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RESEARCH ARTICLE

CASE STUDY: MODEL OF KINETIC STUDY OF OXACILLIN CONSECUTIVE REACTIONS FOR A CONTINUOUS FLOW REACTOR DIMENSIONING

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ABSTRACT

Reactors are equipment in which a chemical reaction takes place. For the chemical engineer, it is an operation of great importance since products that society needs are obtained by chemical transformations of raw materials. It is then fundamental to understand the mathematical models that describe the reacting systems. For a system of sequential reactions the speed law for each participating species is set, obtaining in this way separable differential equations and first order linear differential equations. Undesired reactions that accompany the main reaction can occur in a reactor, so it is relevant to consider all the lateral stages A characteristic example is the antibiotic hydrolysis which can be represented as a series of first order stages in which the desired product is the intermediary [A → I →P]. Hence, it is necessary that the reactors modelling provides the maximum yield through establishing and solving a differential equation per reaction component. This paper presents the conceptual and procedural learning to obtain the sizing for an intermediary product oxacillin reactor [flucloxacillin → oxacillin → meticillin], through establishing the differential equations in which the students apply their knowledge in differential and integral calculus, as well as geometrical interpretation of derivatives and integrals. These concepts are necessary to be applied in the interpretation of the point reactor.

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INTRODUCTION

From a chemical engineer perspective, chemical reactions are extremely important since many raw materials are transformed into products that are destined for society consumption. Reactions take place in industrial quantities in chemical reactors, which can be intermitent or continuous flow. In the first case, when reagents are placed in the reactor, reaction takes place. When the desired conversion occurs, the reactor is emptied with the products, and if necessary, these are separated and purified. On the contrary, continuous flow reactors are constantly fed, so products need to be emptied at the same rate in which reagents are introduced (Fogler, 2016). Inside the continuous flow reactor are two ideal models. The continuous stirred tank reactor, or CSTR, consists of a tank in which reagents are stirred by a propel so that composition is the same at any point of the reactor. The piston flow reactor, or PFR, is a big pipe which length is greater than diameter. In this model, the reaction si assumed to happen throughout the reactor, and not in an axial way in relation to the pipe´s diameter (Levenspiel, 2014). Mathematical modelling for flow reactor consists on balancing product materials and reagents to get a differential equation for each chemical entity.

In some cases, obtained differential equations are of separate variables, but in complex reactions first order linear differential equations are obtained. Even differential equation systems can prevail. During the synthesis processes sequenced reactions can happen, where reagent is transformed into an intermediary and this in turn, becomes a product according to the following model: $A \rightarrow I \rightarrow P$. An example of this are the consecutive reactions that antibiotics present: flucloxacillin hydrolizes into oxacillin, which is then turned into meticillin [$flucloxacillin \overset{k_1}{\rightarrow} oxacillin \overset{k_2}{\rightarrow} meticillin$]. In this particular case, the material balance for each component is necessary, resulting in three differential equations that have to be integrated to obtain the concentrations profile. By solving the equations, the reactor volumen can be obtained, providing the maximum conversión for the intermediary product of our interest, oxacillin. Therefore, the goal of this paper arises, which is to describe the use of math as a tool for sizing a reactor in which the antibiotic hydrolysis sequence occurs. The student then applies the learned tools to solve differential equations and applies these tools to solve industrial problems, such as designing chemical reactors through modelling reacting systems. As such, derivating and integrating, as well as the geometrical implications, are fundamental.

METHODOLOGY

Before modelling complex chemical reactions, the student starts from previous knowledge related to the chemical kynetics subject. By means of a simple chemical reaction, the rate of reaction can be represented as a definition of instant change in a reagent concentration or product in time:

$$aA \overset{k}{\rightarrow} bB$$

in which A is a reaction´s reagent and B is the product, while a and b are the stoichiometrical coefficients. The reaction´s rate can be expressed in eq. 1, wherer represents the rate of the reaction [mol/Ls], C_A and C_B the reagents and products concentration respectively [mol/L], t is time [s], a and b are the stoichiometrical coefficients.

