

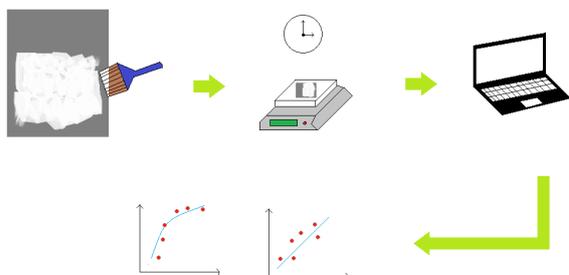
Full Paper | <http://dx.doi.org/10.17807/orbital.v13i1.1508>

# Analysis of Drying Process of Water-Based Architectural Paints

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Due to its low toxicity and because they are environmentally friendly, water-based paints are the most employed in the world, mainly to coat buildings. In these systems, the water evaporation process is important to determine the final paint quality and should be carefully evaluated. This work evaluated the suitability of Crank's model, solution of the Fick's second law, to experimental drying data of water-based architectural paints to better understand this process. Therefore, the data were adjusted to the linearized and original model and the number of terms used in its approximation was varied. For each model, the diffusion coefficient of the water in the coating material and the coefficient of determination were calculated. The results showed that the use of the linearized model is not adequate to determine the diffusion coefficient, but the nonlinear adjustment of the original model can adjust the data for some paints. These results also suggest the addition of terms to the sum of the model to improve its quality in the initial stages of drying.

## Graphical abstract



## Keywords

Architectural paints  
Crank's model  
Diffusion coefficient  
Drying  
Water-based paints

## Article history

Received 08 June 2020  
Revised 12 February 2021  
Accepted 13 February 2021  
Available online 05 March 2021

Editor: Grégoire J. F. Demets

## 1. Introduction

Paint is a mixture, generally liquid, composed of pigments dispersed in a fluid resin which, upon passing through a curing process and being applied into thin film forms an opaque and adhesive layer at the substrate [1, 2]. One of the largest sectors of the paint trade is that of the products used in the real estate industry. In 2004, 800 tons of paint for civil construction were produced in Brazil, corresponding to approximately 54% of the total domestic production volume [3]. Nowadays, architectural painting has not only a decorative

function, but also notably protection of the substrates used in buildings [1].

Resins, pigments, additives and solvents are the main constituents of the building paints. The solvents have the function of solubilizing the resin and keep all the substances in a homogeneous system. They are also responsible for the applicability characteristics of the paints, such as viscosity [2, 4].

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Water-based paints have been increasing their market share since the 1960s and have become the largest volume products produced in the coating materials industry [5]. Water-based paints are manufactured from modified synthetic resins, suitable for using water as a solvent, which reduces the volatile organic compounds in these formulations. Thus, these products are non-flammable, exhibit less toxicity and eliminate 93% of the use of organic solvents and of the volumetric emission of organic vapors [6].

A water-based paint has slower drying kinetics in a natural atmosphere, when compared to solvent-based paint. Drying denotes the changing state of the coating material, from liquid to solid. Therefore, for a water-based paint, this change involves the water evaporation, a process whose duration is a function of the resin nature, film thickness, temperature and humidity. The curing is distinguished from drying by reactions between the resin and a curing agent. Then, paint may be dry and not yet fully cured [7].

The process of water evaporation affects the rheological properties of the paint, influencing on the coating performance characteristics, such as adhesion, leveling and resistance to undesired tensions [8]. One of the simplest methods to study water evaporation from polymeric colloidal dispersions, such as the water-based paints, is the gravimetry, which consists in monitoring the mass as a function of time [9].

The proposition of mathematical models that accurately describe the drying of water-based paints is essential for improving the quality of this product, expanding its market and reducing the environmental impacts associated with architectural coating materials. Croll [10] measured the weight loss of a water-based paint, called Rohm and Haas Rhoplex® AC-388, over time, at temperature of  $22 \pm 1$  °C, relative humidity of  $50 \pm 2\%$ , under ambient conditions or with an air velocity of  $1.8 \text{ m}\cdot\text{s}^{-1}$ . Two drying stages was observed. The first, with constant rate of water evaporation, occurs when the resistance offered by packed particles is minimal and the process depends heavily on ambient conditions and coating temperature, can be modeled by mass and energy balances. The second, with decreasing drying rate, happens when water loss is limited by transport across a coalescing coating, being modeled by a relationship between evaporation rate and water concentration. In contrast, Vanderhoff *et al.* [11] and, more recently, Phillips *et al.* [12] proposed three stages for the drying process of water-based polymeric coatings. Phillips *et al.* [12] studied the water evaporation from aqueous dispersions consisting of an experimentally determined ratio of epoxy resin and nitrile latex, applying gravimetric analysis, at temperature of  $35 \pm 1$  °C and relative humidity of  $35 \pm 7\%$ , in ovens without convective air flow. The first stage described exhibits a zero-order kinetics, when water evaporates from the surface, where it is in direct contact with the atmosphere, at a constant rate. On the following stages, the evaporation is limited by the rate of water diffusion through coalescing coating, that begins as thin layers on the surface (second stage) and evolves into a more developed coalescent material (third stage). To model the process, the Fick's diffusion equation was solved with the Laplace Transform, providing evaporation rate constants and diffusion coefficients.

In this work, a mathematical approach to the water-based paint drying process is proposed, gauging the possibility of encompassing all stages in a single model. In this regard, if the paint film is taken as an infinite plate, considering the mass transport through the plate as the most important phenomenon of the drying process, and assuming that the

transfer occurs in a one-dimensional direction, with constant diffusion coefficient, the solution of the Fick's second law (Equation 1) according to Crank [13] is given by Equation 2:

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} \quad (1)$$

Where  $C$  is the concentration of diffusive substance,  $D$  is the diffusion coefficient,  $t$  is the diffusion time and  $x$  is the position along the direction in which the diffusion takes place.

$$\frac{M_t}{M_\infty} = 1 - \sum_{n=0}^{\infty} \frac{8}{(2n+1)^2 \pi^2} \exp \left[ -\frac{D \left( n + \frac{1}{2} \right)^2 \pi^2 t}{l^2} \right] \quad (2)$$

Where  $M_t$  is the amount of substance that diffused on the plate at time  $t$ ,  $M_\infty$  is the amount of substance that diffused on the plate in an infinite time and  $l$  is half of the plate thickness.

