

## An Approach to the Application of a Modified Fick's Diffusion Model: Development of an Algorithm

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### ABSTRACT

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*Fick, diffusion, model, extraction*

In the present work, we studied the mathematical characteristics of a modified Fick's diffusion model which is widely used for modelling the extraction kinetics of various compounds because it allows to describe the mass transfer in terms of two parameters: washing fraction ( $M_0/M_\infty$ ) and diffusion coefficients ( $D_{eff}$ ). This model also involves an infinite series of terms, obtaining an adequate simplification criterion of the model for each system under study. A calculation algorithm was developed to determine the number of terms of the series that is sufficient. Based on the developed criterion, the data obtained by various authors for different systems were analyzed, finding in general that the number of terms of the series was underestimated, which affected both the parameter values and the analysis of the phenomena involved. The main impact was detected on the parameter associated with the washing phenomenon, observing in general an underestimation of that parameter, whereas a smaller overestimation could be seen for the diffusion coefficient. Our study shows the importance of adopting an adequate simplification criterion when using a diffusion model to avoid errors in the interpretation of the mass transfer phenomena involved.

## 1. INTRODUCTION

The process of solvent extraction of compounds is affected by many physical and chemical variables, difficult to evaluate quantitatively and qualitatively. For example, for the extraction of oilseeds, different models have been proposed to analyze the kinetics of extraction, and Appendix presents the different models used by different authors [1-5].

In this context, one of the models most commonly used for modelling the extraction kinetics of oil and various compounds is the modified diffusion model of Fick's law developed by Perez et al. [5] based on the solution to Fick's equation described by Crank [6]. This modified model considers two main mechanisms: a washing process of the surface of the particles, and a non-stationary diffusion process, suspended in a medium maintained at constant concentration.

The importance of using this model for fitting experimental data lies not only in obtaining high correlation coefficients [7], but also in estimating parameters. The washing fraction ( $M_0/M_\infty$ ), related to the extraction of compounds in an early stages and, which gives a starting point to adjusted model; and diffusion coefficients ( $D_{eff}$ ), related to diffusion phenomena and velocity of convergence to asymptote of the model. These parameters allow to characterize the mass transfer, and thus to analyze and interpret the phenomena involved. In this context, given the nature of the solution to Fick's law (infinite series of terms) and the existence of boundary conditions, it is necessary to determine the criteria for the simplification and boundary conditions for a correct application of the model.

This model has been used in the analysis of the extraction kinetics of oil from different matrices [5, 8-23] and of bioactive compounds from biological matrices [24-25]. Several authors [5, 8-9, 11, 17-19, 22-23] applied the mentioned model for study the kinetics of solvent extraction (hexane and ethanol) of vegetables oils, in a stirred batch device at constant temperature. Also, the model has been used in study of inorganic compounds such as lime [26]. In those works, different simplifications were presented for applying the model and defining the boundary conditions, obtaining the characteristic parameters.

The aim of this work was to study the mathematical characteristics of the modified Fick's diffusion model [5] to develop an adequate simplification criterion for every system under study, and to analyze the results obtained by various authors.

## 2. MATERIALS AND METHODS

### 2.1 Modified Fick's diffusion model

The solution of Fick's law for spherical particles in non-stationary state described by Crank [6] is given by Equation 1:

$$\frac{M_t}{M_\infty} = 1 - \sum_{i=1}^{\infty} \frac{6}{i^2 \pi^2} e^{-i^2 Bt} \quad (1)$$

with  $t$  being the diffusion time in seconds;  $M_t$ , mass of the oil that diffuses at time  $t$ ;  $M_\infty$ , mass of the oil that diffuses at infinite time; and  $B$ , the coefficient of the model.

When the ground sample is heated to the required temperature, the oil moves to the outer surface of the particle, becoming more accessible to the solvent. Then when it is mixed with the oil-free solvent, a series of phenomena take place, such as the washing of the surface oil, the saturation of the solvent, which produces a modification of the structure, and the displacement of the miscella by non-diffusive mechanisms.

