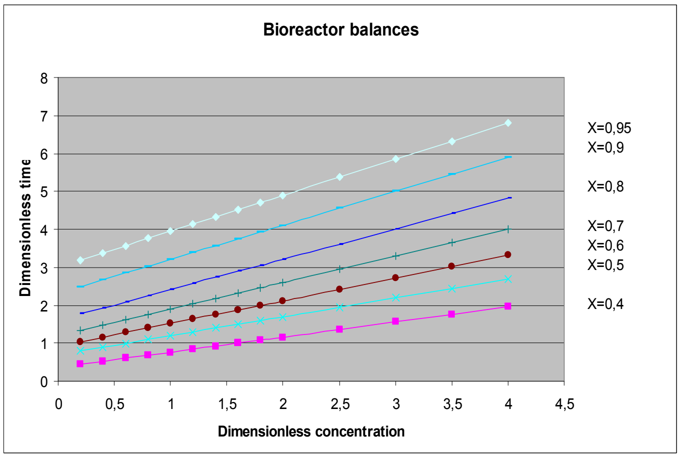
Aw* = Aw/Awo

where Awo is the concentration of alcohol at the value n=0, that is at conversion X=1. Then the dimensionless diagram shows a linear relationship.

4.4 Mass Balance in a Bioreactor

Both in the batch bioreactor and in the PFR reactor the same mass balance equation is valid {1}.

Vmax. t=X[So]-Km. ln(1-X) {1}



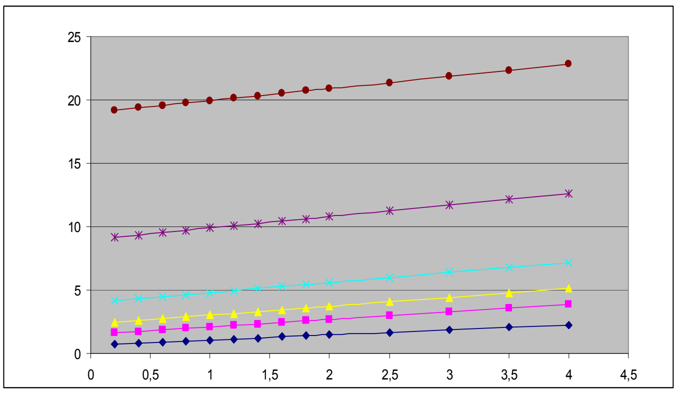


Figure 4 Dimensionless bioreactor mass balance diagram. Dimensionless time is plotted vs the dimensionless initial substrate concentration for various values of the conversion, X. Above the batch and PFR reactors and underneath the CSTR reactor.

ISBN: 978-960-474-261-5

By defining the dimensionless initial substrate concentration as

$So^* = So/Km$ and

the dimensionless time

$t^* = t. Vmax/Km$

the equation {1} becomes:

$t^* = X. So^* - \ln(1-X)$ {5}

whose graphical representation is given in Fig.4.

Straight lines are obtained for each value of X (varying between 0.4 and 0.95). The fact that the slope of each line is equal to X and the distance from the origo at the axis of dimensionless time, is –ln(1-X) for the batch and PFR reactor and X/(1-X) for the CSTR reactor (analysis in 4.5 paragraph) shows the way of the construction of those diagrams.

4.5 The case of the CSTR bioreactor

In the case of the Continuous Stirred Tank Reactor (CSTR) [6] the mass balance equation is

$Vmax.t_R = X.So+Km.X/(1-X)$ {6}

Here the residence time, t_R, is made dimensionless in a similar way as the time, t, in the batch reactor:

$t_R^* = t_R . Vmax/Km$

and the dimensionless initial substrate concentration is made dimensionless as in the case of the previous reactors.

$So^* = So/Km$

Then Eq.6 becomes

$t_R^* = X. So^* +X/(1-X)$

In Figure 4 the underneath diagram concerns the CSTR reactor.

5. Concluding remarks

The aim of this work being a part of the Diploma Thesis of Maria Hadjigeorgiou the aim was to give a helping hand to the practical Scientist or Technologist/Engineering of Biosciences to be able in a simple and easy way to solve grafically everyday problems by using useful dimensionless diagrams. In this paper we have applied Dimensional analysis in four cases and produced dimensionless diagrams in each case, concerning the following applications:

a. Time-Temperature Relationship in the thermal microorganism deactivation processes such as Pasteurization and Sterilization.

b. Michaelis Menten kinetics for applications in the enzymatic reaction

c. In the determination of beer content using the Balling equation diagram

d. In the mass balances of Bioreactors for solving problems of residence time and/or conversion calculations. In this case two diagrams were produced one for the batch and PFR (plug flow reractor) types of reactor and one for the CSTR (Continuous Stirred Tank Reactor).

Use of this kind of diagrams have been demonstrated in the class and were enthusiastically adipted.

6. Acknowledgements

The class (comrades of Maria) of Food Science sector of the Department of Agriculture and Food Science of the Cyprus University of Technology, Limassol, Cyprus, which entered the University in the year 2007 is acknowledged for fruitful discussion and their generous participation in the problem of the present Thesis.

References

[1] Vassilis Gekas, Transport Phenomena of Food and Biological Materials, CRC Press, Boca Raton, 1992

[2] Vassilis Gekas, Modeling with uncertainty, chapter in Advances in Osmotic Dehydration, CRC Press, Boca Raton, 1995

[3] Christina Mandakas, Vassilis Gekas, G. Maniatis and E.Reppas Of the (Boltzmann) method, to be presented in the WSEAS Vouliagmeni Conference, December 2010

[4] Maria Hadjigeorgiou, Diploma Thesis, 2010/11, Department of Agriculture and Food Science of the Cyprus University of Technology, Limassol, Cyprus

[5] F. Devllighere et al. “Predictive Microbiology” in Predictive Modeling and Risk Assessment, Springer Verlag, Eds Rui Costa and Kristberg Kristbergsson, 2008, Reykiavikk, Iceland

[6] T. Godfrey & S.West, Industrial Biotechnology, The Macmillan Press Ltd, Basingstoke, 1996