$$r = -\frac{1}{a}\frac{dC_A}{dt} = \frac{1}{b}\frac{dC_B}{dt} \quad (1)$$

The rate equation for a simple reaction is not that complicated, since the model integration can be done in a separable variable differential equation. The problem arises them in a series of complex reactions (consecutive), in which the reagent in a reaction becomes an intermediary product which posteriorly turns into a final product. The problem presented to students is that of antibiotics series of reactions, in which the desired product is the intermediary one and not the final product of the reaction, as noted in the following case:

$$flucloxacillin \overset{k_1}{\rightarrow} oxacillin \overset{k_2}{\rightarrow} meticillin$$

Flucloxacillin (Fig.1a) is a potent antibiotic against Gram positive bacteria, responsable for hepatic and nephrotic damage. In contrast, oxacillin can attack the same bacteria without being as agressive as flucloxacillin (Fig. 1b)

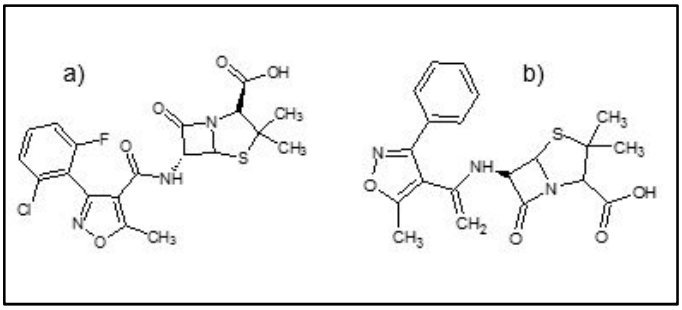

Figure1. Chemical structures for flucloxacillin (a) and oxacillin (b)

It is relevant to note that, in flucloxacillin reaction the hydrolysis does not stop in the desired product (oxacillin), but continues until metilcillin is formed (Fig.2). This antibiotic is not as potent as oxacillin, so even if it is the final product of the reactions´sequence, it is not the one we are looking for.

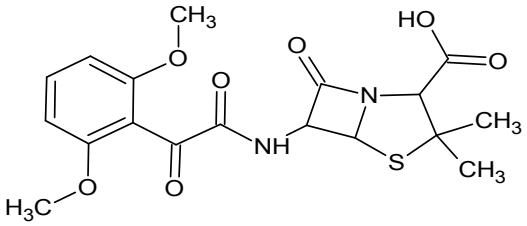

Figure 2. Meticillin chemical structure

This series of reaction can be represented as scheme 1

$$A \overset{k_1}{\rightarrow} I \overset{k_2}{\rightarrow} P \text{(Scheme 1)}$$

Being A fluclosacillin, I the intermediary product oxacillin and P, the final product meticillin. For a continuous flow reactor, the volumen is that to the design parameter we are interested in calculating (independent variable). By manipulating the volumen, the product concentration can be modified. The reactor´s volume is implicit in the residence time, which is defined as the time in which the reacting mixture travels through the reactor, and can be expressed by:

$$\tau = \frac{V}{Q_o} \quad (2)$$

τ is the residence time [min], V the reactor´s volume [L] and Q_o the feeding volumetric flow [L/min]. Then, the rate can be expressed as the change in the concentration in terms of the change in the residence time. Consecutive reactions for flucloxacillin hydrolysis can be expressed as:

$$A \overset{k_1}{\rightarrow} I \text{ (Scheme 2)}$$
$$I \overset{k_2}{\rightarrow} P \text{ (Scheme 3)}$$

As one can observe, reagent A is consumed to form I, and the intermediary product is a product, but it is as well a reagent for the second reaction. To get to the mathematical model that describes the concentration of each chemical entity in terms of the residency time, the rate needs to be calculated for each, as follows:

Rate for reagent A:

$$r = -\frac{dC_A}{d\tau} = k_A C_A \quad (3)$$

Note that 3 is a separable variable equation, so by integrating and evaluating the integrating constant with initial conditions τ=0, C_A=C_{Ao} the following equation arises:

$$C_A = C_{Ao} e^{-k_1 \tau} \quad (4)$$

With this, the concentration profile for reagent A can be constructed in terms of the residency time, once K_1 is known. Then, the rate equation for the intermediary can be calculated:

$$r = \frac{dC_B}{d\tau} = k_1 C_A - k_2 C_B \quad (5)$$

Substitutingeq.4 in eq. 5, eq. 6 is obtained:

$$\frac{dC_B}{d\tau} = k_1 C_{Ao} e^{-k_1 \tau} - k_2 C_B \quad (6)$$

Reordering terms, eq. 7 follows:

$$\frac{dC_B}{d\tau} + k_2 C_B = k_1 C_{Ao} e^{-k_1 \tau} \quad (7)$$

Obtaining a first order linear differential equation, Eq. 8.