These phenomena occur during much shorter periods of time than the molecular diffusion mechanisms [5]. Thus it is considered that they take place instantaneously, removing an oil fraction during the initial period. The boundary conditions established by Pérez et al. [5] are presented in Equations 2-5:

$$t = 0 \quad M = 0 \quad (2)$$

$$t = t_0 \quad M = M_0 \quad (3)$$

$$t = t \quad M = M_t \quad (4)$$

$$t \rightarrow \infty \quad M = M_\infty \quad (5)$$

Under these conditions, the modified diffusion model that considers this initial period is given by Equation 6:

$$\frac{M_t - M_0}{M_\infty - M_0} = 1 - \sum_{i=1}^{\infty} \frac{6}{i^2 \pi^2} e^{-i^2 B(t-t_0)} \quad (6)$$

Rewriting Equation 6, we obtain Equation 7:

$$\frac{M_t}{M_\infty} = 1 - \left(1 - \frac{M_0}{M_\infty}\right) \sum_{i=1}^{\infty} \frac{6}{i^2 \pi^2} e^{-i^2 B(t-t_0)} \quad (7)$$

where,  $B$  is described according to Equation 8:

$$B = \frac{D_{\text{eff}} \pi^2}{R_m^2} \quad (8)$$

with  $D_{\text{eff}}$  being the effective diffusivity ( $\text{m}^2\text{s}^{-1}$ ), and  $R_m$ , the mean particle radius.

## 2.2 Simplified model

For extraction times that are sufficiently long, Pérez et al. [5] considered as a valid simplification taking into account only the first term of the series, and so the simplified model can be expressed as:

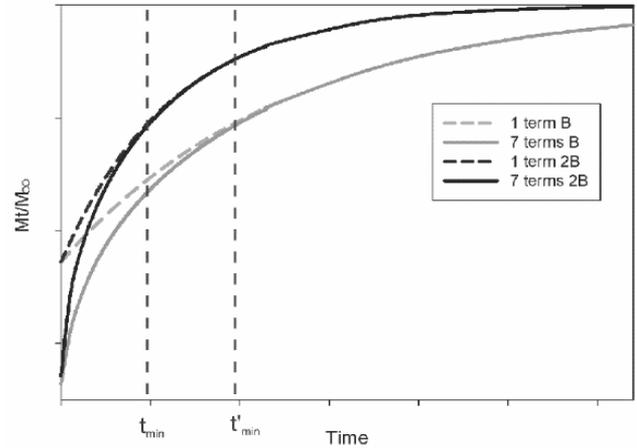
$$\frac{M_t}{M_\infty} = 1 - A e^{(-Bt)} \quad (9)$$

where,

$$A = \left(1 - \frac{M_0}{M_\infty}\right) \frac{6}{\pi^2} e^{Bt_0} \quad (10)$$

This simplification has been used by a number of authors [5, 8-12, 16, 20-21, 24-25]; however, a detailed analysis of the mathematical series shows that the assumed validity of this

simplification (considering sufficiently long times) varies according to parameter  $B$ , as shown in Figure 1.



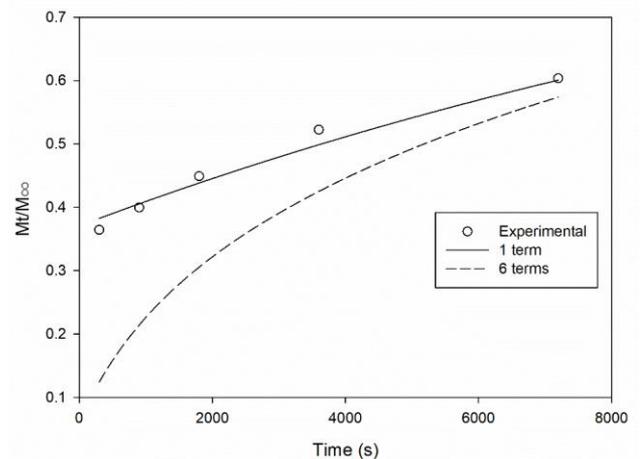
Note: Dotted lines indicate the time from which the simplification is valid for each case;  $t_{\min}$  and  $t'_{\min}$ , time from which the simplification is valid.