In practice, it is impossible to perform this summation with infinite terms and it is common to approximate it by the first terms (Equation 3). The higher the term  $\frac{Dt}{l^2}$ , fewer terms are required to achieve the desired accuracy.

$$\frac{M_t}{M_\infty} = 1 - \sum_{n=0}^{n'} \frac{8}{(2n+1)^2 \pi^2} \exp \left[ -\frac{D \left( n + \frac{1}{2} \right)^2 \pi^2 t}{l^2} \right] \quad (3)$$

Where  $n'$  is an integer greater than or equal to zero being common practice makes it equal to zero approaching the value of the summation by the first term. Therefore, the aim of this work is evaluating the suitability of Crank's Model to experimental drying data of water-based building paints obtained by Guío [14].

## 2. Results and Discussion

There are two ways to perform the desired modeling: through Linearized Crank's Model, Equation 4, where  $n'=0$  (approximation by the first term) and  $P$  is given by Equation 5, or through Crank's Model (Equation 3) [9].

$$P = Dt \quad (4)$$

$$P = -\frac{4l^2}{\pi^2} \ln \left[ \frac{\pi^2}{8} \left( 1 - \frac{M_t}{M_\infty} \right) \right] \quad (5)$$

In this work three different analyses were performed on the data: Analysis A, B and C.

### Analysis A

The diffusion coefficient of water in each paint sample was calculated using Linearized Crank's Model (Equation 4). The coefficient of determination of Linearized Crank's Model (Equation 6 - see section 3. Methods) was also calculated for each sample.

### Analysis B

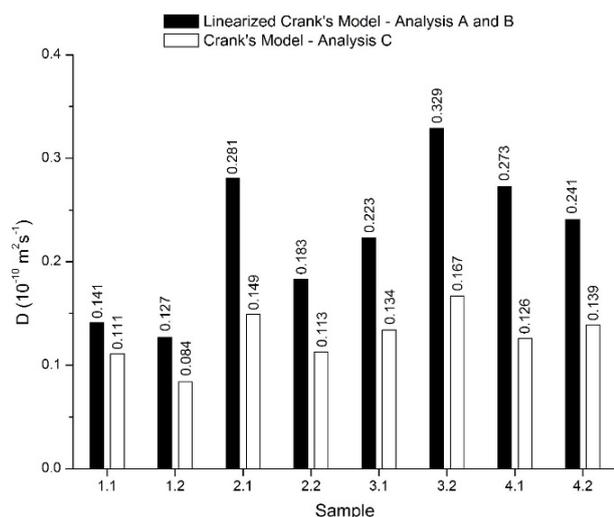
The diffusion coefficient of water in each paint sample was calculated using Linearized Crank's Model (Equation 4). The coefficient of determination of Crank's Model (Equation 7 - see section 3. Methods) was also calculated for each sample. This analysis was performed to evaluate the possibility of applying to the original data a diffusion coefficient calculated from a linearized model.

### Analysis C

The diffusion coefficient of water in each paint sample was calculated using Crank's Model (Equation 3). The coefficient of determination of Crank's Model (Equation 7 - see section 3. Methods) was also calculated for each sample. The procedures of Analysis C were carried out for values of  $n'$  varying between 0 and 5 to evaluate the influence of the

number of terms of the summation of Equation 3 used in its approximation on its performance.

The water diffusion coefficient in the paint calculated for each sample using Linearized Crank's Model and Crank's Model is presented in Figure 1. It can be observed that the values obtained by the linearized model are higher than the values calculated using the original model for all samples. Comparing the values determined by the two procedures, it is noted that they are discrepant since the diffusion coefficients calculated by Analyzes A and B are, on average, 73% higher than those calculated by Analysis C.



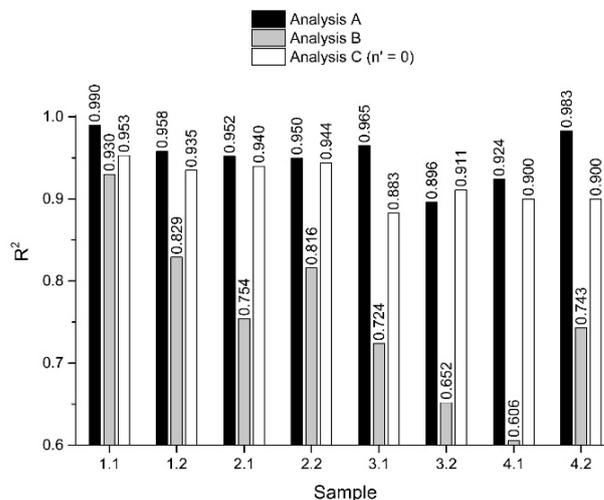
**Fig. 1.** Comparison of water diffusion coefficients in paints calculated by Linearized Crank's Model and Crank's Model.

The coefficients of determination obtained when performing Analyzes A, B and C ( $n' = 0$ ) are shown in Figure 2. In this figure, it is noted that the coefficients of determination obtained by Analysis A are, on average, 28% higher than those obtained by Analysis B and, moreover, the average of the coefficients of determination found in Analysis B is low (0.757). This indicates that the coefficient of determination of Linearized Crank's Model (Analysis A), even with high values and showing a good fit quality that can be seen in Figure 3, can not be used as a parameter to evaluate the ability of a diffusion coefficient to represent the original (non-linearized) data.

It is also shown in Figure 2 that the coefficients of determination obtained by Analysis C are, on average, 23% higher than those obtained by Analysis B, indicating that the non-linear fit allows the calculation of a diffusion coefficient best suited to representing the real data than that obtained by the linear fit. Moreover, it is noted that the linear fit is not even able to determine which samples will be best fitted by the non-linear model. For example, sample 3.1 has the third highest coefficient of determination for Analysis A, however it has the worst coefficient of determination for Analysis C. It can be said that the information taken from the Figures 1 and 2 indicates that linearization is not a good tool for calculating water diffusion coefficients in building paints and should only be used as an initial estimate of the order of magnitude of these coefficients.

The water diffusion coefficient in the paint calculated for each sample by the non-linear fit of Crank's Model (Analysis C) is shown in Figure 1. The fit was performed for  $n'$  ranging from 0 to 5, however, it was noticed that the addition of terms

to the summation did not change the value of the calculated diffusion coefficients, so there is only one calculated diffusion coefficient value for each sample. The coefficients of determination found for Crank's Model with  $n'$  ranging from 0 to 5 are shown in Figure 4. Unlike the diffusion coefficients, the coefficients of determination were affected by the addition of terms to the summation.

