Numerical Solution of the Equations of Salt Diffusion into the Potato Tissues

Behrouz Mosayebi Dehkordi, Frazaneh Hashemi, and Ramin Mostafazadeh

Abstract—Fick's second law equations for unsteady state diffusion of salt into the potato tissues were solved numerically. The set of equations resulted from implicit modeling were solved using Thomas method to find the salt concentration profiles in solid phase. The needed effective diffusivity and equilibrium distribution coefficient were determined experimentally. Cylindrical samples of potato were infused with aqueous NaCl solutions of 1-3% concentrations, and variations in salt concentrations of brine were determined over time. Solute concentrations profiles of samples were determined by measuring salt uptake of potato slices. For the studied conditions, equilibrium distribution coefficients were found to be dependent on salt concentrations, whereas the effective diffusivity was slightly affected by brine concentration.

Keywords—Brine, Diffusion, Diffusivity, Modeling, Potato

I. INTRODUCTION

There are two important solid-liquid diffusion processes utilized in the food industry. Leaching, the transfer of solutes from a solid to an adjacent liquid is used to extract sugar, vegetable oils, tea, gelatin, pectin and other food solutes. Garrote et al. [1] examined a two stage soaking process with water as the solvent to leach glucose from the potato slices at various temperatures. Some mathematical models to simulate the leaching of potato have been reported, such as glucose leaching [2,3], potassium and magnesium leaching [3], and nutrient loss [4].

Infusion, the transfer of solutes from a liquid into a solid is also an important food processing operation which is used to transfer colors, flavors and curing and conditioning agents into foods. Smoking, salting, and the addition of certain additives (e.g., sodium nitrite for sausage) are diffusion applications that play important roles in meat processing. Infusion of salt into meat was investigated by Wistreich et al. [5,6] who first tried to simulate a one-dimensional infusion process by constructing an empirical equation which included the effects of solution concentration, soaking time and volume. In Stahl and Loncin study [7], potato samples were infused in 0.5-1% Cyclohexanol solutions. The diffusion coefficients and solute concentrations profiles of samples were determined by measuring the Cyclohexanol uptake of potato samples. Wang and Sastry [8] found an analytical model for concentration profiles to be in good agreement with experimental results.

The objectives of this research were: a) to determine the equilibrium distribution coefficient (m) and diffusivity (D_s) of salt (sodium chloride) in potato tissue in an infusion process and b) to develop a numerical solution for the two-dimensional diffusion equation.

II. MATERIALS AND METHODS

Fresh, peeled white potato samples were selected and used for the experiments. Cylindrical potato pieces with 3.5 cm length and 3 cm diameter were cut and soaked in beakers containing 200 ml of 1%, 2%, and 3% (w/v) brine. Lateral surfaces of the cylinders were sealed properly to ensure one-dimensional diffusion. The beakers were covered with parafilm to avoid vaporization. The temperature controlled at 24 °C for all experiments. Electrical conductivity of each brine sample was measured using "Cryson" liquid conductivity meter every 15 minutes. Three replications for each experiment were carried out and the mean values of results were used for calculations.

Solute concentration profiles of potato samples at equilibrium were determined by cutting the samples into slices and measuring salt uptakes.

In the following calculations X and Y denote to solid and liquid solute concentrations and F and L denote to solid and liquid volumes respectively.

A. Determination of equilibrium distribution coefficient (m)

During the diffusion process, solute transfers from brine to solid until the system reaches to equilibrium. The solute concentration of solid at equilibrium can be calculated from:

\[ X_e = \frac{(Y_0 - Y_s) L}{F} \]

in which \( Y_0 \) and \( Y_s \) are initial and equilibrium concentrations of solute in brine.

The equilibrium equation will be \( Y_e = mX_e \) instead of \( Y_e = X_e \) [7], which results in calculating \( m \):

\[ m = \frac{Y_e}{X_e} \]

(2)
B. Determination of diffusion coefficient \((D_s)\)
The diffusion phenomenon for cylindrical geometry is given by Fick's second law [9]:

\[
\frac{\partial c}{\partial t} = D_s \left( \frac{\partial^2 c}{\partial r^2} + \frac{1}{r} \frac{\partial c}{\partial r} \right) \tag{3}
\]

And for slab geometry will be reduced to:

\[
\frac{\partial c}{\partial t} = D_s \frac{\partial^2 c}{\partial x^2} \tag{4}
\]

Where \(x = 0\) at the center and \(x = \pm L\) at the surfaces. The initial condition is:

\[
at t = 0\; \text{for all} \; x
\]

