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Influence of film coefficient during multicomponent diffusion – KCl/NaCl in biosolid for static and agitated system using 3D computational simulation

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Abstract

The influence of film coefficient formed during the diffusion of inorganic salts (NaCl and KCl) in biosolids was studied using a 3D computer modeling by Finite Elements Method (FEM) in COMSOL Multiphysics® software combined with SOM-type Artificial Neural Networks (ANN). Such tools have shown that the influence of the film formed in the biosolid/solution interface occurs in a heterogeneous manner and is due to the matrix geometry, the type of system (agitated or static) and the ion size (Na^+ or K^+). The influence of film coefficient was more pronounced for K^+ ion, and for a static system. Comparing the geometry of biosolids, ion diffusion was more pronounced in the (Y±) axis in relation to other axes, X (±) and Z (±), as well as in between the poles (±) of this axis. FEM simulation associated with SOM-type ANN were efficient tools to evaluate this complex and unknown biophysical phenomenon.

Keywords: finite elements method; mass transfer; modeling; brines.

Practical Application: To simulate situations for the food industry in order to improve the quality and uniformity of food biosolids.

1 Introduction

Salting by immersion in a solution containing sodium chloride is one of the oldest and most commonly used treatments for food preservation, since this salt not only has antimicrobial activity, but also promotes chemical and nutritional changes, enhancing the flavor, texture, color and regulating moisture in the final product (Thibaudeau et al., 2015). Various types of foods, such as meat, fish, eggs, cheese, olives, pickles, potatoes, carrots, among others, are still obtained through the use of this preservation process (Dixit et al., 2018; Bordin et al., 2018).

Brining quail eggs is usually performed by immersion in brine where the migration of sodium ions into the biosolid occurs by diffusion. Borsato et al. (2012) studied brining quail eggs in static and agitated systems with a mixture of NaCl and KCl at a ratio of 70 to 30% (m/m) in brine, respectively, and compared them with commercial samples containing only NaCl. Sensory analysis showed that the proportion of salts presented no significant difference between samples.

Many models of solute diffusion from liquids to solids can be described by Fick's 2nd law in non-stationary system. A wide variety of solutions to this law is comprehensive presented by Crank (1975). Schwartzberg & Chao (1982) have also reviewed the literature on the diffusivity of solutes in solids, particularly in food and gels. Currently there are mathematical models seeking to model diffusion processes and other phenomena. A method that is commonly used is the Finite Element Method (FEM), which is basically the domain discretization in several elements (Hao et al., 2016; Angilelli et al., 2015). The FEM is used as a tool in several areas of engineering, chemistry and physics. Studies related to the transfer of heat and/or mass in food applying FEM in different biosolids are described in literature, specifically the component diffusion process (Ramya & Kumar, 2015; Harkouss et al., 2018). However, there is little knowledge about the influence of the film formed during the diffusion process.

According to Schwartzberg & Chao (1982), when fluid is in contact with a solid, a film is formed on its surface. If there is a mass transfer between the fluid and the surface, the current must go through the stationary layer, which acts as a resistive barrier. Angilelli et al. (2015) evaluated the influence of the film coefficient in multicomponent diffusion during the dehydration of melon using a fructo-oligosaccharide (FOS) and sucrose solution, concluding that the presence of the film formed on the solution/solution solid interface influences the diffusion process.

When it comes to food biosolids diffusion on the surface as well as the formation of the film may be dependent on the geometry and the morphology of the same. In this sense some data analysis tools such as artificial neural networks (ANN) are necessary to better understand the effects of these factors during the process (Cremasco et al., 2016). The interesting thing about this tool is that the result can be observed through a topological map whose function is to facilitate the interpretation of results (Cremasco et al., 2016). This study aims at investigating the

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influence, formation and distribution of the film in multicomponent diffusion of NaCl and KCl during the brining process of quail eggs in a static and agitated brine system.

2 Materials and methods

2.1 Egg preparation and brining

Quail (*Coturnix coturnix japonica)* eggs were purchased from Yamada Horticultural Trade Ltda, based in Londrina-PR, Brazil. The static and agitated brines were prepared with a saline concentration of approximately 3% (m/v) according to Borsato et al. (2012), in which the quantity of salt was divided into portions of 30% potassium chloride (KCl) and 70% sodium chloride (NaCl). A pump with a 500 L/h circulation flow was used for agitation. A pump with a 500 L/h circulation flow was used for agitation.

2.2 Scanning Electron Microscopy (SEM)

The microstructures of egg whites cooked and after brining were observed under a field emission scanning electron microscope (SEM). The samples were immobilized by immersion in 1ml 2.5% glutaraldehyde and 2% paraformaldehyde in 0.1M sodium phosphate buffer (pH 7.0) for 1h and then post-fixed in 1% Osmium Tetroxide for 1h. The fixed material was dehydrated in an ethanol series (70, 80, 90 and 100%), and were dried to the critical point in CO_2 and coated with a 20-30 nm layer of gold. They were viewed under a FEI Quanta 200 scanning electron microscope, at an accelerating voltage of 30 kV.