$$\frac{dy}{dx} + p(x)y = g(x) \quad (8)$$

Given that the independent variable (y), is the residence time and the dependent variable (x) is C_B, the equation can be shaped into equation 9, in the following way:

$$\frac{dC_B}{d\tau} + p(\tau)C_B = g(\tau) \quad (9)$$

Being for equation 6, $7p(\tau) = k_2$ y $g(\tau) = k_1 C_{Ao} e^{-k_1\tau}$

When this mathematical model is reached, it can be solved in class by using two methods: integrating factor or parameter variation.

With the integrating factor method, (Carmona, 2011), Eq. 10 is obtained.

$$u(\tau) = e^{\int p(\tau)d\tau} = e^{\int k_2 d\tau} = e^{k_2\tau} \quad (10)$$

Therefore, C_B can be described as in equation 11, calculated as:

$$C_B = \frac{1}{u(\tau)} \int u(\tau) g(\tau) d\tau = \frac{1}{e^{k_2\tau}} \int e^{k_2\tau} k_1 C_{Ao} e^{-k_1\tau} d\tau \quad (11)$$

Solving the integral from Eq. 11, Eq. 12 follows:

$$C_B = \frac{k_1 C_{Ao}}{k_2 - k_1} [e^{-k_1\tau} + Ce^{-k_2\tau}] \quad (12)$$

With initial conditions τ=0, C_B=0the integration constant to obtain equation 13 can be calculated, achieving the mathematical model that describes B´s concentration variation in terms of the residency time.

$$C_B = \frac{k_1 C_{Ao}}{k_2 - k_1} [e^{-k_1\tau} - e^{-k_2\tau}] \quad (13)$$

Expressing the rate of the reaction for the product formation B P, Eq. 14 can be obtained.

$$r = \frac{dC_P}{d\tau} = k_2 C_B = k_2 \frac{k_1 C_{Ao}}{k_2 - k_1} [e^{-k_1\tau} - e^{-k_2\tau}] \quad (14)$$

This differential equation is considered as separable variables, so integrating and evaluating the constant in initial conditions τ=0, C_P=0, equation 15is reached.

$$C_P = \frac{C_{Ao}}{k_2 - k_1} [k_2(1 - e^{-k_1\tau}) - k_1(1 - e^{-k_2\tau})] \quad (15)$$

RESULTS AND ANALYSIS

Once obtained the integrated equations, the concentrations profile can be elaborated in terms of the residency time with the kinetic constants from the reactions sequence already known (Sinko and Singh, 2011).

$k_1 = 0.01277\ min^{-1}$ *y* $k_2 = 0.00638\ min^{-1}$

By substituting the constant values in equations 4, 7 13 and 15, with an initial concentration value C_{Ao}=0.001 M, the concentrations profile assigning values to the residency time can be graphed:

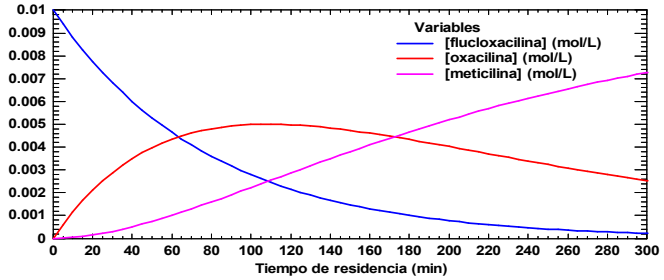

Figure 3. Concentration profiles in terms of flucoxacillin, oxacillin and meticillin time