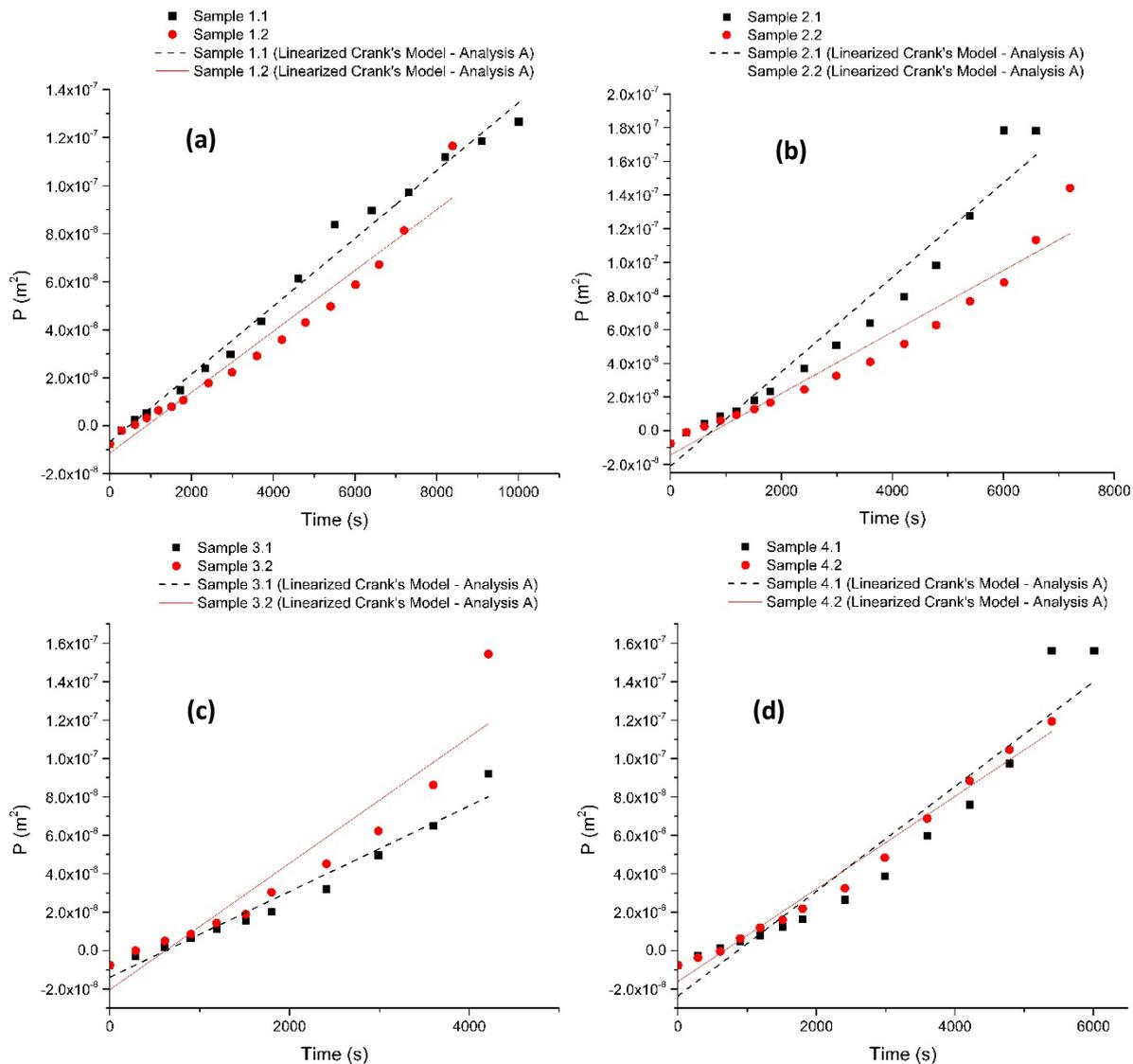


**Fig. 2.** Comparison of coefficient of determination for the three different analyzes.

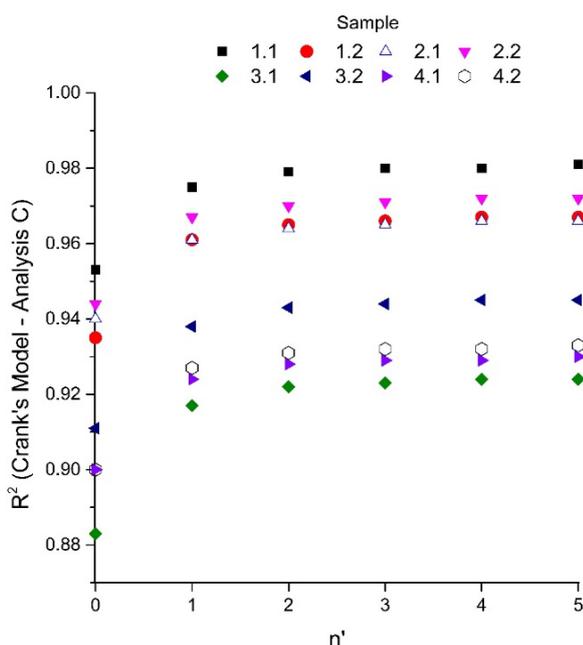
Noting Figure 4, it is possible to realize that the influence of the addition of a term to the summation of the model in its capacity to represent the experimental data reduces when the number of terms becomes high. Therefore, the change from  $n'$  value of 0 (a term) to 1 (two terms) is the one that most impacts the values of the coefficients of determination. These results make it possible to say that, if the interest is restricted to the calculation of the diffusion coefficient of water in architectural paints, the approximation by the first term of the summation of Equation 3 ( $n' = 0$ ) is adequate to determine the desired values. However, if the objective is to model the drying data of these paints, adding terms to the summation of the model becomes necessary to improve its performance. Experimental data and drying models of all samples are presented in Figure 5.

An examination of Figure 5 confirms that the greater the term  $\frac{Dt}{l^2}$ , less terms are required to achieve a desired accuracy. It can be observed for all samples that for the high  $t$  values both the approximation by the first term of the summation ( $n' = 0$ ) and by its sixth term of it ( $n' = 5$ ) present similar results. The advantage of adding terms to the summation would be, in this case, to improve drying modeling in low time values for all samples.

It is also noticed that in a given interval (ranging from 80% to 93% of the total drying) the inversion in the quality of the models occurs, wherein the value of the diffusion coefficient obtained by the linearized model becomes better to represent the drying phenomenon. Among the explanations for the fact that Crank's Model presents worse results in the representation of the final moments of drying than in the initial ones, it is possible that some of the approximations used in the application of the model are not reasonable, as for example, since the weight loss is quite significant in the samples (44.6% to 54.8%), the reduction of the paint layer thickness during drying may not be negligible and the consideration of a constant value impacts the model.