2.3 Modeling and determination of film coefficient

The mathematical model used was based on a generalization of Fick's 2nd law and on Onsager equation (1945). The finite element formulation considering the simultaneous three-dimensional mass transfer of two solutes is described by Borsato et al. (2012) and Angilelli et al. (2015). Some simplifying assumptions were made according to Angilelli et al. (2015). The solute diffusion occurred in a three-dimensional volume $\Omega \subset R^3$ associated with a set of coordinates X, Y, Z, the hypothesis that the diffusion coefficient or diffusivity is constant over the concentration regardless of the position and the immersion time of the solid is accepted, the diffusion of the solvent, the solute was considered as the predominant process in the mobility and the process takes place under substantially isothermal conditions and the contraction of the sample during the procedure was negligible. The $C_1(x,y,z,t)$ and $C_2(x,y,z,t)$ concentrations of the NaCl and KCl solute, respectively, at the point $P(x,y,z) \in \Omega$ and the instant t can be described by the Onsager (1945) equations for the solute concentrations (Equation 1).

$$\frac{\partial C_1}{\partial t} = D_{11}\nabla^2 C_1 + D_{12}\nabla^2 C_2 \ \ and \ \frac{\partial C_2}{\partial t} = D_{21}\nabla^2 C_1 + D_{22}\nabla^2 C_2 \quad (1)$$

Where Dii are the main coefficients, Dij are the crossed that combine the flows and $\nabla^2(\cdot)=\nabla\cdot\nabla(\cdot)$, is the Laplacian operator. The initial conditions of the salting process are given by Equation 2.

$$C_1(x,\ y,\ z,\ 0) = C_{1,0} \ \ and \ \ C_2(x,\ y,\ z,\ 0) = C_{2,0}; \quad x,\ y,\ z\ \in \Omega \quad (2)$$

For the surface conditions at the diffusion process, the following Equation 3 was applied:

$$\frac{\partial C_1(\pm R,t)}{\partial n} = \frac{Bi}{a}\left[C_1 - C_{1,s}\right], \qquad R\epsilon\ \partial\Omega, t > 0$$
$$\frac{\partial C_2(\pm R,t)}{\partial n} = \frac{Bi}{a}\left[C_2 - C_{2,s}\right] \quad (3)$$

where $\partial\Omega$ is the set of points that describe a contour surface of the solid; $C_{1,s}$ and $C_{2,s}$ are the concentrations of solutes in direct contact with the surface of the egg; $\partial/\partial n$ is the normal derivative operator; a is the half width in the Z–axis; and B_i is the Biot number that expresses the mass ratio between the internal resistance and external resistance mass transfer. Knowing the diffusion coefficient (D_{ii}) value, the term h_m, which is the mass transfer coefficient of the solute in the film formed around the egg, can be determined from Equation 4 (Schwartzberg & Chao, 1982).

$$Bi = \frac{h_m.m.a}{D_{ii}} \quad (4)$$

2.4 Simulation by Finite Elements Method (FEM)

The simulation was performed using the COMSOL Multiphysics® software and the default physical interface "*Transport of Diluted Species (tds)*". The parameters used in the simulation were: main diffusion coefficients, crossed diffusion coefficients and mass Biot number, adjusted by Borsato et al. (2012). Figure 1 presents the solid automatically generated by the software with extremely fine mesh type. All simulations were performed with a 3D geometry modeling where the area was already subdivided into a tetrahedral finite element mesh comprised of 85,297 elements with 24,1104 degrees of freedom; the mean dimensions of the quail eggs used in the simulation and convention were adopted for the imaginary axis. The experimental data used are presented in Borsato et al. (2012).

2.5 Artificial Neural Networks (ANN)

The Kohonen Self-Organizing Map (SOM) algorithm starts by initializing the first grid with random synaptic weights and no organization being applied to the map. After initialization, there are three key processes: competition, cooperation and synaptic adaptation (Haykin, 2001). The function chosen to represent the topological neighborhood was Equation 5.

$$h_{j,i} = \exp(-d_{j,i}^2 / 2\sigma^2) \quad (5)$$

where σ is the effective radius of the topological neighborhood, and $d_{j,i}$ is the lateral distance between the winning neuron *i* and the excited neuron *j*.

Over the training epochs, there is a reduction in the size of the neighborhood due to an exponential decay (Equation 6).

$$\sigma(n) = \sigma_0 \exp(-n/\tau_1) \quad n = 0,\ 1\ ,\ 2,\ ... \quad (6)$$

where σ_0 is the effective radius in the initialization of the algorithm, τ_1 is the time constant, with $\tau_1 = 1{,}000/\log \sigma_0$ being recommended and *n* is the number of training epochs. During

the adaptive process, it is necessary to modify the synaptic weight vector (w_j) of the *j* neuron in the grid in relation to the input vector x. The modification process is a modification of the Hebb postulate of learning, described by Equation 7.

$$w_j(n+1) = w_j(n) + \eta(n) h_{j,i(x)} \left(x - w_{j(n)}\right) \quad (7)$$

where $\eta(n)$ is the learning rate, which, as shown, is variable and decreases during the training epochs, *n*. The learning rate decrease may be modelled by an exponential decay, as described in Equation 8. In this equation, η_0 is the initial learning rate and τ_2 is another time constant; the recommended values are respectively 0.2 and 1,000:

$$\eta(n) = \eta_0 \exp(-n/\tau_2) \quad (8)$$

The SOM applied to each ion in each isolated system consists of a 3×3 hexagonal topology with 7,000 training epochs. The initial neighborhood relationship was 1.0, with an initial learning rate of 0.2, decaying exponentially with the training epochs to 1.8238×10^{-4} (Haykin, 2001; Cremasco et al., 2016).

2.6 Computer processing and program

The COMSOL Multiphysics® version 5.2 (COMSOL, Inc., Burlington, MA) software packaged based on the FEM was used to simulate the influence of the formed film during the multicomponent diffusion of NaCl and KCl in different systems. The neural network routine developed was used according to the algorithm described in Haykin (2001), and was processed by the Matlab® R2010a software.