**Figure 1.** Exponential series for different parameter  $B$  values

It can be observed that for increasing  $B$  values, the minimum time ( $t_{\min}$ ) that can be considered long enough decreases, and thus the validity of the assumed simplification depends on the system under study.

In addition, given the boundary condition of the parameter  $M_0/M_\infty$ , the value of that parameter affects the magnitude of the difference observed between simplified models.

Since the solution to Fick's equation obtained by Crank [6] involves an infinite series of terms, any model with a finite number of terms will be a simplification. If the simplification is correct, when applying a model with a larger number of terms, the obtained curves should overlap. The simplified model (equation 9) can be applied to the experimental data, obtaining high correlation coefficients; however if the simplification is not valid, an error will be observed for the obtained parameter values in the verification with a model with a larger number of terms, as exhibited in Figure 2.



Notes: Fits with models with 1 and 6 terms of the series, for  $t_0=0$ .  $A = 0.6294$ ;  $B = 6.32 \times 10^{-5}$  obtained using SigmaPlot software 12.2.0.45 [27].

**Figure 2.** Experimental data obtained by Sánchez et al. [19] at 298K

The parameter values obtained with the model with 1-term series do not match the optimum values expressed by Crank's solution [6] for this system. It is worth noting that the greatest

difference between the curves is observed for the shorter times; therefore, with a term selection criterion that decreases the difference for the shorter experimental times, a smaller error would be yielded at longer times.

The error in the parameter values propagates to the estimation of the diffusion coefficients ( $D_{\text{eff}}$ ) and the washing fractions ( $M_0/M_\infty$ ), and thus it can lead to an erroneous interpretation of the phenomena.

### 2.3 Calculation algorithm for determination of the number of terms of the series needed

On the basis of this analysis, it is necessary to evaluate the nature of the experimental data represented by their optimum fitting parameters in order to determine the number of terms that are necessary.

A calculation algorithm was developed defining

$$\frac{M_t}{M_\infty} = 1 - \sum_{i=1}^n R_i \quad (11)$$

where, 
$$R_i = \left(1 - \frac{M_0}{M_\infty}\right) \frac{6}{i^2 \pi^2} e^{-i^2 B t} \quad (12)$$

And taking as acceptable error the equivalent to the minimum error observed by the authors for the experimental yields (0.001) of different systems [8, 11, 19, 22-23].

The scheme of calculation algorithm is shown in Figure 3 and the steps are described as follow:

Step 0. To start the calculation, it is necessary to define the washing time ( $t_0$ ) and the lowest extraction time observed experimentally ( $t_i$ ).

Step 1. Adjustment of the experimental data with appropriate software by applying Fick's modified diffusion model with a quantity of  $k$  terms obtaining the values of the parameters  $M_0/M_\infty$  and  $B$ .

Step 2. Analysis of the value of  $R_i$  for an initial value 1 and compare it with the established error (0.001)

Step 3. If  $R_i$  is greater than the established error, repeat step 2 with a value of  $i$  greater than the previous one. Then repeat until  $R_i$  is lower than or equal to the established error.

Step 4. When the value of  $R_i$  reaches a value less than or equal to the established error, the value of  $i$  will correspond to the new number of terms of the model ( $n$ ). Compare the value of  $n$  with the amount of terminus used in the initial fitting ( $k$ ).

Step 5. If  $n$  is not equal to  $k$ , repeat Steps 1, 2, 3 and 4 with  $k = n$ .

Step 6. When  $n$  is equal to  $k$ , select the model and the parameters obtained by fitting the model with the  $k$  terminus.

