A Grey Wolf Optimizer-based Fractional Calculus in Studies on Solar Drying

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Abstract

In this novel article, a comparative study has been conducted between analytical and fractional solution of Fick’s first- and second-order of diffusion to model the solar drying process of different products and dryers under different operating parameters. Laplace and Laplace’s inverse transform have been used to obtain the solution in function with two parameters: the order index \( n \) and the fractional time index \( \alpha \) of the above Fick’s laws, and their parameters have been non-linearly optimised using a grey wolf optimisation (GWO) algorithm. The results showed that the anomalous diffusion phenomenon during the drying process is best described by the fractional-order model. Values obtained using the model MR12 were in better agreement with the experimental data than the values obtained using the other selected models with very acceptable statistical parameters.

Keywords

Fractional calculus, solar drying, modelling, Grey Wolf Optimizer, moisture ratio

1 Introduction

The drying process of wet agricultural products is the oldest and most important process for preservation of their original characteristics to be stored for a longer period.\(^1\)\(^,\)\(^2\) When moisture content increases in food products, the activity of microorganisms and biochemical reactions increase and cause irreversible damage to the product.\(^3\)

During the drying process, two phenomena occur concurrently: transfer of heat energy to the product via conduction, convection, and radiation transfer, and movement of internal moisture to the surface of the product where it is evaporated by appropriate hot air.\(^4\)

Due to several limitations of the mathematical models for describing the drying process of food represented, for instance, by the deep knowledge of the process mechanism and many experimental governing parameters, and which soft computing modelling approach can easily solve with high performances.\(^1\) Lately, fractional calculus modelling in drying has been shown as a potential tool to generalise mathematical models providing a description of the process by differential equations of arbitrary order.\(^5\)

The prediction of the drying characteristics and behaviours using mathematical models, multiple linear regression (MLR) or artificial intelligence methods, such as artificial neural network (ANN),\(^6\)\(^-\)\(^8\) Bayesian extreme learning machine (BELM), extreme learning machine (ELM), support vector machine (SVM), adaptive neuro-fuzzy inference system (ANFIS), fuzzy inference system (FIS), and response surface methodology (RSM), have been reported in numerous research papers such as\(^9\)\(^-\)\(^15\). Results from these papers show that ANFIS is the most convenient approach to model drying kinetics of agricultural products.

However, according to our knowledge, only a few research investigations report the use of fractional calculus modelling of the drying process of food materials, such as\(^16\)\(^-\)\(^18\). In addition to the application of the classical optimisation methods, recently, a Grey Wolf Optimizer (GWO), as one of the powerful evolutionary algorithms, has successfully been used for solving various optimisation problems.\(^19\),\(^20\) It is well-acknowledged that experimental measurements are expensive, time-consuming and cumbersome especially due to the highly nocuous H2S. As a direct consequence, a new meta-heuristic technique namely grey wolf optimiser-based support vector machine (GWO-SVM) The objective of this work was to study the applicability of the fractional calculus with non-integer order as fractional numbers with respect to time derivatives in Fick’s first and second laws of anomalous diffusion. The fractional calculus model parameters have been optimised using a GWO. The performance of the best model was approved based on the statistical parameters compared to the experimental data collected from the previously published papers in the literature.
2 Materials and methods

2.1 Experimental procedure

The database was collected from scientific papers covering different agricultural products under various drying and dryer types in different countries, as summarised in Table 1. The database was extracted from the papers using the software Digitizer. The experimental data were extracted as the moisture ratio in function of time to be used to adjust the parameters and compare the proposed models in this work.

The kinetics of the moisture content loss of thin layer and uniform washed samples the size of about 10 cm length and 1 cm thickness of fresh red tomatoes was determined by\(^{26}\) at temperatures of 38 °C, 44 °C, 50 °C, 57 °C, and 64 °C at a drying air flow rate of 1 m\(^{-1}\).