3 Results and discussion

The parameters optimized by the super-modified simplex method for the diffusion process during the brining by immersion of quail eggs are presented in Table 1. The main and cross coefficients and the Biot number were used to determine the influence of the diffusion coefficient of the film formed on the egg surface during the brining under agitated and static system. The simulations were performed at the following times: 0, 0.001, 0.01, 0.02, 0.05, 0.1, 0.25, 0.5, 1.0, 2.5, 5.0, 7.5, 10, 15, 20, 25, 30, 50, 70, 90, 120, 150 and 200 hours.

Regarding agitated and static systems, there was no difference in the values of main and cross coefficients, which indicates how much the flow of one solute interferes with the flow of the other. With respect to Na^+ and K^+ ions, it could be observed that the lower main and cross coefficient values have been assigned to K^+. However, the difference between the cross coefficients was small, indicating that diffusion, in relation to its own gradient, was more important than the interference of a solute in the flow of another solute.

The main K^+ diffusion coefficient is approximately 7-fold lower when compared to Na^+, which contradicts the literature (Schwartzberg & Chao, 1982). The diffusion coefficient is related to ion mobility in solution and, according to Lee (1996), in an

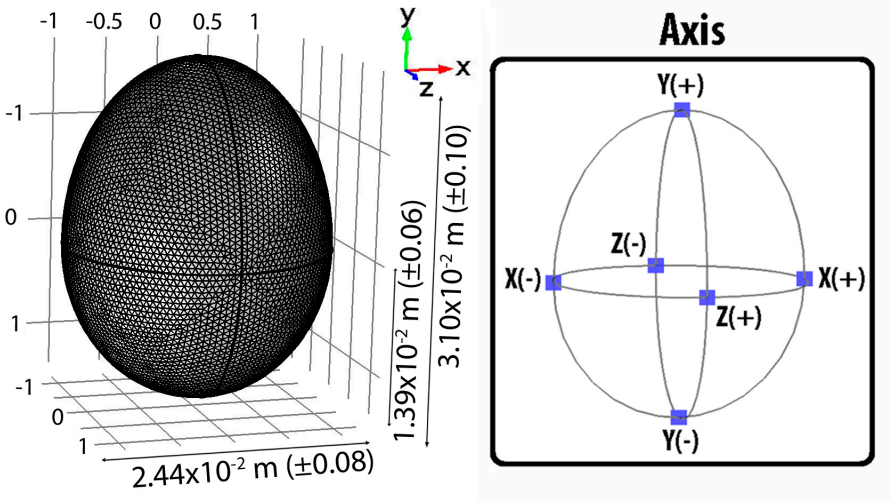

Figure 1. Dimensions and guidelines of the quail eggs used in the simulation.

Table 1. Adjusted values for main and crossed diffusion coefficients, mass Biot number and film coefficient(h_m).

	Static brine		Agitated brine	
	Na^+	K^+	Na^+	K^+
Main coefficients (m^2/s)	8.047×10^{-10}	1.185×10^{-10}	8.047×10^{-10}	1.185×10^{-10}
Crossed coefficients (m^2/s)	5.787×10^{-11}	5.752×10^{-11}	5.787×10^{-11}	5.752×10^{-11}
Mass Biot number	46.61	46.61	167.99	167.99
h_m (m/s)	3.07×10^{-6}	4.53×10^{-7}	1.11×10^{-5}	1.63×10^{-6}

Adapted from Borsato et al. (2012).

aqueous medium, the mobility of K^+ is higher than that of Na^+ because, being a larger ion, K^+ has lower charge density and, thus, provides less attraction over water molecules when compared to Na^+ and consequently, has a lower hydration layer, facilitating their motion in solution. In food, water can be linked to protein (hydration water) or it can be free. The hydration water is linked by hydrogen bonds and hydrophilic groups. Free water is immobilized in the three-dimensional network of protein strands, joined by cross-linking and electrostatic attraction (Sgarbieri, 1996). Ion diffusion takes place in the same occluded water, therefore, the ratio of sodium and potassium diffusion should be similar to that observed in aqueous solution.

The greater diffusion coefficient of Na^+ in relation to K^+ in this experiment can be attributed to the high percentage of egg protein (being mainly composed of three proteins, namely, ovalbumin, ovotransferrin, and ovomucoid), which has high water affinity (Hashiba et al., 2008). Introducing Na^+ in a higher hydration layer, it enters the solid from the biosolids/solution interface, which can be facilitated by the attraction between the ion hydration layer and the egg protein.

One possible theory suggests that the transfer resistance in each phase is set in a film along the surface interface (Coulson & Richardson, 1965). According to Bona et al. (2007), the influence of the film can be measured by the mass Biot number. If this value is above 100, the diffusion process is limited by internal mass transfer. According to Table 1, the optimized Biot values for static and agitated systems were 46.61 and 167.99, respectively. Another parameter to be evaluated is the film coefficient (h_m). The h_m values presented in Table 1 for the agitated system were approximately 10-fold higher when compared to the static system for both ions, indicating less influence on the film diffusion. In both systems, Na^+ also presents h_m values approximately 10-fold higher when compared to K^+, therefore, it has greater diffusion facility on film.