### 2.4 Determination of the number of terms of the series for different systems

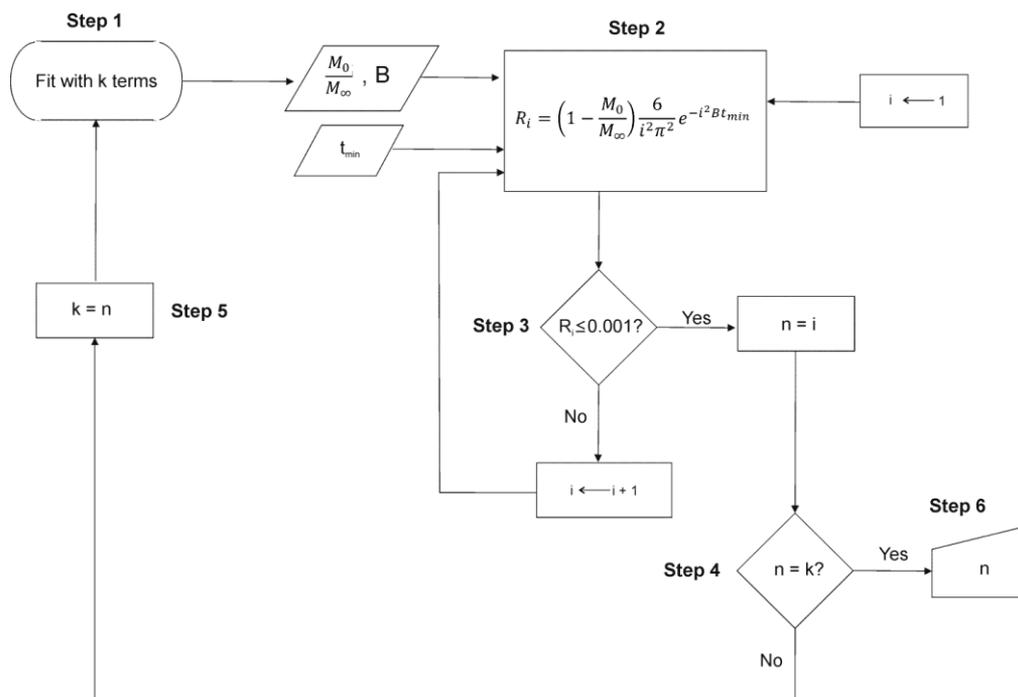
A calculation algorithm was programmed with the Dev-C++ 5.5.3 software [28] that allows to determine the number of terms needed for fitting each particular case.

The models applied by different authors were analyzed: Inanc et al. [26], Sun et al. [24], Najdanovic-Visak et al. [20], Sánchez et al. [19], Colivet et al. [16], Zárata et al. [11], Bäumlér et al. [9], Amarante et al. [10], Fernández et al. [8] and Pérez et al. [5].

For the fit carried out with the experimental data obtained by Sánchez et al. [19], the SigmaPlot 12.2.0.45 software [27] was used, and in order to compare the error made by using a smaller number of terms than needed, the percentage relative error (RE%) of the predicted yield for the shortest experimental time ( $t_i$ ) was calculated:

$$RE\% = \left| \frac{Y_1 - Y}{Y_1} \right| \times 100 \quad (13)$$

where,  $Y_1$  is the yield predicted by the model with 1-term series for the shortest experimental time ( $t_i$ ), and  $Y$  is the yield predicted by the model with the necessary number of terms calculated for the shortest experimental time ( $t_i$ ).



Note:  $k$ , number of terms entered for the data fitting;  $M_0/M_\infty$ , model parameter obtained from the fitting;  $B$ , model parameter obtained from the fitting;  $t_{\text{min}}$ , lowest experimental extraction time;  $i$ , counter;  $n$ , number of necessary terms for the fitting.

Figure 3. Calculation algorithm for the number of terms of the series

### 3. RESULT AND DISCUSSION

#### 3.1 Analysis of the model used by Sánchez et al. [19]

For the experimental data obtained by Sánchez et al. [19], considering a washing time equal to 0 ( $t_0=0$ ), the fit was performed with the 1-term model. Based on the obtained parameters, we applied the calculation algorithm, obtaining the number of necessary terms for the first iteration and the relative errors made with the 1-term model for the prediction of the first analyzed extraction time ( $t_i$ ). The results are shown in Table 1.