Crank [9] gave a general solution for (2) considering the boundary condition of:

\[
at x = 0\; \text{for all} \; t
\]

\[
at x = \pm L \; \text{and} \; X = X_e; \text{ for all} \; t
\]

Crank solution is as follows:

\[
\begin{align*}
Y-Y_e &= \sum_{n=1}^{\infty} \frac{2\alpha(1+\alpha)}{1+\alpha+\alpha^2} q_n^2 D_s t \exp(\frac{-q_n^2 D_s r^2}{l^2}) \tag{5} \\
X-X_e &= \sum_{n=1}^{\infty} \frac{2(1+\alpha)}{1+\alpha+\alpha^2} \cos(q笋 x/L) \exp(\frac{-q_n^2 D_s r^2}{l^2}) \tag{6}
\end{align*}
\]

In which \(\alpha\) is the effective volume ratio, \((\alpha = mL/F)\) and \(q_n\) is a constant calculated from the roots of \(\tan(q_n) = -\alpha q_n\). A solution for this equation has been given by Crank:

\[
\begin{align*}
q_1 &= 1.57141 + \left[0.8535\exp(-\frac{\alpha}{0.3112}) + 0.5484\exp(-\frac{\alpha}{1.416}) \right] \\
&+ [0.1656\exp(-\frac{\alpha}{9.726})] \tag{7} \\
q_2 &= 4.68453 + \left[0.9929\exp(-\frac{\alpha}{0.1612}) + 0.4868\exp(-\frac{\alpha}{0.7189}) \right] \\
&+ [0.1187\exp(-\frac{\alpha}{10.52})] \tag{8} \\
q_3 &= 7.86682 + \left[0.9542\exp(-\frac{\alpha}{0.1014}) + 0.4707\exp(-\frac{\alpha}{0.3646}) \right] \\
&+ [0.1331\exp(-\frac{\alpha}{2.0025})] \tag{9} \\
q_4 &= 11.0035 + \left[1.094\exp(-\frac{\alpha}{0.08243}) + 0.3908\exp(-\frac{\alpha}{0.3832}) \right] \\
&+ [0.07801\exp(-\frac{\alpha}{2.746})] \tag{10} \\
q_5 &= 14.13436 + \left[1.017\exp(-\frac{\alpha}{0.06799}) + 0.3579\exp(-\frac{\alpha}{0.3342}) \right] \\
&+ [0.06891\exp(-\frac{\alpha}{2.212})] \tag{11} \\
q_6 &= 17.2858 + \left[1.087\exp(-\frac{\alpha}{0.5424}) + 0.3886\exp(-\frac{\alpha}{0.2308}) \right] \\
&+ [0.08849\exp(-\frac{\alpha}{1.478})] \tag{12}
\end{align*}
\]

The \(q_n\) can be then calculated from:

\[
q_n = \sum_{i=1}^{n} \frac{q_i}{n} \tag{13}
\]

A plot of the logarithm of \([Y-Y_e]/(Y_r-Y_e)\] against \(t\) should yield a straight line and the slope is \(-q_n^2 D_s / 2.303 t^2\) in which \(D_s\) can be calculated.

C. Solute concentration profile in potato samples using numerical analysis:

In order to determine the salt concentration profiles in potato tissues the relevant governing partial differential equations were solved by implicit method applying the following boundary conditions:

One-dimensional unsteady state diffusion in \(r\) direction:

\[
\frac{\partial c}{\partial t} = D_s \left( \frac{1}{r} \frac{\partial}{\partial r} \left( \frac{\partial c}{\partial r} \right) \right) \tag{14}
\]

at \(t = 0\) : \(X = 0\) ; for all \(r\)

at \(r = 0\) : \(\frac{\partial c}{\partial r} = 0\) ; for all \(t\)

at \(r = R\) : \(X = X_e\) ; for all \(t\)

Two-dimensional unsteady state diffusion in \(x\) and \(r\) directions:

\[
\frac{\partial c}{\partial t} = D_s \left( \frac{\partial^2 c}{\partial x^2} + \frac{1}{r} \frac{\partial c}{\partial r} \right) \tag{3}
\]

at \(t = 0\) : \(X = 0\) ; for all \(x\) and \(r\)

at \(x = 0\) : \(\frac{\partial c}{\partial x} = 0\) ; for all \(t\) and \(r\)

at \(x = \pm L\) : \(X = X_e\) ; for all \(t\)

at \(r = 0\) : \(\frac{\partial c}{\partial r} = 0\) ; for all \(t\) and \(x\)

at \(r = R\) : \(X = X_e\) ; for all \(t\) and \(x\)

The created set of equations was solved using Tomas method [10].