The influence of the film formed during the diffusion process can be analyzed by also analyzing the solute concentration data regarding biosolid radius at different times. In Figure 2,

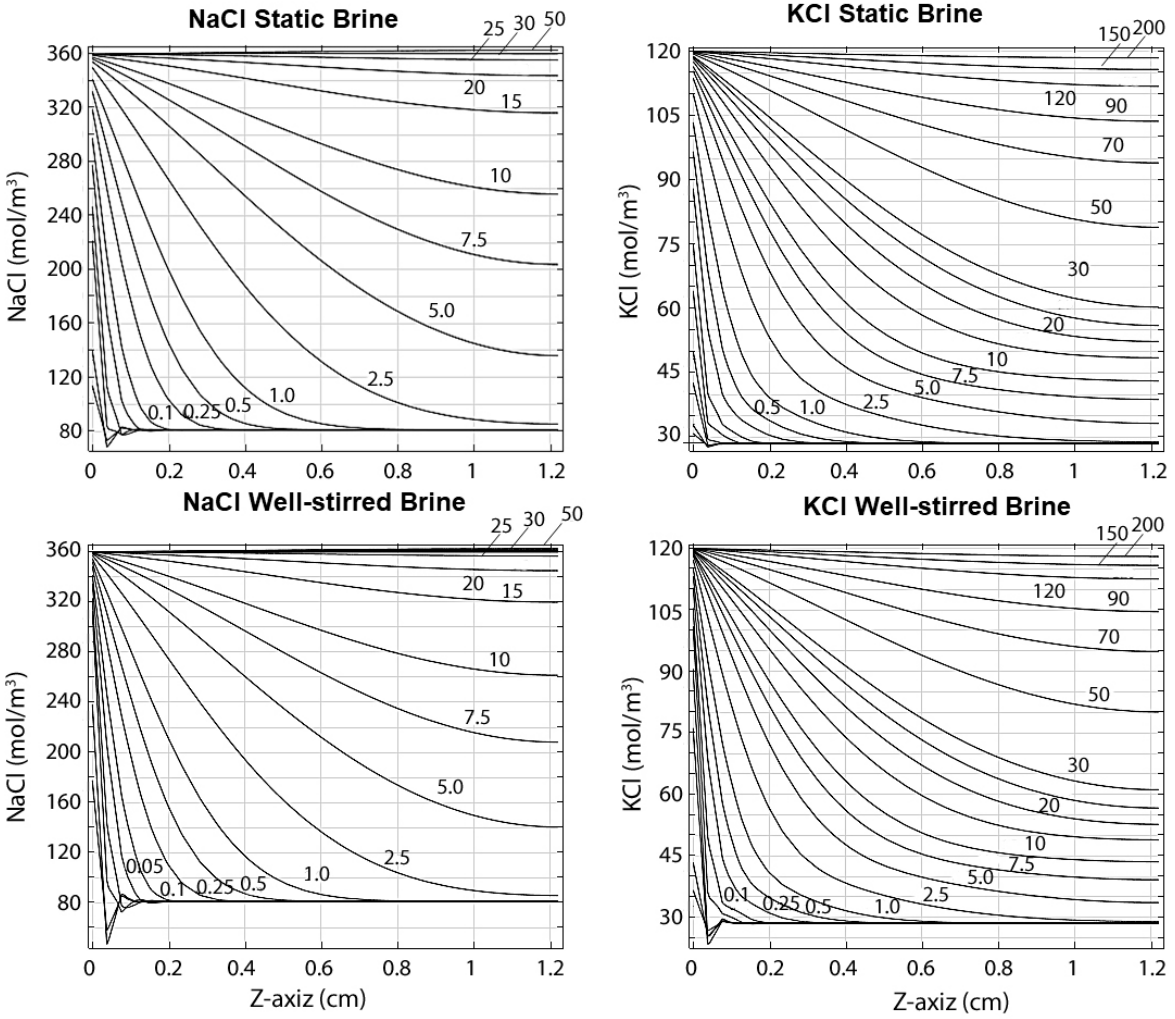

Figure 2. Distribution profile of concentration during 200 h in simulating of multicomponent diffusion process on radius in Z(-) axis (10^{-2} m) in quail eggs.

the graphs show the diffusion profile of Na^+ and K^+ where the distance 0 represents the surface at point Z(-) (Figure 1) and 1.2 cm is the center of the biosolid.

The initial concentration of Na^+ and K^+ in quail eggs was 81.0 and 28.6 mol/m^3, respectively, so it is not possible for any part of the solid that the concentration of these salts may be lower than the time 0 h. Lower values than the initial ones are seen in Figure 2, and this can be caused by oscillation due to the limitation of the method but this oscillation does not compromise the analysis of the influence of the film.

The concentrations of Na^+ and K^+ in the brines used were 360 and 120 mol/m^3, respectively; these concentrations would be expected for the egg surface immediately after immersion if there were no influence of the film. According to Figure 2, there is clear evidence that the film influences the diffusion process in both systems. For example, in agitated brine at time 0.001 h on the egg surface, the concentration of these salts were 238.29 mol/m^3 for Na^+ and 43.35 mol/m^3 for K^+ while at the same time, in the static system, the concentrations were 139.80 and 32.83 mol/m^3, respectively. The same behavior is observed for other times. At 0.5 hour, for instance, the concentrations of Na^+ and K^+ in agitated system were 352.23 and 113.22 mol/m^3, and in static system, they were 332.17 and 96.62 mol/m^3, respectively. The estimated time for each ion in each system, wherein the concentration of the surface comes into equilibrium with the brine, are shown in Table 2. The existence of the film is verified due to the time spent for the concentration of ions on the egg surface to come into equilibrium with the brine. Otherwise, the equilibrium would be reached almost immediately upon the immersion of the biosolid into the brine. Table 2 also shows the percentage of ion concentrations in relation to the brine value at random times of the simulation.