It can be observed that, for the analyzed systems, up to 9 terms of the series are needed to correctly fit the modified Fick's diffusion model to the data, registering relative errors of up to 70 % in the predicted yield at  $t_i$ , and thus confirming that the use of a 1-term model would not be adequate for these systems.

In order to evaluate the influence of these simplification errors on the phenomena involved (washing and diffusion), the washing fractions ( $M_0/M_\infty$ ) and the diffusion coefficients ( $D_{eff}$ ) were calculated for a 1-term model fitting, and then they were compared with those obtained by other authors using 8 terms. The results are presented in Table 2.

As for the  $D_{eff}$  value, relative errors of up to 36.68 % were observed, whereas the errors for the washing fractions were

higher. It is worth noting that, in some cases, for the washing fraction negative values were obtained with the 1-term model, which do not have a physical meaning. By applying an adequate simplification (8 terms), washing fraction values over 0.2 were estimated, confirming the importance of the washing phenomenon in these systems. The error of considering as a valid assumption the simplification with 1 term leads to an underestimation of the washing phenomenon and an overestimation of the diffusion phenomenon.

**Table 1.** Analysis of the model with 1-term series applied to the experimental data obtained by Sánchez et al. [7] using the proposed algorithm

Assay	1-term Model			Minimum Terms Needed (at least)	RE% at $t_i$ (%)
	A	$M_0/M_\infty$	$B \times 10^5$		
1	1.03	-0.03	6.32	9	70.1
2	1.04	-0.04	10.92	8	61.1
3	1.02	-0.02	12.34	7	55.4
4	1.03	-0.03	15.98	7	50.9
5	1.00	0.01	18.06	6	44.4
6	0.99	0.01	26.20	5	35.5
7	0.93	0.07	25.46	5	31.3
8	0.97	0.03	43.15	4	23.2

Note: RE%, percentage relative error.

**Table 2.** Comparison of the parameters obtained with models with 1 and 8 terms for the experimental data obtained by Sánchez et al. [19], considering a washing time equal to 0 ( $t_0=0$ )

Assay	1 term				8 terms			Relative error %	
	A	$B \times 10^5$	$M_0/M_\infty$	$D_{eff} \times 10^{13}$	$M_0/M_\infty$	$B \times 10^5$	$D_{eff} \times 10^{13}$	$D_{eff}$	$M_0/M_\infty$
1	1.03	6.32	-0.04	6.76	0.26	4.00	4.28	36.68	69.6
2	1.04	10.90	-0.04	11.69	0.23	7.33	7.84	32.88	39.1
3	1.02	12.34	-0.02	13.21	0.24	9.00	9.63	27.09	127.7
4	1.03	15.98	-0.03	17.11	0.24	10.50	11.24	34.31	74.7
5	1.00	18.06	0.00	19.32	0.26	12.00	12.84	33.54	$\infty$
6	0.99	26.20	0.01	28.04	0.25	17.50	18.73	33.21	869.5
7	0.93	25.46	0.07	27.25	0.28	19.50	20.87	23.42	8.8
8	0.97	43.15	0.03	46.18	0.23	34.16	36.56	20.83	34.9

#### 3.2 Analysis of the model applied by different authors

The works reported by various authors were also analyzed, assuming a washing time equal to zero, and the results are shown in Table 3.

Among the analyzed systems, it can be observed that the 1-term simplification shows relative errors below 4 % for the shortest extraction time in the systems studied by Pérez et al. [5], and Najdanovic-Visak et al. [20], with the latter being the work where the modified Fick's diffusion model was presented.

On the other hand, the systems analyzed by Inanc et al. [26] and Sun et al. [24] exhibited negative washing fractions, which do not have a physical meaning. The application of the calculation algorithm for the conditions described by these authors shows the need for up to 11 terms of the series for the data fitting, registering relative errors of up to 663.6 % in the predicted yield for  $t_i$ .