2.2 Theory of first/second Fick’s laws

This work is based on the normal and fractional resolution of the first and second Fick’s laws, the models’ parameters have been determined using an optimisation algorithm of grey wolf implemented in the Matlab software by minimising the objective function. This model considers that the moisture rate variation in agricultural products is directly proportional to their own moisture. The negative sign in Eq. 1 indicates that moisture will drop over time:\(^{27}\)

\[
d^{\alpha}X(t) = -k \left( X(t) - X_e \right)^\alpha
\]

where \(X(0) = f(0) = X_0\), \(k\) is the kinetic constant of the model, \(X_0\) is the initial moisture content, \(X_e\) is the equilibrium moisture content, \(X(t)\) is the moisture content at time \(t\), and \(\alpha\) the fractional time index where \(0 < \alpha < 1\) with \(\alpha \in \mathbb{R}^{28}\) and can be represented by the Caputo derivative\(^5\)

\[
D^\alpha_t X(t) = \frac{1}{\Gamma(m-\alpha)} \int_0^t (t-\tau)^{m-\alpha-1} X^m(\tau) \, d\tau
\]

for \(m-1 < \alpha < m\).\(^5\) The solution of Eq. 1 has been discussed according to the kinetic order and the derivative order – Table 1 summarises the proposed models which are based on Fick’s first law.\(^29\) The moisture can be expressed in Eq. 2.

\[
MR(t) = \frac{X(t) - X_e}{X_0 - X_e} \approx \frac{X(t) - X_e}{X_0 - X_e}
\]

The moisture ratio can be simplified into the following formula, and after considering that \(X_e\) is too small compared to \(X(t)\) and \(X_0\):

\[
MR(t) = \frac{X(t) - X_e}{X_0 - X_e} \approx \frac{X(t) - X_e}{X_0}
\]

The solution of this differential equation of non-integer order as fractional number model representing mass transfer behaviour during the drying process is solved using Laplace’s direct and inverse transform. Eq. 6 shows the correlation to obtain Laplace’s transform of an arbitrary-order equation for \(\alpha\) as a non-whole number, for \(m-1 < \alpha < m\).\(^27\)

\[
\mathcal{L} \left[ f^{(\alpha)}(s) \right] = s^\alpha \mathcal{L} \left[ f(t) \right] - s^{\alpha-1} f(0)
\]

If \(0 < \alpha < 1\), this equation can be simplified into equation 7 where \(f(0) = X_0\):

\[
\mathcal{L} \left[ f^{(\alpha)}(s) \right] = s^\alpha \mathcal{L} \left[ f(t) \right] - s^{\alpha-1} f(0)
\]

A demonstration of the ordinary \(n\)-order and fractional \(n\)-order, Fick’s equation respectively is presented in the

<table>
<thead>
<tr>
<th>Authors</th>
<th>Product</th>
<th>Drying type</th>
<th>Thickness / m</th>
<th>T / °C</th>
<th>Country</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>E. K. Akpinar</td>
<td>Mint leaves</td>
<td>Solar dryer Open sun</td>
<td>/</td>
<td>35-60</td>
<td>Turkey</td>
<td>21</td>
</tr>
<tr>
<td>O. Badaoui</td>
<td>Tomato</td>
<td>Solar drying</td>
<td>0.007</td>
<td>36</td>
<td>Algeria</td>
<td>22</td>
</tr>
<tr>
<td>S. Boughali</td>
<td>Tomato</td>
<td>Indirect active hybrid solar-electrical dryer</td>
<td>0.01</td>
<td>50 65 75</td>
<td>Algeria</td>
<td>23</td>
</tr>
<tr>
<td>N. Kumar</td>
<td>Carrot pomace</td>
<td>Air drying</td>
<td>0.01</td>
<td>60 65 70 75</td>
<td>India</td>
<td>24</td>
</tr>
<tr>
<td>O. Ismail</td>
<td>Purslane</td>
<td>Open-air sun drying</td>
<td>/</td>
<td>28-52</td>
<td>Turkey</td>
<td>25</td>
</tr>
<tr>
<td>S. B. Mariem</td>
<td>Tomato slices</td>
<td>Hot air blowing (Air drying)</td>
<td>0.01</td>
<td>38 44 50 57 64</td>
<td>Tunisia</td>
<td>26</td>
</tr>
</tbody>
</table>
The derivation of the above equation gives:

\[ \frac{dX(t)}{dt} = (X_0 - X_e) \frac{dMR(t)}{dt} \]  