It can be seen that, for both ions, the film influence is more pronounced in the static system, since the percentages of the species concentration are lower than those for the agitated system. According to Coulson & Richardson (1965), the film can be interpreted as a physical barrier, which does not accumulate any substance, and the h_m value depends on the concentration gradient of the species and the thickness of the film. The film thickness varies with the degree of disturbance - the faster the agitation of the system, the smaller the film thickness and the higher the diffusivity. This agitation also favors the collision of ions with the film, promoting the diffusion.

Comparing the ions in the same system, a greater influence of the film can be observed always for K^+. It is known that the hydrated sodium radius is larger than the hydrated potassium radius (Lee, 1996). However, considering the film as a physical barrier, it does not behave like an aqueous medium, and therefore, it does not present a hydration layer during the passage of the ions in the film. Although the ionic radius size is not the only factor, it is nonetheless quite important. Potassium has a larger ionic radius when compared to Na^+, with ionic radius values of 137×10^{-12} m and 99×10^{-12} m (Lee, 1996), respectively, and thus, it is more difficult to cross the film.

According to Table 2, at 0.5 h in the agitated system, the concentration of both ions on the surface were of more than 94% of the solution concentration; and in static system, the percentage was 92% for Na^+ and 81% for K^+. The time required for the Na^+ and K^+ ions to reach the solution/surface equilibrium were 15 and 25 hours (agitated system) and 20 and 70 h (static system), respectively. This time interval between 0.5 hour, already has a high concentration, and the equilibrium time is due to the dependence of the mass transfer rate in relation to the concentration gradients. As the concentration of the surface approaches to the values of the solution, the gradient decreases, and diffusion becomes slower. Figures 3a and 3b show 3D images of the multicomponent diffusion on the biosolid surface at different times (0-200 h) in the simulation for ions (Na^+ and K^+) in the static system.

Figures 3a and 3b suggest that there may be variation in the film influences in the diffusion process with the biosolid surface region, which can be observed by the color scale indicating different ion concentrations on the surface throughout the discretized geometric domain. From the time 0.05 h for Na^+ (Figure 3a) and 0.25 h for K^+ (Figure 3b), there is the formation of a region of higher concentration of ions around the poles of the Y (±) axis (Figure 1). This behavior can be more noticeable in the 0.5-15 h interval times for Na^+ and 1.0-15 h for K^+, where the poles are more evident. This same interpretation can be applied to the agitated system.

The color legend does not show much difference between the concentration values. However, it is not possible to estimate the size of this difference based only on observations. Thus, there is the need for further detailed study on the behavior of the biophysical process with the application of SOM-type ANN, based on not very conventional statistical principles (Haykin, 2001; Cremasco et al., 2016).

The ion concentration values at the axis points X(±), Y(±) and Z(±) indicated in Figure 1 and the total concentration on the egg surface for all simulated times were presented to the SOM network for diffusion analysis of both systems. The distribution map (Figure 4) presents the classification of the axes and the total surface for the concentration for each ion and independent system. The SOM network classifies the input data as clusters, which can be formed by one or more neurons (Cremasco et al., 2016). The definition of the groups is characterized by the presence of empty neurons among the clusters. Therefore, it can be concluded that the network was able to identify differences in the diffusion process at different points on the biosolid for both systems, with the formation of 3 different groups for all cases.

Table 2. Percentage concentrations of ions in the surface of the species in relations to the expected values.

	Agitated brine		Static brine	
	Na^+	K^+	Na^+	K^+
Brine (mol/m^3)	360	120	360	120
0.001 h	86%	48%	51%	30%
0.5 h	98%	95%	93%	81%
100%*	15 h	25 h	20 h	70 h

*Time for the ions concentration on the surface and in solution come into equilibrium.