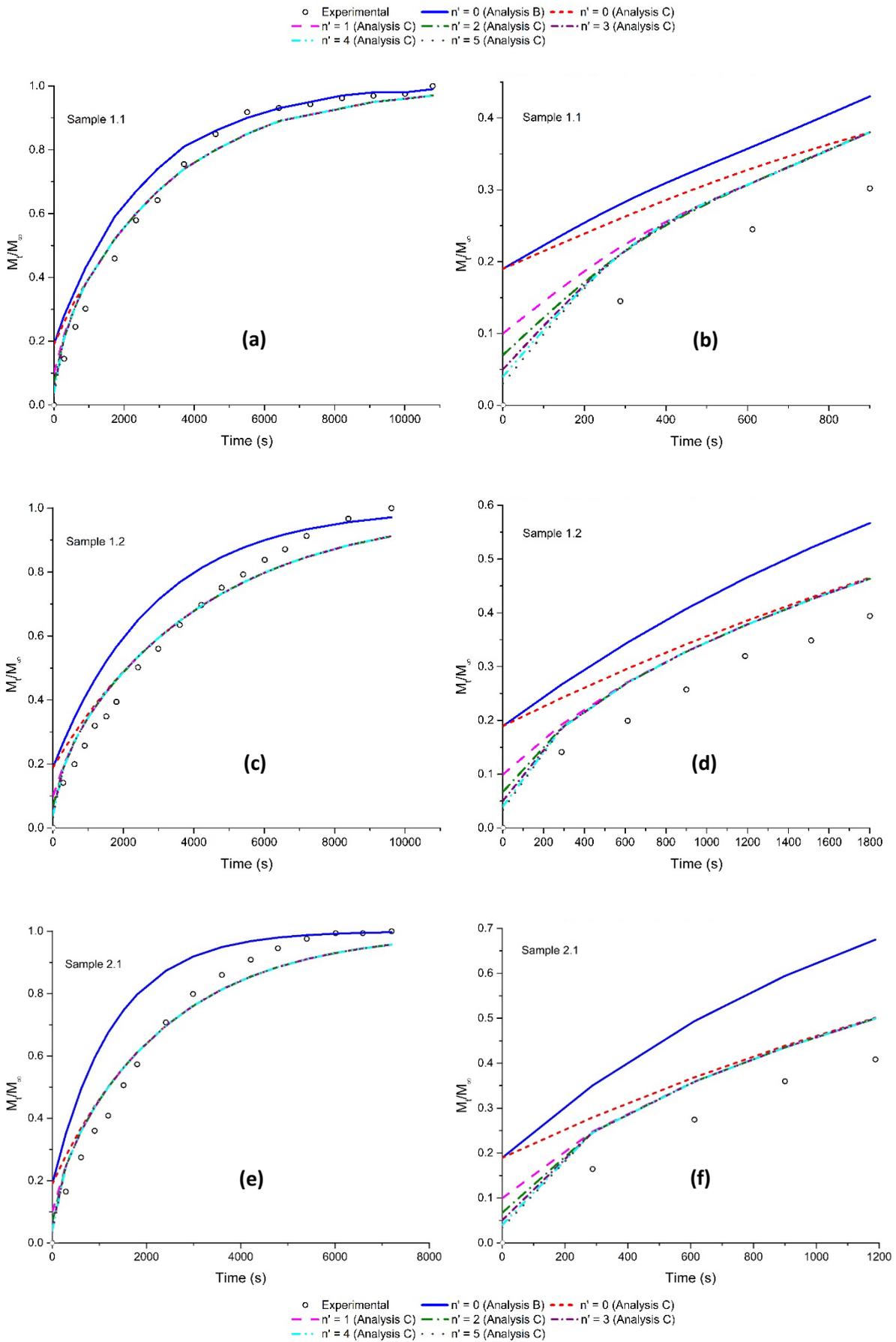
**Fig. 3.** Application of Linearized Crank's Model to the drying data of the acrylic paints - (a) manufacturer 1 (b) manufacturer 2 (c) manufacturer 3 (d) manufacturer 4.