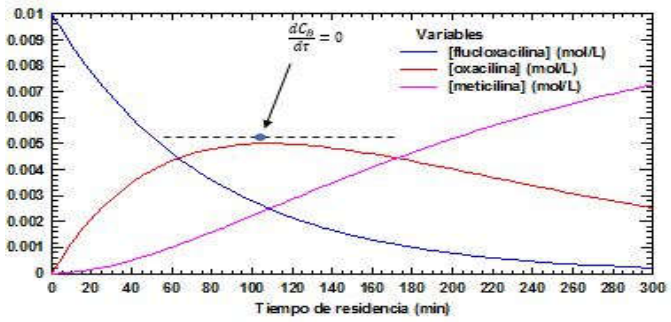

Figure 4. Derivate application to calculate optimal residency time

As can be observed in figure 3, the concentration profile described by the red curve corresponds to the oxacillin concentration. Given that the aim is to obtain as higher concentration as possible, it is essential to determine the residence time which provides the greater oxacillin conversion. This curve presents a maximum in which the derivate value is 0.

Thus, derivating equation 15 ,13, eq. 16 is obtained:

$$\frac{dC_B}{d\tau} = \frac{k_1 C_{Ao}}{k_2 - k_1} [-k_1 e^{-k_1\tau} + k_2 e^{-k_2\tau}] \quad (16)$$

By applying $\frac{dC_B}{d\tau} = 0$, the residency time is optimal since it refers to the value in which the maximum concentration for the intermediary (oxacillin) is found. As such, eq. 17 is obtained by clearing residency time.

$$\tau_{optimal} = \frac{1}{k_1 - k_2} ln \left[\frac{k_1}{k_2}\right] \quad (17)$$

Since kinetic constants are known, the residency time and optimal conversion can be calculated. In this case, it is equivalent to 107.7 min.

$$\tau_{optimal} = \frac{1}{0.01277\ min^{-1} - 0.00638\ min^{-1}} Ln \left[\frac{0.01277\ min^{-1}}{0.00638\ min^{-1}}\right] = 107.7\ min$$

By knowing the optimal residency time (Froment, Bischoff and Wilde, 2010), it is possible to know the optimal conversion. From equation 8, Eq. 18 can be obtained finding an optimal conversion of 0.745.

$$X_A = \frac{C_{Ao} - C_A}{C_{Ao}} \quad (18)$$

Substituting eq. 4 in 18:

$$X_A = 1 - e^{-k_1\tau} \quad (19)$$

Substituting the optimal residency time (eq. 17) in eq. 19, optimal conversion can be calculated:

$$X_{A\,op} = 1 - \left(\frac{k_1}{k_2}\right)^{\frac{k_1}{k_2 - k_1}} \quad (20)$$

Substituting K_1 and K_2 values:

$$X_{A\,op} = 1 - \left[\frac{0.01277\ min^{-1}}{0.00638\ min^{-1}}\right]^{\frac{0.01277\ min^{-1}}{0.01277\ min^{-1} - 0.00638\ min^{-1}}} = 0.745$$

Finally, the volumen of the reactor can be calculated, which is one of the objectives. Since the optimal residence time is

known, the reactor´s optimal volumen can be calculated through equation 2, assuming a 1L per minute flow.

$$V = \tau Q_o = (107.7\ min)\left(1\frac{L}{min}\right) = 107.7\ L$$

Conclusion

Using Maths as a tool in chemical kinetics for chemical engineers is fundamental, since reacting systems can be described by using differential equations, as well as sizing a chemical reactor. As in the flucloxacillin example, a complex reaction is exposed that through establishing differential equations correspond to separable and linear variable models. When they are solved, it is possible to know the optimal time for an intermediary, the optimal conversion and the reactor´s volume. The learning and teaching process applied to chemical kinetics and catalysis by using Maths in a reacting system.

REFERENCES

Carmona, J. I. 2011. *Ecuaciones diferenciales***,** 5 ed. Pearson, México

Fogler, S. 2016. *Elements of Chemical Reaction Engineering*. Prentice Hall, 5 Ed. USA

Froment, G.; Bischoff, K.; De Wilde, J. 2010. *Chemical Reactor Analysis and Design.*Wiley, 3 Ed. USA

Levenspiel, O. 2014. *Chemical Reaction Engineering*, Wiley, 3 Ed. USA.

Sinko, P.J. & Singh, Y. Eds, 2011. *Martin´s physical pharmacy and pharmaceutical Science:* Physical Chemical and Biopharmaceutical Principles in the Pharmaceutical Science. 6a Ed. Wolters Kluwer Lippincott Williams & Wilkins: New York.

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