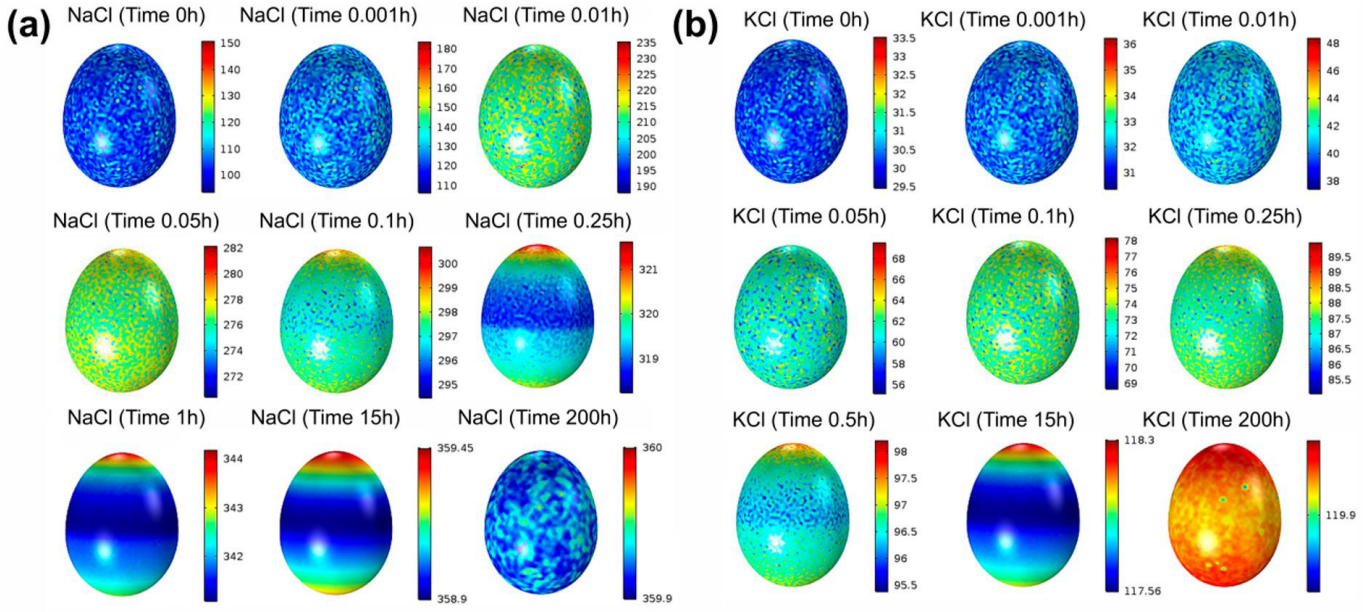

Figure 3. 3D – Concentration distribution field of Na^+ (a) and K^+ (b) in mol/m^3 in biosolid surface for the static system at different time intervals.

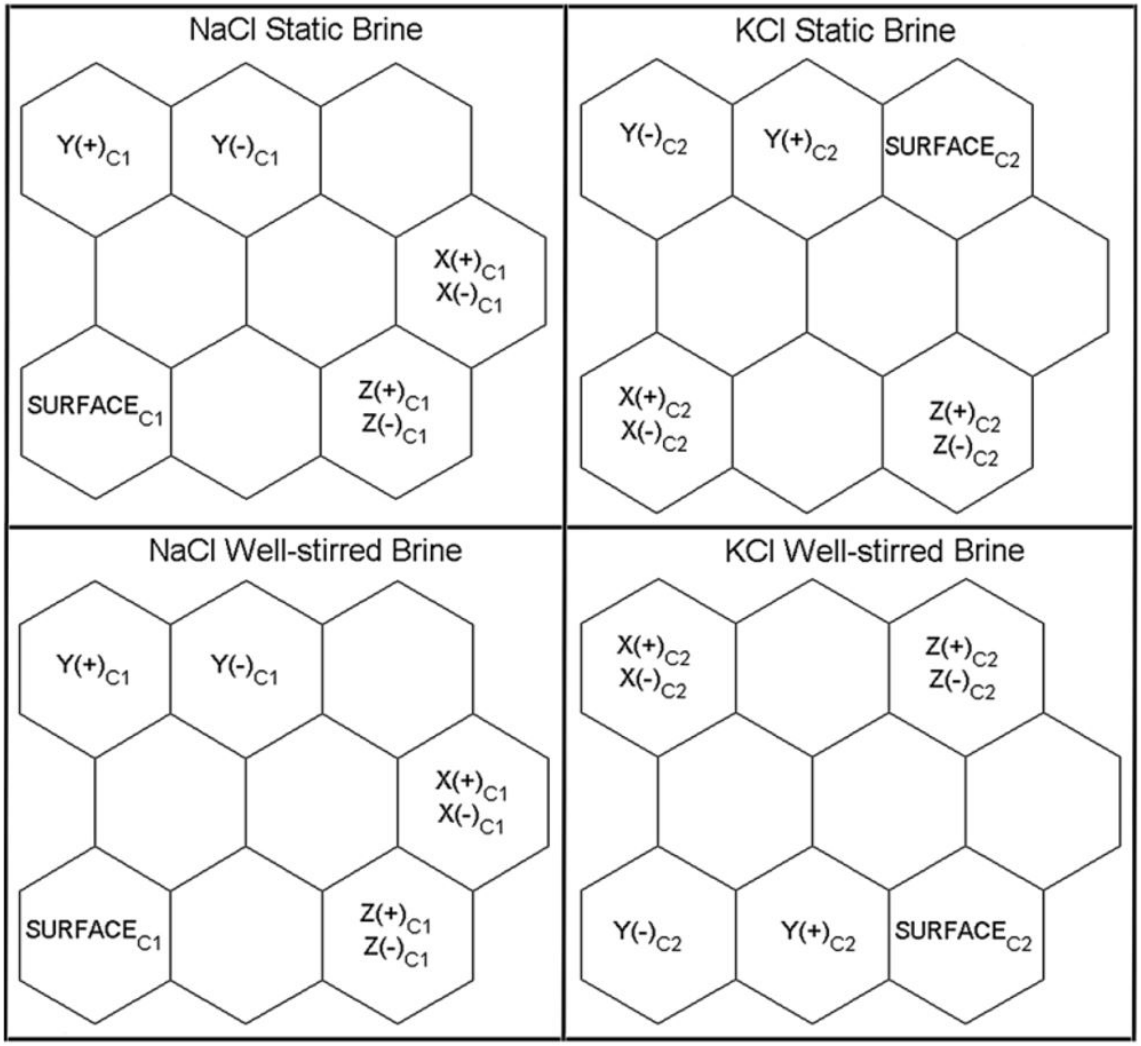

Figure 4. Axis distribution according to the winning neuron for each individual ion and system. **(C1)** – Na^+ and **(C2)** – K^+.