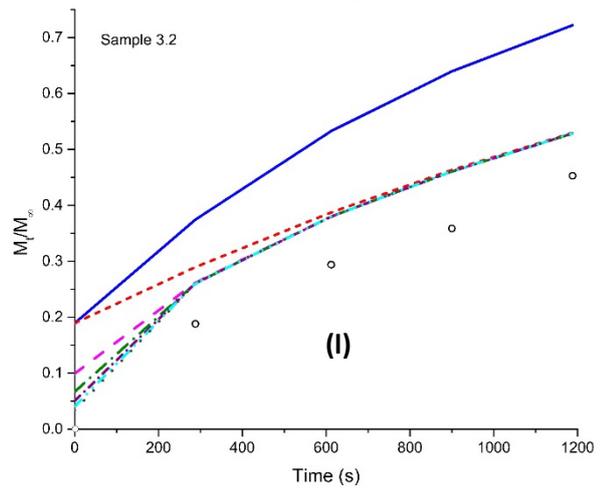
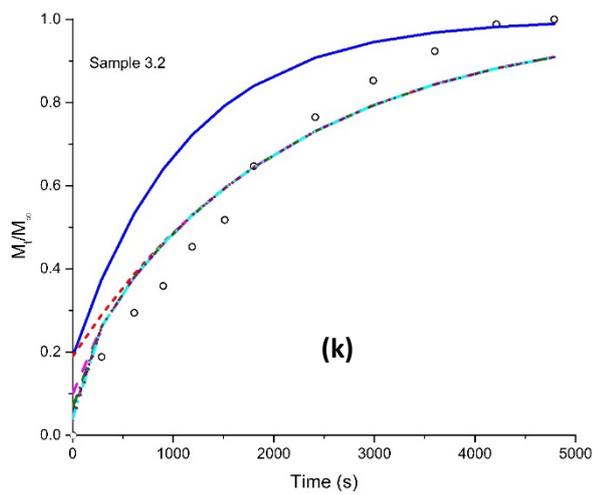
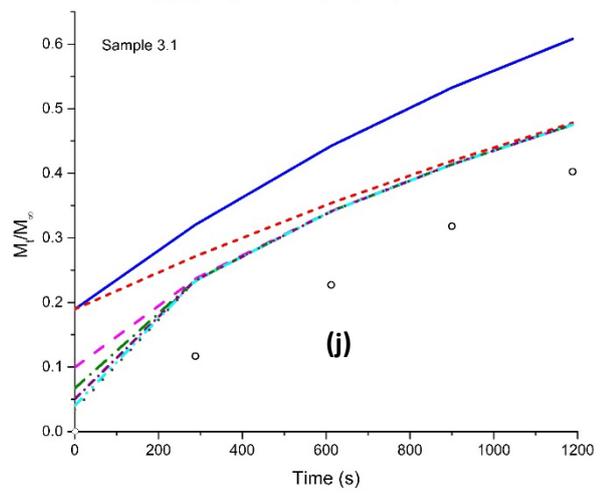
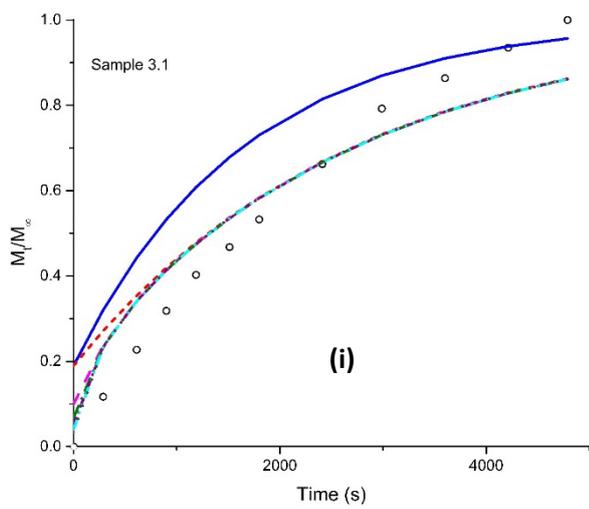
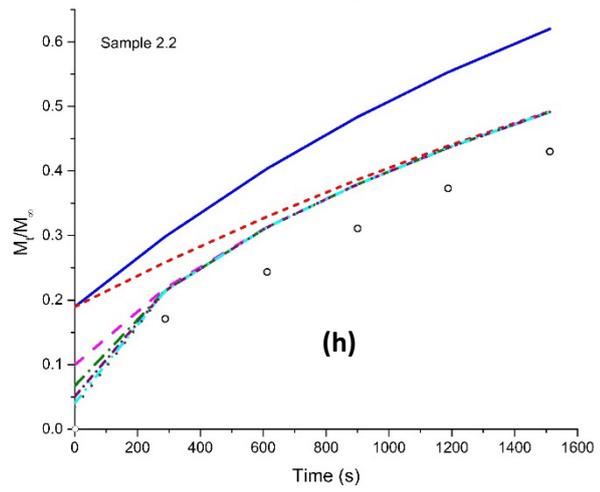
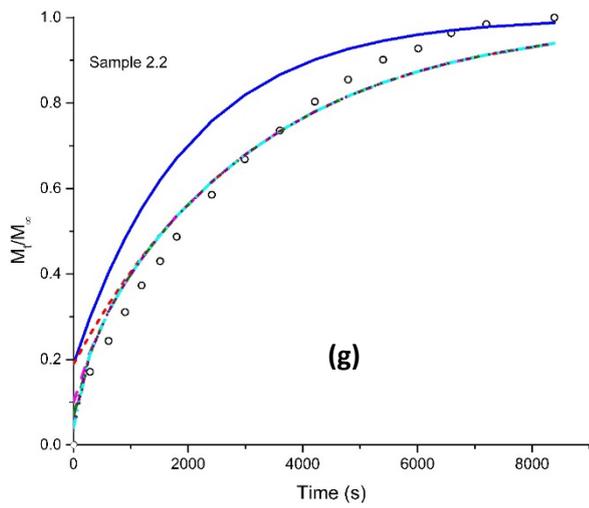


**Fig. 4.** Influence of increasing number of terms of Crank's Model summation on its coefficient of determination.

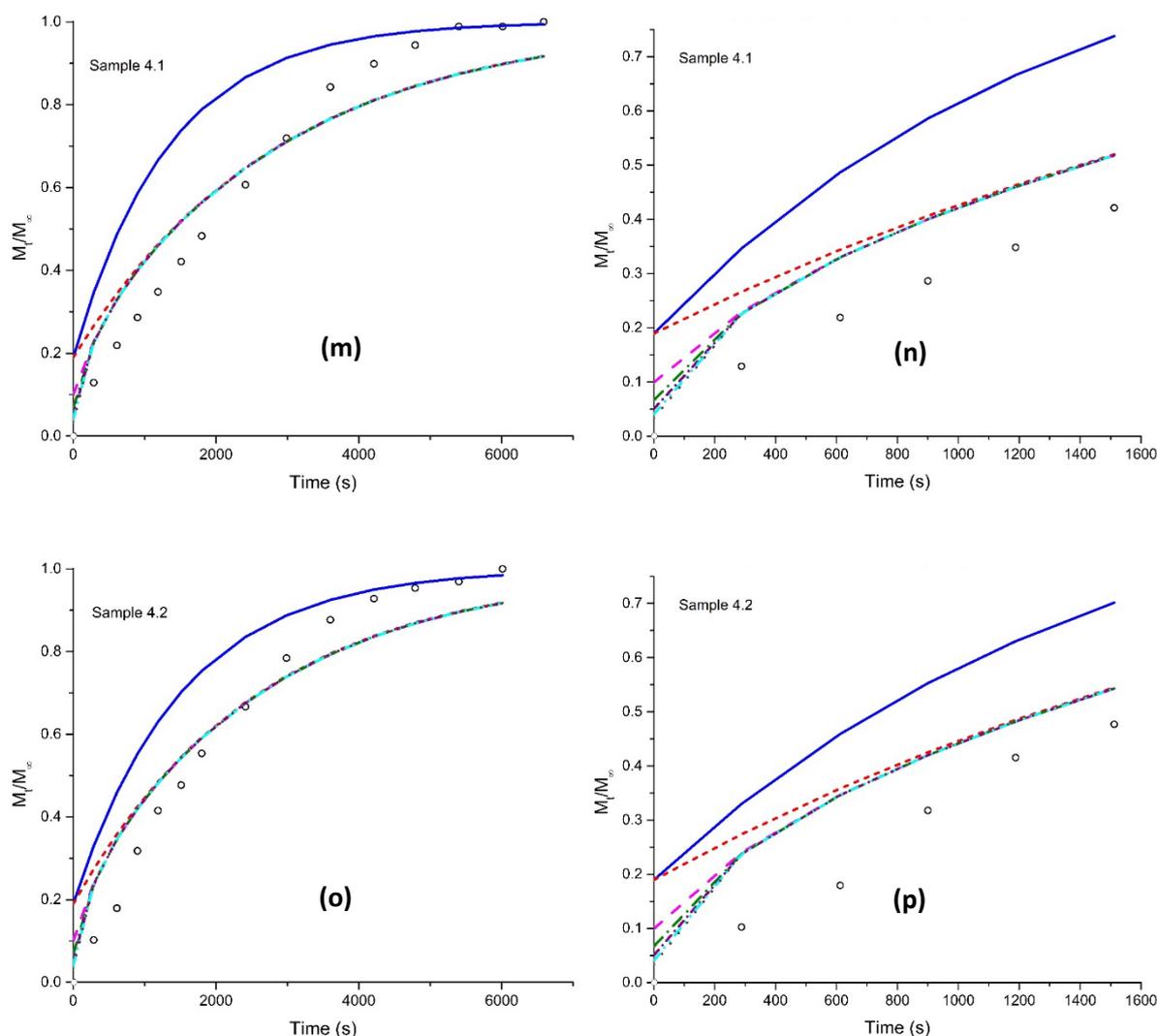
Another approach that may have decreased the accuracy of the model near the end of drying is the consideration of a constant diffusion coefficient throughout the process. This consideration may not be valid because during the drying of a coating material its physical state changes from liquid to solid, which could change the value of the water diffusion coefficient in the material.