(7)

By the equality of Eqs. 7 and 1 when \( \alpha = 1 \), we can obtain Eq. 8:

\[ (X_0 - X_e) \frac{dMR(t)}{dt} = -k_n (X(t) - X_e)^\alpha = -k_n (X_0 - X_e)^\alpha MR^n \]  

(8)

This equation can be written as:

\[ \frac{dMR(t)}{dt} = -K_n MR^n \quad \text{where} \quad K_n = k_n (X_0 - X_e)^{n-1} \]  

(9)

where \( K_n \) is the effective drying velocity constant, and \( k_n \) is the drying velocity constant. The solution of this equation can be expressed as in MR6:

\[ MR = 1 - \frac{k_n}{(X_0 - X_e)^{n-1}} \]  

(10)

The same demonstration has been done for the fractional order. The fractional form of Eq. 9 can be written as follows:

\[ \frac{d^\alpha X}{dt^\alpha} = D^\alpha_a MR = -k_n (X_0 - X_e)^{n-1} MR^n \]  

(11)

and can be simplified by performing a change-of-variable transformation \( M(t) = MR(t)^{1/n} \) or \( M(t) = MR(t)^{1/n} \).

\[ D^\alpha_a M(t) = k_n (n-1)(X_0 - X_e)^{n-1} \]  

(12)

Laplace transform was applied to Eq. 13 by using the relationship given by Eq. 5.

\[ \mathcal{L} \left[ \frac{d^\alpha M(t)}{dt^\alpha} \right] (s) = S^\alpha M(s) - S^{n-1} M(0) = \frac{k_n (n-1)(X_0 - X_e)^{n-1}}{s^{n-1}} \]  

(13)
\[ M(S) = \frac{1}{S} + k_n(n-1)(X_0 - X_e)^{n-1} \frac{1}{S^{n+1}} \]  
where \( M(0) = 1 \)  
\( (14) \)

Eq. (15) shows Laplace’s inverse transform to generalise the model’s equation.

\[ \mathcal{L}^{-1}\left[\frac{1}{S}\right] = \sum_{n=0}^{\infty} \frac{t^n}{\Gamma(n+1)} \]

By using Laplace’s inverse transform of \( \frac{1}{S} \), the gamma function is defined by the following integral and can be related to the factorials for any natural \( n \) \( \Gamma(n) = (n-1)! \) and also satisfies the following functional equation \( \Gamma(x+1) = x\Gamma(x) \), where \( x \in \mathbb{R}^+ \). This function is already implemented in the MatLab software and can be used directly as \( \text{gamma}(x) \).

The final solution of Eq. 15 is presented in Eq. 16:

\[ M(t) = 1 + k_n(n-1)(X_0 - X_e)^{n-1} \frac{t^n}{\Gamma(n+1)} \]  
\( (16) \)

And finally, by replacing \( M(t) \) with \( MR(t) \), we will have the final solution expressed in Eq. 17 and MR12 in Table 2.

\[ MR = \left[ \frac{1}{S} + k_n(n-1)(X_0 - X_e)^{n-1} \frac{t^n}{\Gamma(n+1)} \right] \]  
\( (17) \)

Eqs. 10 and 16 can be used for all kinetics except for \( n = 1 \), which can be done separately in an easy manner.