The network indicates that different systems for the same ion presented the same clusters and the same neighborhood relations. Therefore, despite the influence of the film being different in different systems, they have the same tendency regarding the position on the solid. The analysis of the distribution of data regarding the position of neurons can be interpreted in accordance with the distance. As the distance increases, the lower the neighborhood relationship, thus decreasing the similarity between them. For both ions, no difference was observed between the points on the X-axis (±) because they were classified in the same neuron; the same is also valid for the points in the Z-axis (±).

For K^+, the (±) points at the X and Y axes are not part of the same cluster because there is an empty neuron between each axis group, indicating that they are different. In the case of Na^+, the (±) points at the X and Y axes belong to the same cluster since they belong to nearby neurons, and thus, despite having a small difference, such difference is lower than that observed for K^+. For Na^+, the surface forms an independent cluster and the (±) points in the Y axis are also classified into neighbor neurons, thus, despite being part of the same group, there is a difference between their extremities. For K^+, the interpretation for this axis is similar, differing only in that the surface is part of this group.

The main information obtained from the network, and that reinforces the conclusions suggested by the 3D simulation images obtained, is that there is difference in the diffusion of ions in the Y(±) axis in relation to the other axes and between the poles (±) of this axis. Figures 5a and 5b present the weight maps at the different times evaluated in the (FEM) simulation for the Na^+ and K^+ ions in the static system. It is possible to identify that there are differences on the ion concentration values in relation to the diffusion time in different points of the biosolid. It is important to note that the values of surface concentrations were higher than the other points and axes, followed by the values of the Y(+) axis, then by Y(-), regardless of ions or system. The same interpretation can be made for the agitated system.

As mentioned, the film acts as a variable physical barrier, the thinner it is, the easier it is for diffusion to occur. Thus, the results suggest that the thickness of the film formed on the Y(+) axis is lower than in the other axes. This phenomenon may be related to the geometry of biosolids.

Due to the factors presented, there is the need of a better understanding of the egg surface morphology, which can be observed by the SEM analysis on the egg surface after it has been cooked and after brining (Figure 6).

In the micrographs in Figure 6, it can be observed that the surfaces of both samples are irregular, with structural organization due to the joining of several interconnected globular proteins, which form filaments with defined directions, overlapped in different planes, forming a tridimensional network (Sgarbieri, 1996). These irregularities favor the formation of the film on interfaces with rough surfaces. This would explain why the use of stirring in the brine was not able to completely extinguish the influence of the film, just minimizing its interference in the diffusion.

According to the SEM analysis, there was a morphological change in the surface of the egg subjected to brining, since its roughness is more pronounced. The probable cause of this morphological change is associated with the entry of salts in the biosolid. The interactions between the salts and the protein molecules during diffusion may be causing their rearrangement, since the main difference is between the arrangement of the planes between the filaments in relation to the egg that has only been boiled.

The heterogeneity of Na^+ diffusion observed in the simulation can be attributed to its higher affinity for egg protein, due to its greater hydration layer. According to Hashiba et al. (2008), after cooking, the pores of the protein matrix (surface) are filled with water, which increases the diffusivity. However, since the surface presents some porosity and tortuosity, the diffusion process may suffer inferences. Such heterogeneity is found in all food products rich in protein, although different according to the matrix used (Hashiba et al., 2008).

Further studies are necessary on how salts interacts with protein during the diffusion process, orientation and arrangement

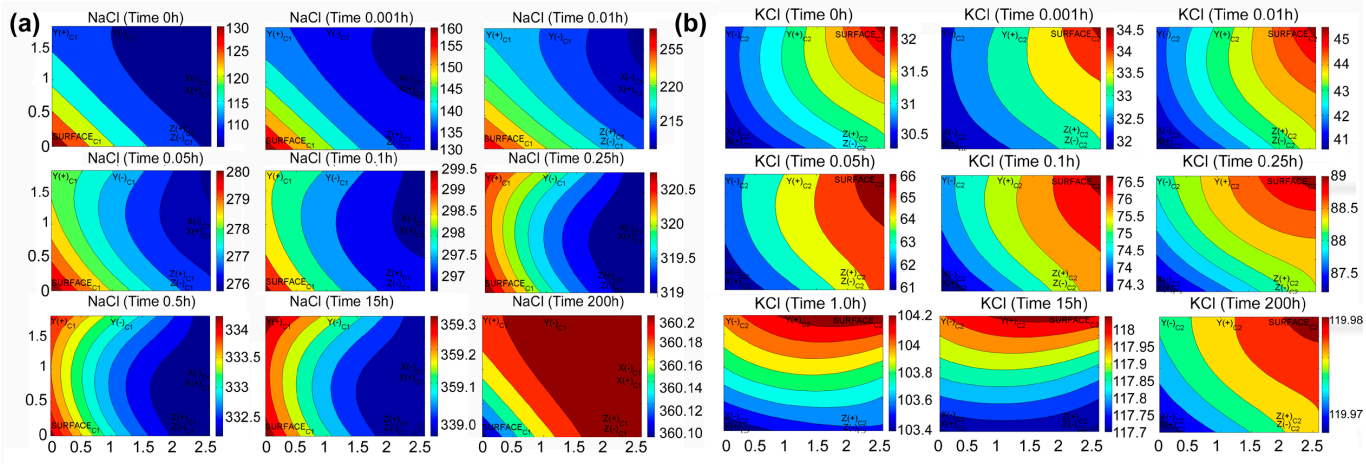

Figure 5. Weight map of the variable Na^+ (a) and K^+ (b) in mol/m^3 for the static system.