It is also possible to observe in Figure 4 that the samples studied can be divided into two groups: the first group of those that reached a coefficient of determination greater than 0.95 for the non-linear fit of Crank's Model with six terms ( $n' = 5$ ), in other words, despite the simplifications, the model was able to represent the data well (more than 95% of the data variance is explained by the model) and the second group of those that did not reach a coefficient of determination greater than 0.95. It is realized that, at least for paints with drying curves that resemble those of the second group (acrylic paints - manufacturer 3 and 4), the consideration that drying takes place in one step may compromise the suitability of the model to the data. So, for them, the division of the process into two or three steps, as proposed by Croll [10], Vanderhoff *et al.* [11] and Phillips *et al.* [12], may be required in applications that require a more precise model, with consequent loss of simplicity.





○ Experimental    —  $n' = 0$  (Analysis B)    - -  $n' = 0$  (Analysis C)  
 - -  $n' = 1$  (Analysis C)    - -  $n' = 2$  (Analysis C)    - -  $n' = 3$  (Analysis C)  
 - -  $n' = 4$  (Analysis C)    - -  $n' = 5$  (Analysis C)



**Fig. 5.** Experimental data and Crank's Model calculated using the diffusion coefficients obtained by the linearized (Analysis B) and original (Analysis C) models for sample (a) 1.1 (c) 1.2 (e) 2.1 (g) 2.2 (i) 3.1 (k) 3.2 (m) 4.1 (o) 4.2 and enlarged graphs to make it possible to see the influence of increasing number of terms of Crank's Model summation on its quality to fit the data for sample (b) 1.1 (d) 1.2 (f) 2.1 (h) 2.2 (j) 3.1 (l) 3.2 (n) 4.1 (p) 4.2.

The calculated mean diffusion coefficients of water in each of the four paints (arithmetic mean between diffusion coefficients calculated for samples of the same paints by the non-linear model with  $n' = 5$ ) are presented in Table 1.

**Table 1.** Water diffusion coefficients in the four water-based paints studied.

Paint	Diffusion coefficient (D) ( $10^{-11} \text{ m}^2 \cdot \text{s}^{-1}$ )
Acrylic paint - manufacturer 1	0.97
Acrylic paint - manufacturer 2	1.31
Acrylic paint - manufacturer 3	1.51
Acrylic paint - manufacturer 4	1.33

As expected, water presented close values of diffusion coefficient in the different paints, given that the nature of the solvent is one of the factors that have the greatest impact on the diffusion coefficient. It should be noted, however, that because they are of different brands, the paints have different formulations and consequently different mass transfer

resistance, which already brings a natural variability to the diffusion coefficient. At the same time, it was important to evaluate the data of these paints of such different brands and formulations because in practice, to be considered a good model, it needs to represent well the drying of all water-based paints available on the market. In addition, due to this wide variety, it was possible to verify whether the considerations adopted (paint film is taken as an infinite plate, mass transport through the plate as the most important phenomenon of the drying process, transfer occurs in a one-dimensional direction, constant diffusion coefficient, constant paint layer thickness, all weight loss is due to water evaporation) were valid for different paint compositions.

Comparing the values in Table 1 and the diffusion coefficient of water vapor in air at 21 °C ( $2.44 \cdot 10^{-5} \text{ m}^2 \cdot \text{s}^{-1}$ ), temperature close to Guío's [14] experimental condition (24 °C), they are much smaller, confirming that the paint actually offers a resistance to mass transfer [17]. Water diffusion coefficient values between  $10^{-10}$  and  $10^{-13} \text{ m}^2 \cdot \text{s}^{-1}$ , which includes the data in Table 1, suggest that water diffusion in the studied paints occurs through a polymeric membrane formed during the coalescence of the coating material [17].

Philips *et al.* [12], in considerably more abrupt drying conditions ( $35 \pm 1 \text{ °C}$  and relative humidity of  $35 \pm 7\%$ ) than

those of Guío's work [14] (24 °C and relative humidity of 74%), divided the drying curve into two stages and obtained a water diffusion coefficient in an aqueous dispersion consisting of an experimentally determined ratio of epoxy resin and nitrile latex of  $2.55 \cdot 10^{-11} \text{ m}^2 \cdot \text{s}^{-1}$  for the second stage, coefficient larger than those calculated in this work, but with similar order of magnitude, as expected.

### 3. Material and Methods

Guío [14] measured weight loss over time for samples of the six most commonly used water-based building paints in the city of São Carlos (located in the state of São Paulo in Brazil) following ISO 1513-2010 and ISO 15528-2000 [14,15,16]. The paints were applied to aluminum plates (100 mm x 100 mm x 2 mm) using a 600  $\mu\text{m}$  quadrangular applicator in a room with 74% of relative humidity and temperature of 24 °C [14-16]. Although in practice other materials, such as concrete, are more commonly covered by architectural paints than aluminum, the execution of paint drying experiments on plates of this metal is important to allow the comparison of the results of this work with the results of the works reported in literature. This is because most of these studies also use aluminum containers, as is the case of the study by Phillips *et al.* [12] and the calculations of transmission rates for liquid water and water vapor performed by Vanderhoff *et al.* [11].