Other authors considered that the washing stage does not occur instantaneously, selecting a washing time  $t_0$  larger than 0. Toda et al. [14] worked with a washing time of  $t_0=600$  s, while Amarante et al. [10] selected a washing time of  $t_0=1800$ . However, these authors used the experimental data obtained at times lower than  $t_0$  for the model fitting and to solve the

diffusion coefficient, and therefore the resolution of the model does not have physical or mathematical consistency.

For a given  $t_0$ , it is necessary to use experimental initial times higher than  $t_0$ . The analysis of the models that consider washing times equal to zero and those selected by the authors for the experimental initial times used in each work and using higher initial times than the selected  $t_0$  are shown in Table 4 and 5.

As the shortest experimental time reported by Amarante et al. [10] was 30 s, the most adequate combination would be  $t_0=0$  and  $t_i=30$  s, for which up to 15 terms of the series are necessary, with a RE% of up to 50.22 %. For the washing time selected by the authors, the necessary terms decrease to 5 with a RE% of up to 16.82 % for  $t_i=2700$  s (higher than the washing time), an assumption that would rule out 86% of the adjustable experimental data obtained for times below 2700 s due to the mathematical inconsistency.

Negative values of washing fractions were observed when using the washing time equal to zero or those selected by Toda [14]. Likewise for all the analyzed combinations of  $t_0$  and  $t_i$ , relative errors larger than 5 % were observed for the predicted yield at  $t_i$ , being necessary the use of up to 5 terms of the series. Since the authors selected experimental values from  $t=300$  s for the model fitting, the most adequate combination for the

calculation of the number of necessary terms and subsequent fit would be  $t_0=0$  (or a time lower than  $t_i$ ) and  $t_i=300$  s, for which the largest relative errors were obtained (up to 952.54 %), what would explain the negative values observed

for the washing fractions. It is worth noting that for a  $t_i$  lower than the selected  $t_0$  it is not possible to apply the calculation algorithm because a mathematical inconsistency would arise.

**Table 3.** Analysis of the models applied by different authors using the proposed algorithm, for a washing time equal to zero ( $t_0=0$ )

Assay	1 term model				Minimum terms needed (at least)	RE% at $t_i$ (%)
	A	$M_0/M_{\infty}$	$B \times 10^5$			
Inanc et al. [26] $t_i = 300$ s	1	0.91	-0.50*	199.00	2	4.2
	2	0.85	-0.40*	114.00	3	14.6
	3	0.76	-0.25*	38.00	5	50.8
	4	0.88	-0.44*	18.00	7	161.9
	5	0.95	-0.57*	5.00	11	663.6
Sun et al. [24] $t_i = 300$ s	6	0.82	-0.35*	36.00	5	68.2
	7	0.80	-0.31*	38.00	5	57.6
	8	0.82	-0.35*	52.00	4	46.5
	9	0.81	-0.32*	59.00	4	37.2
	10	0.83	-0.37*	39.00	5	66.3
	11	0.79	-0.30*	46.00	4	46.2
	12	0.81	-0.34*	56.00	4	40.7
	13	0.78	-0.28*	57.00	4	34.9
	14	0.77	-0.27*	29.00	5	65.0
	15	0.68	-0.12*	30.00	5	43.6
	16	0.73	-0.20*	47.00	5	53.7
	17	0.79	-0.30*	67.00	4	29.3
Najdanovic-Visak et al. [20] $t_i = 100$ s	18	0.19	0.68*	410.00	2	1.1
	19	0.14	0.77*	572.00	2	0.4
	20	0.15	0.75*	677.00	2	0.3
	21	0.14	0.77*	760.00	2	0.2
Colivet et al. [16] $t_i = 180$ s	22	-	0.00	54.00	5	31.6
	23	-	0.00	54.00	5	31.5
	24	-	0.00	56.00	5	30.7
	25	-	0.35	58.00	5	13.6
	26	-	0.35	57.00	5	13.8
	27	-	0.35	76.00	4	11.1
	28	-	0.64	123.00	3	3.1
	29	-	0.64	93.00	3	4.1
	30	-	0.64	92.00	3	4.1
	31	0.45	0.25	24.00	5	21.6
Zárate et al. [11] $t_i = 300$ s	32	0.45	0.25	42.00	4	14.6
	33	0.45	0.25	56.00	4	11.6
	34	0.30	0.50	73.00	3	4.8
	35	0.20	0.66	23.00	5	7.1
Baümler et al. [9] $t_i = 300$ s	36	0.20	0.66	4.00	8	11.8
	37	0.46	0.24	10.00	8	32.1
Fernández et al. [8] $t_i = 300$ s	38	0.46	0.24	13.00	7	29.3
	39	0.46	0.24	16.00	6	27.0
	40	0.46	0.24	25.00	5	21.9
	41	0.48	0.21	10.00	8	33.8
Pérez et al. [5] $t_i = 2000$ s	42	0.14	0.78*	11.90	3	1.7
	43	0.15	0.75*	15.30	3	1.4
	44	0.14	0.77*	16.60	2	1.0
	45	0.14	0.76*	20.90	2	0.7
	46	0.14	0.76*	40.20	2	0.1
	47	0.11	0.81*	51.00	1	<0.1
	48	0.21	0.65*	10.40	3	3.2
	49	0.19	0.68*	11.90	3	2.5
	50	0.18	0.70*	13.50	3	2.0