### 2.3 Theory of Fick’s second law

The aim of this part was to mathematically model the drying kinetics of food slices using the analytical series solution of Fick’s second law of diffusion given by the following equation, where \( D_{\text{eff}} \) is considered as diffusion constant:

\[ \frac{\partial^\alpha X(x, t)}{\partial^\alpha x} - \frac{1}{D_{\text{eff}}} \frac{\partial X(x, t)}{\partial t} = 0 \]  
\( (18) \)

Considering the initial and boundary conditions:

\[ \begin{align*}
X(t = 0, x) &= X_0 \\
\frac{\partial X}{\partial t}(t, x = 0) &= 0 \\
X(t, x = \pm \frac{e}{2}) &= 0
\end{align*} \]
\( (19) \)

The use of fractional time derivatives has been substantiated by studies indicating that porous materials are well characterised with respect to both super-diffusive and sub-diffusive behaviours using only temporal fractional orders. The value of \( \alpha \) can distinguish some domains of anomalous transport:

\[ 0 < \alpha < 1 \rightarrow \text{sub-diffusion} \]
\[ \alpha > 1 \rightarrow \text{super-diffusion} \]

Threshold between the two anomalous transport domains \( \rightarrow \) normal Brownian diffusion

In fractional calculus, the Mittag–Leffler’s function \( E_{\alpha}(x) \) has the same meaning as base exponential function. This function has the form presented in the equation

\[ E_{\alpha}(x) = \sum_{k=0}^{\infty} \frac{x^k}{\Gamma(1+ak)} \]

If \( \alpha = 1 \) and for long drying times, the Mittag–Leffler equation converges to exponential function based on Taylor series and expressed by the relation

\[ E_1(x) = \sum_{k=0}^{\infty} \frac{x^k}{\Gamma(1+k)} = e^x. \]

This simplification makes the fundamental equation of anomalous diffusion (Eq. 4) the fundamental Fick’s equation with the analytical solution, which is done by Crank for long drying times assumption (MR13), and the solution of the fractional anomalous diffusion for long drying times assumption is given by MR14. This analytical solution

| Table 3 – Ordinary vs. fractional solution of Fick’s second law |
|-------------------|------------------------|-------------------|
| Code              | Ordinary model         | Fractional model  |
| MR13              | \( \alpha = 1, \beta = 2 \) | \( \alpha = 1, \beta = 2 \) |
| \( MR = \frac{X(t) - X_e}{X_0 - X_e} = \frac{8}{\pi} \sum_{n=0}^{\infty} \left( \frac{1}{(2n+1)} \exp \left( -D_{\text{eff}} \left( \frac{(2n+1)\pi}{l} \right)^2 t \right) \right) = \frac{8}{\pi} \exp \left( -D_{\text{eff}} \left( \frac{\pi}{l} \right)^2 t \right) \) |
| MR14              | \( \alpha = \text{fractional}, \beta = 2 \) | |
| \( MR = \frac{X(t) - X_e}{X_0 - X_e} = \frac{8}{\pi} \sum_{n=0}^{\infty} \left( \frac{1}{(2n+1)} \frac{E_{\alpha} \left( \frac{(2n+1)\pi}{l} \right)^2 t^\alpha \right) \right) = \frac{8}{\pi} \exp \left( -D_{\text{eff}} \left( \frac{\pi}{l} \right)^2 t^\alpha \right) \) where \( D_{\text{eff}} \left( \frac{m^\alpha}{s^\alpha} \right) \) |
has been obtained considering assumptions like the food was an infinite slab, the initial moisture content ($X_0$) was uniform, and the moisture transfer was defined as one-dimensional.