III. Results

For the all experiments no meaningful changes in brine concentrations were observed during first 30 minutes of contact between brine and solid.

A. Solute equilibrium distribution coefficient \((m)\)

TABLE I contains values of the equilibrium distribution coefficient \(m\) and the equilibrium concentrations. It can be denoted that \(m\) decreases when the salt concentration of brine \((Y_e)\) increases, however, the relationship was not linear. Two important parameters \(\alpha\) and \(q_n\), can be determined from the results of \(m\). The effective volume ratio \((\alpha)\), can be calculated by its definition \(\alpha = mL/F\), and \(q_n\), can be determined from equations (7) to (13). Both parameters are required for calculating \(D_s\).
TABLE I

<table>
<thead>
<tr>
<th>Y₀ (%)</th>
<th>Y₁₀⁻⁻</th>
<th>X₁₀⁻⁻</th>
<th>m</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.01</td>
<td>0.0081</td>
<td>0.0076</td>
<td>1.06</td>
</tr>
<tr>
<td>0.02</td>
<td>0.0188</td>
<td>0.0097</td>
<td>1.93</td>
</tr>
<tr>
<td>0.03</td>
<td>0.0277</td>
<td>0.0185</td>
<td>1.49</td>
</tr>
</tbody>
</table>

**B. Diffusion coefficient in sample (Dₛ)**

Values of $Dₛ$ were determined from the slopes of plots of

$$\log \left( \frac{Y - Y_0}{Y_0 - Y_∞} \right)$$

against $t$, for brine initial concentrations ($Y_0$) of 1%, 2% and 3%. Since the regression-based slopes were equal to $-\frac{q^2Dₛ}{2.303\tau}$, $Dₛ$ could be determined. The calculated $Dₛ$ values are tabulated in TABLE II.

**TABLE II**

VALUES OF MEASURED SALT DIFFUSIVITIES INTO THE POTATO TISSUES

<table>
<thead>
<tr>
<th>Y₀ (%)</th>
<th>$Dₛ$ (m²/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>3.45</td>
</tr>
<tr>
<td>2</td>
<td>4.39</td>
</tr>
<tr>
<td>3</td>
<td>4.33</td>
</tr>
</tbody>
</table>

**C. Model Verification**

For one-dimensional diffusion, the equilibrium salt concentrations were determined by cutting the potato samples into equal slices and measuring the salt uptake of each slice. TABLE III compares these concentrations which are in good agreement.

**TABLE III**

CALCULATED AND MEASURED SALT CONCENTRATIONS IN THE POTATO

<table>
<thead>
<tr>
<th>r (mm)</th>
<th>Calculated $X \times 10^{-3}$</th>
<th>Measured $X \times 10^{-3}$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$Y₀=10$</td>
<td>$Y₀=20$</td>
</tr>
<tr>
<td>0</td>
<td>5</td>
<td>12.40</td>
</tr>
<tr>
<td>5</td>
<td>5.51</td>
<td>13.22</td>
</tr>
<tr>
<td>10</td>
<td>7.43</td>
<td>15.95</td>
</tr>
<tr>
<td>15</td>
<td>9.52</td>
<td>19.32</td>
</tr>
</tbody>
</table>

**D. Salt distribution in the potato tissue – diffusion in r direction:**

Fig. 1 to 3 represent the salt distribution in the potato tissues after 300 minutes immersing in 1%, 2% and 3% brines. The salt diffusion is considered only in r direction.

**E. Salt distribution in the potato tissue – diffusion in x and r directions:**

Fig. 5 to 7 represent salt concentration profiles in the potato tissues after 300 minutes immersing in 1%, 2% and 3% brines.
IV. DISCUSSION

Determination of diffusivity is recognized as one of the initial steps in investigating of diffusion dependent phenomena. The needed effective diffusivity for modeling the salt diffusion into the potato tissues was determined experimentally. A summary of the results are as follows:

- At the initial contact of brine and potato it takes 30 minutes for salt species to start diffusing.
- For the studied conditions, equilibrium distribution coefficients \((m)\) were found to be dependent on salt concentrations, whereas the effective diffusivity was slightly affected by brine concentration.
- The equilibrium distribution coefficient decreases when the salt concentration of brine \((Y_\infty)\) increases; however, the relationship is not linear.
- Diffusion coefficient of salt in potato tissue was measured to be \((3.45-4.39) \times 10^{-9} \text{ m}^2/\text{s}\).
- Crank solutions represented for Fick's low equations in mass transfer gives precise and satisfactory explanation for the diffusion of salt into potato tissues.

REFERENCES