Note: \* Calculated from A. RE%: Percentage Relative Error.

**Table 4.** Analysis of the 1-term model applied to the experimental data obtained by Amarante et al. [10] using the proposed algorithm

Assay	57	58	59	60
A	0.48	0.48	0.47	0.44
$B \times 10^5$	8.97	9.24	10.20	11.10

		$M_0/M_\infty^*$ ( $t_0=1800$ s)	0.33	0.34	0.35	0.41
		$M_0/M_\infty^*$ ( $t_0=0$ s)	0.21	0.22	0.22	0.28
$t_0 = 0$ s	ti=30 s	Minimum terms needed (at least)	15	15	15	14
		RE% at ti (%)	50.2	26.5	48.5	41.8
	ti=2700 s	Minimum terms needed (at least)	3	3	3	3
		RE% at ti (%)	8.3	7.9	6.8	5.4
$t_0=1800$ s	ti=30 s	Minimum terms needed (at least)	-	-	-	-
		RE% at ti (%)	-	-	-	-
	ti=2700 s	Minimum terms needed (at least)	5	5	5	5
		RE% at ti (%)	16.8	16.2	14.7	12.1

Note: \* Calculated from A. RE%: Percentage Relative Error.

**Table 5.** Analysis of the 1-term model applied to the experimental data obtained by Toda et al. [14] using the proposed algorithm

		Assay	51	52	53	54	55	56
		A	1.02	1.10	1.06	1.31	1.21	0.95
		$B \times 10^5$	67.00	68.00	73.00	49.00	56.00	58.00
		$M_0/M_\infty^*$ ( $t_0=600$ s)	-0.12	0.47	0.53	0.11	0.28	0.45
		$M_0/M_\infty^*$ ( $t_0=0$ s)	-0.68	-0.80	-0.75	-1.15	-0.98	-0.57
$t_0=0$ s	ti=300 s	Minimum terms needed (at least)	4	4	4	5	4	4
		RE% at ti (%)	81.0	135.7	87.8	176.8	952.5	72.7
	ti=900 s	Minimum terms needed (at least)	3	3	3	3	3	2
		RE% at ti (%)	5.5	5.2	4.3	36.9	15.3	6.8
$t_0=600$ s	ti=300 s	Minimum terms needed (at least)	-	-	-	-	-	-
		RE% at ti (%)	-	-	-	-	-	-
	ti=900 s	Minimum terms needed (at least)	4	3	3	4	4	4
		RE% at ti (%)	20.4	5.6	4.4	17.7	11.5	7.1

Note: \* Calculated from A. RE%: Percentage Relative Error.