### 2.4 Grey Wolf Optimisation (GWO) algorithm

Optimisation problems refer to the search of a maximum or minimum for a given function within an available interval. Most of the usual optimisation techniques are based on the derivative information of the concerned functions, which is not always possible. Among the nature-inspired algorithms, swarm intelligence methods are popular and have an excellent optimisation ability due to their numerous advantages to escape from local optima and derivative-free mechanism. The Grey Wolf Optimizer (GWO) considered as recent swarm-based optimisation algorithm simulates social hierarchy and hunting behaviour of grey wolves in nature, where the chasing and hunting behaviour of wolves to catch their prey represent the searching path to the optimal solution. This technique was proposed by Mirjalili et al. and has been successfully applied to solve various optimisation problems.

In this study, GWO was programmed in MATLAB to optimise Fick’s law parameters in order to match the forecasted output with the real produced output. A full description of this method is presented in paper.

### 2.5 Effective moisture diffusivity and activation energy calculation

The performance of the tested models was conducted on five kinetics of 0.01 m tomato slices drying at different temperatures. An investigation was conducted to determine which model was capable of modelling the 05 selected kinetics. The results show that MR12 gave best statistical parameters with an optimised kinetic order and fractional order.

Fig. 1 shows the performance of model MR12, which was obtained with very acceptable $R^2$ and very low RMSE. These results prove the superiority of model MR12 in modelling the 05 selected kinetics of 0.01 m of tomato slices drying at different temperatures.

The performance of the proposed models has been generalised using other products and under different parameters. Model MR12 presented its best fitting performance and statistical evaluations in comparison to the other models when modelling 11 kinetics of various products, as presented in Fig. 2.

It has been reported that the effective moisture diffusivity ($D_{eff}$) value for food materials is within the range of $10^{-11}$–$10^{-9}$. Fick’s second law was applied in this work to determine the $D_{eff}$ and to model foods that have undergone dehydration processes. As $D_{eff}$ increased with increasing temperature, the lowest $D_{eff}$ was at 38 °C and the maximum at 64 °C for the fractional and ordinary solutions.

The performance of the selected models was done using the coefficient of determination ($R^2$) and root mean square error (RMSE) given by the following equations:

$$R^2 = 1 - \frac{\sum_{i=1}^{N} (MR_{pre,i} - MR_{exp,i})^2}{\sum_{i=1}^{N} (MR_{pre,i} - MR_{exp,i})^2}$$

$$RMSE = \sqrt{\frac{1}{N} \sum_{i=1}^{N} (MR_{pre,i} - MR_{exp,i})^2}$$

The deviation observed between experimental and analytical or fractional equations is because all selected kinetics where highly fitted by $n$-fractional-order model obtained using Fick’s first law (MR12). Namely, results showed that MR13/14 was not the best when fitted with the selected drying kinetics. In addition, in this work, the $D_{eff}$ was optimised by GWO in comparison to other selected works, and with this parameter, it was determined by the simple analytical solution given by Crank for long drying times. Table 5 presents the RMSE between effective moisture diffusivities of tomato drying kinetics at different temperatures.
The relationship between temperature and effective diffusivity may be well presented by an Arrhenius-type model:\textsuperscript{18}

\[
D_{\text{eff}} = D_0 e^{-\frac{E_a}{RT}}
\]  

(22)

where \(D_0\) is the pre-exponential factor of the Arrhenius model (m\(^2\) s\(^{-1}\)), \(E_a\) is the activation energy (kJ mol\(^{-1}\)), \(R\) is the universal gas constant (8.3143 kJ mol\(^{-1}\) K\(^{-1}\)), and \(T\) is the absolute temperature (K). The natural logarithm of \(D_{\text{eff}}\) as a function of absolute temperature was plotted. \(E_a\) could be calculated by the linearisation of Eq. 20, and using the slope = \(-E_a/R\). \(E_a\) is presented in Table 5, and it follows the interval proposed in the literature for foods, ranging from 10 to 120 kJ mol\(^{-1}\).
Table 5 – Effective moisture diffusivities of tomato drying kinetics and activation energy values