Kiil [17] developed a novel drying model for water-based coatings and verified it using Croll's data [10]. It was noted that the adjustable parameters, such as the diffusion coefficient for the second stage, are independent of initial wet film thickness, considering a range of values from 89 to 1322  $\mu\text{m}$  [17]. Therefore, although architectural coatings are often applied with a wet film thickness of 30 to 100  $\mu\text{m}$  per layer, the results obtained for paint samples with a higher thickness (in this case, 600  $\mu\text{m}$ ) are probably representative of the actual application condition.

Each paint was tested in duplicate. One of the aluminum plates after paint application is shown in Figure 6 [14].

In this work, among the paints analyzed by Guío [14], the four whose duplicates presented closest drying data were studied. The paint samples, the formulation provided by the

manufacturer on the product label, the initial weight of each sample, the time required to stabilize its weight (determined when the paint weight was constant for 3 consecutive measurements), and the total weight loss are shown in Table 2 [14]. Guío [14] also presents the results of gas chromatography-mass spectrometry experiments (GC-MS) for wet and dry samples that were carried out to evaluate the presence of volatile organic compounds in the studied paints. However, the discussion of these results is outside the scope of this work and the reading of Guío's work [14] is recommended for further information.



Fig. 6. Aluminum plate after paint application [14].

In addition to the data presented in Table 2, Guío also indicates the value of  $l$  (semi-thickness of the paint layer) of 300  $\mu\text{m}$  and the weight values obtained from the time of paint application until the moment where its weight stabilizes, allowing the calculation of  $M_t$  (difference between the weight of the paint at instant  $t$  and initial weight) and  $M_\infty$  (difference between the constant weight of the paint and the initial weight). Guío suggests as a good approximation to consider that all weight loss is due to water evaporation [10].

Table 2. Water-based paints studied [14]

Paint (Formulation)	Samples	Initial weight (Kg)	Time required to weight stabilization (s)	Weight loss (%)
<b>Acrylic paint - manufacturer 1</b> (Water, aqueous dispersion resin of modified acrylic copolymers, organic and inorganic pigments, mineral fillers, specific additives, glycols, thickening agents, microbicides, aliphatic hydrocarbons)	1.1	$3.01 \cdot 10^{-4}$	$1.08 \cdot 10^4$	52.8
	1.2	$4.58 \cdot 10^{-4}$	$9.61 \cdot 10^3$	52.6
<b>Acrylic paint - manufacturer 2</b> (Water, aqueous dispersion resin of styrene acrylic copolymers, heavy metal free pigments, inert mineral fillers, glycols and surfactants)	2.1	$3.09 \cdot 10^{-4}$	$7.20 \cdot 10^3$	53.1
	2.2	$3.52 \cdot 10^{-4}$	$8.39 \cdot 10^3$	54.8
<b>Acrylic paint - manufacturer 3</b> (Water, modified acrylic polymer, lead and chromate-free organic and inorganic pigments, calcium carbonate, aluminum silicate, titanium dioxide, glycol ethers, isothiazolinones, aliphatic hydrocarbons)	3.1	$3.18 \cdot 10^{-4}$	$4.79 \cdot 10^3$	48.4
	3.2	$3.52 \cdot 10^{-4}$	$4.79 \cdot 10^3$	48.3
<b>Acrylic paint - manufacturer 4</b> (Water, aqueous dispersion resin based on acrylic and vinyl polymers, heavy metal free pigments, inert fillers, glycols, ethoxylated and carboxylated surfactants, isothiazolinones.)	4.1	$3.70 \cdot 10^{-4}$	$6.59 \cdot 10^3$	48.1
	4.2	$4.37 \cdot 10^{-4}$	$6.01 \cdot 10^3$	44.6

### Linearized Crank's Model

It is possible to obtain the value of the diffusion coefficient of Equation 4 that best fits the data obtained by Guío [14] using the Linear Fit tool from Excel software. For Linearized Crank's Model, the coefficient of determination ( $R^2$ ) is given by Equation 6.

$$R^2 = 1 - \frac{\sum_{i=1}^j [(\widehat{P})_i - (P)_i]^2}{\sum_{i=1}^j [(P)_i - \overline{(P)}]^2} \quad (6)$$

Where  $(\widehat{P})_i$  is the estimated value for  $P$  using Equation 4,  $(P)_i$  is the experimental value for  $P$  and  $\overline{(P)}$  is the average value of the  $j$  terms  $(P)_i$  for each sample [18].

### Crank's Model

It is possible to obtain the value of the diffusion coefficient of Equation 3 that best fits the data obtained by Guío using the Solver tool from Excel software [10]. This tool is used to maximize the coefficient of determination ( $R^2$ ) of Crank's Model, Equation 7, by varying the diffusion coefficient ( $D$ ).

$$R^2 = 1 - \frac{\sum_{i=1}^j \left[ \left( \frac{M_t}{M_{\infty}} \right)_i - \left( \frac{M_t}{M_{\infty}} \right)_i \right]^2}{\sum_{i=1}^j \left[ \left( \frac{M_t}{M_{\infty}} \right)_i - \overline{\left( \frac{M_t}{M_{\infty}} \right)} \right]^2} \quad (7)$$

Where  $\left( \frac{M_t}{M_{\infty}} \right)_i$  is the estimated value for  $\frac{M_t}{M_{\infty}}$  using Equation 3,  $\left( \frac{M_t}{M_{\infty}} \right)_i$  is the experimental value for  $\frac{M_t}{M_{\infty}}$  and  $\overline{\left( \frac{M_t}{M_{\infty}} \right)}$  is the average value of the  $j$  terms  $\left( \frac{M_t}{M_{\infty}} \right)_i$  for each sample [13].

### Analysis C - Choice of the number of terms

For  $n'$  smaller than 5 the addition of one more term to the summation results in a change in the value of  $\frac{M_t}{M_{\infty}}$  represented with two decimal digits. The value of 5 was determined by obtaining the integer part of the solution of Equation 8 for  $t = 0$ , where the unknown is the value of  $n'$ .

$$\frac{8}{(2n'+1)^2 \pi^2} \exp \left[ -\frac{(2n'+1)^2 D \pi^2 t}{4l^2} \right] = y \quad (8)$$

Where the term to the left of the equality is the value that is subtracted from  $\frac{M_t}{M_{\infty}}$  for each term added to the summation and has maximum modulus value when  $t = 0$ . The highest value this term can assume given the necessity that this term does not change the value of  $\frac{M_t}{M_{\infty}}$  represented with  $w$  decimal digits is represented by  $y$ , and can be calculated by Equation 9.

$$y = \frac{10^{-w}}{2} \quad (9)$$

The minimum  $n'$  values as a function of the number of desired decimal digits ( $w$ ) are presented in Table 3.