#### 4. CONCLUSIONS

The analysis of a mathematical diffusion model based on a modified form of Fick's law allowed us to determine a criterion for the simplification of the model according to the system under study, developing an algorithm for calculating the number of terms of the series that are necessary for the model fitting and for obtaining the parameters from a given error (related to the experimental error 0.001). The calculation algorithm is described by 7 steps, including an initial fit of experimental data, a calculation of error associated to assumptions and comparison with a tolerable value, and a recalculation of model with fixed number of terms. The data obtained by various authors for different systems were studied using the proposed algorithm, finding in general that the number of terms of the series of the model was underestimated, which led to differences in the calculation of the model parameters and the analysis of the phenomena involved. The greatest difference was seen for the parameter related to the washing phenomenon, observing an underestimation in the models with fewer terms of the series than necessary, while the diffusion coefficient ( $D_{eff}$ ) was overestimated. The results obtained in this work show the importance of adopting an adequate simplification criterion in a physical model, which would allow to explain mass transfer phenomena, avoiding errors in their interpretation.

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## NOMENCLATURE

M	mass of solute that diffuses (kg solute kg dry meal <sup>-1</sup> )
M <sub>0</sub> /M <sub>∞</sub>	Washing fraction (dimensionless)
B	model-fitting parameters (s <sup>-1</sup> )
D <sub>eff</sub>	effective diffusion coefficients (m <sup>2</sup> s <sup>-1</sup> )
R <sub>m</sub>	average particle radius of the extreme values (m)
t	diffusion time (s)
A	model-fitting parameters (dimensionless)
t <sub>min</sub> , t' <sub>min</sub>	lowest experimental extraction time
RE%	percentage relative error
Y <sub>1</sub>	yield predicted by the model with 1-term series for the shortest experimental time
Y	yield predicted by the model with the necessary number of terms calculated for the shortest experimental time
K	number of terms entered for the data fitting.
i	counter
n	number of necessary terms for the fitting.

## Subscripts

0,1,2,...,n	series terms
0	washing stage
∞	infinite time
t	at time t

APPENDIX

Mathematical models used to describe the kinetics of vegetable oil extraction

Models	Attributes	References
$E = \frac{8}{\pi^2} \sum_{n=0}^{\infty} \frac{1}{(2n+1)^2} 10^{[-(2n+1)\frac{\pi D t}{4e^2}]}$	Flakes	Boucher et al. [1]
$\frac{dE}{dt} = -\frac{12D}{\varepsilon e^2} (C_s - C_0)$	Flakes	Karnofsky [2]
$\frac{dC_{oil}}{dt} = \frac{C_{eq} - C_{oil}}{\left[ \frac{A}{k_E} + \frac{B}{D_E} \left( \frac{1}{r} - \frac{1}{R} \right) \right]}$	Ethanol, Spherical particles	Chien et al. [3]
$C_L = A_L [1 - e^{(-B_L t)}]$ $C_D = A_D [1 - e^{(-B_D t)}]$	Dehulled sunflower	Patricelli et al. [4]
$\frac{M_t}{M_{\infty}} = 1 - \left( 1 - \frac{M_0}{M_{\infty}} \right) \frac{6}{\pi^2} e^{[-B(t-t_0)]}$	Spherical particles	Pérez et al. [5]

Note: E: fraction of total oil not extracted. D: diffusion coefficient. e: flake thickness. t: time. ε: fraction of voids in the flakes. C<sub>s</sub>: average oil concentration in the film at time t. C<sub>0</sub>: concentration of the miscella used in the experience. C<sub>oil</sub>: oil concentration in the enveloping phase. C<sub>eq</sub>: oil concentration under equilibrium conditions. r: radius of the unextracted area. R: particle radius. k<sub>E</sub>: convective transfer coefficient. D<sub>E</sub>: diffusive transfer coefficient. C<sub>L</sub>: concentration of oil for the washing stage. C<sub>D</sub>: oil concentration for the diffusion stage. M<sub>t</sub>: mass of oil diffusing over time t. M<sub>∞</sub>: mass of oil that diffuses at infinite time. M<sub>0</sub>: mass of oil obtained at the washing stage. t<sub>0</sub>: time of the washing stage.