<table>
<thead>
<tr>
<th>$T/K$</th>
<th>$D_{\text{eff}}$ literature</th>
<th>$D_{\text{eff}}$ RMSE</th>
<th>$D_{\text{eff}}$ ordinary</th>
<th>$D_{\text{eff}}$ RMSE</th>
<th>$D_{\text{eff}}$ fractional</th>
<th>$D_{\text{eff}}$ RMSE</th>
</tr>
</thead>
<tbody>
<tr>
<td>38</td>
<td>$3.0722 \times 10^{-9}$</td>
<td>0.573</td>
<td>$4.3983 \times 10^{-8}$</td>
<td>0.0697</td>
<td>$6.6396 \times 10^{-9}$</td>
<td>0.0262</td>
</tr>
<tr>
<td>44</td>
<td>$3.622 \times 10^{-9}$</td>
<td>0.533</td>
<td>$5.2767 \times 10^{-8}$</td>
<td>0.0628</td>
<td>$8.4435 \times 10^{-9}$</td>
<td>0.0203</td>
</tr>
<tr>
<td>50</td>
<td>$4.048 \times 10^{-9}$</td>
<td>0.5774</td>
<td>$6.9408 \times 10^{-8}$</td>
<td>0.0510</td>
<td>$2.3063 \times 10^{-9}$</td>
<td>0.0292</td>
</tr>
<tr>
<td>57</td>
<td>$4.7995 \times 10^{-9}$</td>
<td>0.576</td>
<td>$8.9339 \times 10^{-7}$</td>
<td>0.0509</td>
<td>$3.8331 \times 10^{-9}$</td>
<td>0.0363</td>
</tr>
<tr>
<td>64</td>
<td>$6.7881 \times 10^{-9}$</td>
<td>0.551</td>
<td>$1.0468 \times 10^{-7}$</td>
<td>0.0675</td>
<td>$2.5467 \times 10^{-9}$</td>
<td>0.0354</td>
</tr>
</tbody>
</table>

Mean RMSE: 0.5662, 0.0604, 0.0295

$E_a/\text{kJ mol}^{-1}$: 10.6700, 30.2452, 55.8922

3 Conclusions

A comparison between analytical and fractional solution of Fick’s first and second laws of anomalous diffusion to model the drying process of different products and dryers under different operating parameters was conducted in this study. Results showed that the performance of Fick’s first law with $n$-order kinetic fractional model (MR12) was higher compared to the other models, as well as to the second-order kinetic fractional model. Model MR12 is potentially capable of fitting the whole set of experimental data from time 0 to the end of the experiment, and provides satisfactory predictions for various agricultural drying processes under different operating parameters. The parameters of each model were optimised using the GWO algorithm. Finally, the determination of the effective moisture diffusivities of some drying kinetics was calculated and found to be in the interval given in literature.

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References

Literatura


SAŽETAK

Frakcijski račun temeljen na “algoritmu sivog vuka” u studijama o solarnom sušenju

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U ovom novom članku provedena je usporedna studija između analitičkog i frakcijskog rješenja Fickove difuzije prvog i drugog reda kako bi se modelirao solarni postupak sušenja različitih proizvoda i sušila pod različitim radnim parametrima. Laplaceova transformacija i Laplaceova inverzna transformacija primijenjene su za dobivanje rješenja u funkciji s dva parametra: indeksom reda \( n \) i razlomljenim vremenskim indeksom \( \alpha \) gore navedenih Fickovih zakona, a njihovi parametri nelinearno su optimirani pomoću “algoritma sivog vuka” (engl. Gray Wolf Optimizer, GWO). Rezultati su pokazali da fenomen anomalne difuzije tijekom postupka sušenja najbolje opisuje model frakcijskog reda. Vrijednosti dobivene primjenom modela MR12 bolje su se slagale s eksperimentalnim podacima od vrijednosti dobivenih primjenom ostalih odabranih modela s vrlo prihvatljivim statističkim parametrima.

Ključne riječi
Frakcijski račun, solarno sušenje, modeliranje, algoritam sivog vuka, omjer vlage

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