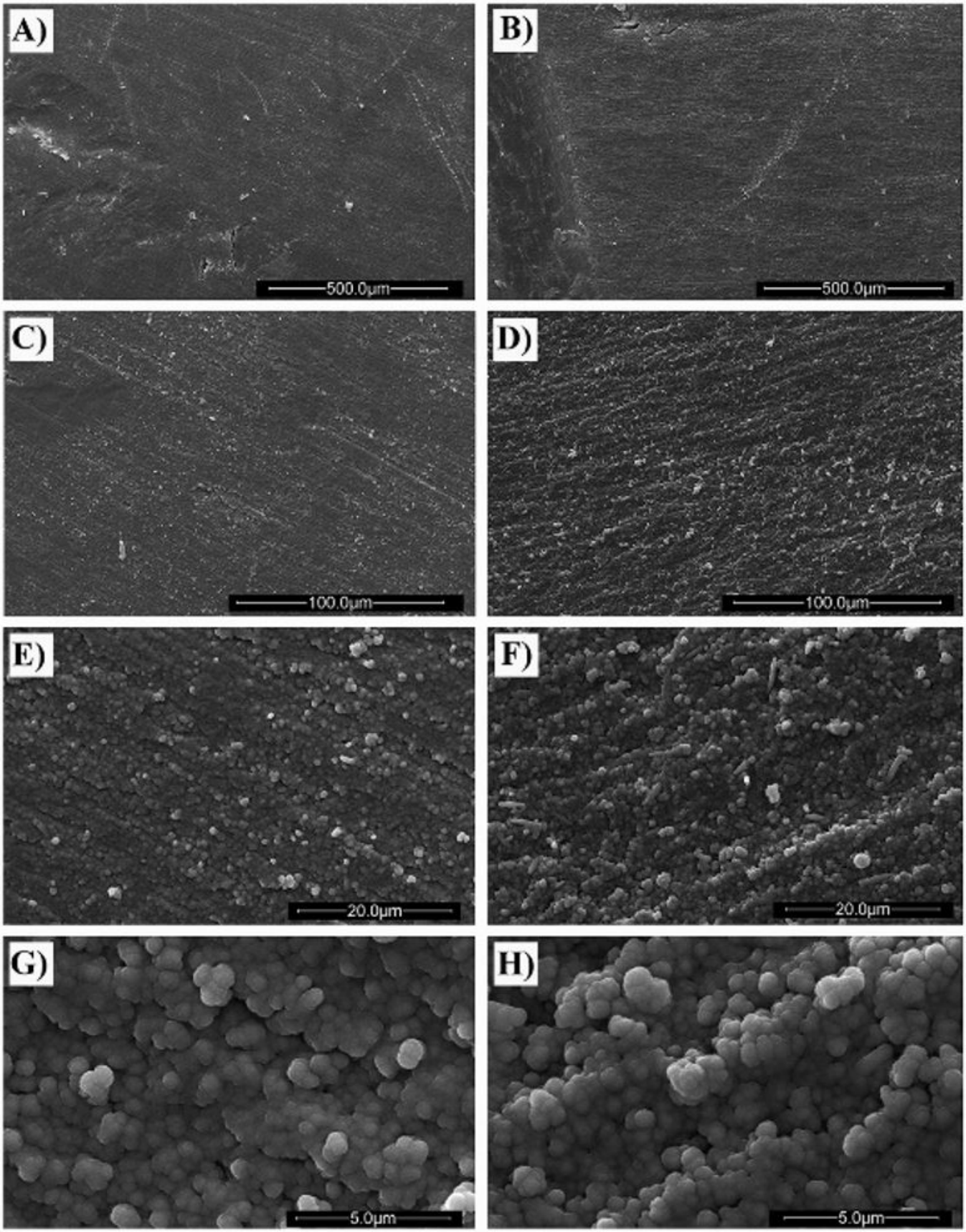

Figure 6. SEM micrographs of the boiled egg surface before brining (A, C, E and G) and after a 200-hours immersion in brine (B, D, F and H). Scale bar: 500.0 x10^{-6} m (140×), 100.0 x10^{-6} m (800×), 20.0 x10^{-6} m (3,000×) and 5.0 x10^{-6} m (12,000×).

of protein filaments along the curvature of the matrix surface, which may be associated with the fact that the diffusion depends on the position on the surface. It is also necessary to investigate if the rugosity provided by these filaments can be distorted at the egg edges and its influence regarding the formation, adhesion and stability of the film in relation to the arrangement of these filaments.

4 Conclusions

The diffusion process is difficult due to the influence of a film formed in biosolid/solution interface, which varies according to the type of system used, the ions and the biosolid geometry. The film interfered more strongly in the diffusion of both ions in the static system as expected since perturbations make it difficult to form. Through the agitation it was possible to increase the value of the film coefficient and, with it, decrease the external resistance facilitating the entrance of the ions on the surface of the quail egg. The influence of the film between the ions for the same system was higher for the sodium ion. The values of film coefficients of Na^+ and K^+ were 3.07×10^{-6} and 4.53×10^{-7} m/s respectively for the static brine and 1.11×10^{-5} and 1.63×10^{-6} m/s for the agitated brine. The FEM simulation combined with SOM-type ANN was an effective tool to evaluate this behavior, having proven that this complex and often disregarded in mass transfer studies in food biophysical complex is heterogeneously formed on the surface and influences the diffusion time. This indicates that diffusivity is not constant and independent of the solid position, such condition being assumed in most simulations involving mass transfer in foods, enabling an improvement in productivity and better control of process quality.

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