Analyzing the Table 3, it can be seen that it would take 20 terms ( $n = 0$  to  $n = 19 = n'$ ) for the term to the left of Equation 8 does not affect the calculated value for  $\frac{M_t}{M_{\infty}}$  represented with three decimal digits. This value would be too high and it was chosen to use representations with 2 decimal digits, sufficient for this work and that can be reached with a reasonable number of terms ( $6, n = 0$  to  $n = 5 = n'$ ).

**Table 3.** Determination of the upper bound of the summation of Crank's Model

$w$	$y$	$n'$
1	0.05	1
2	0.005	5
3	0.0005	19

## 4. Conclusions

The results obtained in this work indicate that the use of a linearized model is not adequate to determine the diffusion coefficient since the values obtained by this technique differed on average 73% of the values obtained by the nonlinear adjustment, even though they presented high coefficients of determination for the linearized model. It was also observed that for the nonlinear model the addition of terms to the summation does not change the calculated value of the diffusion coefficient, but it alters the coefficient of determination of the model being the change of one term ( $n' = 0$ ) for two terms ( $n' = 1$ ) the most significant.

The water diffusion coefficient in each of the four tested paints was determined using Crank's model. It has been shown that Crank's model is capable of representing well the drying data of some water-based building paints, but for others, splitting the drying data into two or three intervals followed by applying different models for each interval may be necessary. It is suggested the addition of terms to the summation of the model as a way to improve its quality in the representation of the initial stages of drying and control of the thickness of the paint layer during the experiment to determine a more reliable model to the final drying stages.

Taking into account that this work has already shown that the modeling method described here can be applied to analyze the drying data in the conditions normally adopted in laboratory tests (using aluminum as a substrate, for example), a possibility for future works would be to evaluate how paint drying behaves under different conditions of temperature, humidity and application on different substrates, such as concrete, a material that is more commonly covered by architectural paints than aluminum. The ability of Crank's model to represent the phenomenon can be analyzed and the water diffusion coefficient in the paints in each of these scenarios can be calculated.

## Acknowledgments

This research did not receive any specific grant from funding agencies in the public, commercial, or not-for-profit sectors.

## Author Contributions

Gustavo Feliciano de Jesus Barcelos contributed with conceptualization, formal analysis, investigation, methodology and writing – original draft.

Paula Duarte de Carvalho Souza contributed with investigation, visualization, writing – original draft and writing – review & editing.

Fernando Cotting contributed with writing – review & editing.

## References and Notes

- [1] Lambourne, R.; Strivens, T. A. Paint and Surface Coatings: Theory and Practice, 2nd ed. Sawston: Woodhead Publishing, 1999.
- [2] Bierwagen, G. P.; Huovinen, A. M. Paint Formulation. In: Cottis, B.; Graham, M.; Lindsay, R.; Lyon, S.; Richardson, T.; Scantlebury, D.; Stott, H. (eds). Shreir's Corrosion. Amsterdam: Elsevier, 2010.

- [3] A Profile of the Brazilian Paint Industry. *Pigm. Resin Technol.* **2005**, 34. [\[Crossref\]](#)
- [4] Tiarks, F.; Frechen, T.; Kirsch, S.; Leuninger, J.; Melan, M.; Pfau, A.; Richter, F.; Schuler, B.; Zhao, C-L. *Prog. Org. Coat.* **2003**, 48, 140. [\[Crossref\]](#)
- [5] Waters, J. A. Latex Paint Formulations. In: Asua, J. M. (eds). *Polymeric Dispersions: Principles and Applications*. Dordrecht: Kluwer Academic Publishers, 1997.
- [6] Elliott, P. T.; Glass, J. E. Water-Born Coatings. In: Craver, C. D.; Caharrer, C. E. (eds.). *Applied Polymer Science 21st Century*. Amsterdam: Elsevier, 2000.
- [7] Felton, L. A. *Int. J. Pharm.* **2013**, 457, 423. [\[Crossref\]](#)
- [8] Eley, R. R. Applied Rheology and Architectural Coating Performance. *J. Coat. Technol. Res.* **2019**, 16, 263. [\[Crossref\]](#)
- [9] Keddie, J. L.; Routh A. F. *Fundamentals of Latex Film Formation: Processes and Properties*. Dordrecht: Springer, 2010.
- [10] Croll, S. G. *J. Coat. Technol. Res.* **1987**, 59, 81.
- [11] Vanderhoff, J. W.; Bradford, E. B.; Carrington, W. K. *J. Polym. Sci.* **1973**, 41, 155. [\[Crossref\]](#)
- [12] Phillips, S. L.; Davis, M. T.; Phillips, D. J. *J. Coat. Technol. Res.* **2004**, 1, 315. [\[Crossref\]](#)
- [13] Crank, J. *The mathematics of diffusion*. Oxford: Clarendon Press, 1970.
- [14] Guío, L. M. P. Volatile Organic Compounds in Real Estate Paints: Characterization and Effects on Indoor Air Quality. [Master's Thesis] São Carlos, Brazil: Universidade de São Paulo, Instituto de Arquitetura e Urbanismo, 2013. [\[Link\]](#)
- [15] ISO 1513:2010(E), Paints and Varnishes - Examination and Preparation of Test Samples. 2010, The International Organization for Standardization: Switzerland.
- [16] ISO 15528:2000(E) Paints, Varnishes and Raw Materials for Paints and Varnishes – Sampling. 2000, The International Organization for Standardization: Switzerland.
- [17] Kiil, S. *Prog. Org. Coat.* **2006**, 57, 236. [\[Crossref\]](#)
- [18] Edgar, T. F.; Himmelblau, D. M.; Lasdon, L. S. *Optimization of Chemical Processes*. New York: McGraw Hill, 2001.

### How to cite this article

Barcelos, G. F. J.; Souza, P. D. C.; Cotting, F. *Orbital: Electron. J. Chem.* **2021**, 13, 1. DOI: <http://dx.doi.org/10.17807/orbital.v13i1.1508>