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Modelling the Drying Kinetics of Apple (Golab Variety): Fractional Calculus vs Semi-empirical Models

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Abstract

In this work, two novel models have been proposed based on semi-empirical and fractional calculus incorporating non-integer time derivatives in the Fick's first law of anomalous diffusion. The experimental data has been collected from literature of 15 kinetics investigated in a convective dryer under the effect of temperatures ranging from 40 to 80 °C at 10 °C interval, and thickness of the slices of 2 to 6 mm at 2 mm interval. The collected experimental dataset was of apple slices (Golab variety). Results from this study were compared with a set of 64 thin-layer drying models previously published in the literature. The fitting capability of the models was compared using the mean of root mean square error MRMSE (%) of all kinetics and the global determination coefficient R^2 . All models' constants and coefficients were optimised by dragonfly algorithm programmed in MATLAB software. Results showed that the fractional model is highly capable of describing the drying curve of the apple slices with a determination coefficient (R^2) of 0.99981, and average root mean square error (MRMSE) of 0.43 % in comparison to the best empirical models with R^2 of 0.99968 and MRMSE of 0.61 %.

Keywords

Thin-layer solar drying, fractional calculus, semi-empirical modelling, apple slices

1 Introduction

Drying is an important unit operation the role of which is to reduce the water content of the treated products.¹ Aimed at neutralizing bacterial activities and fungi, drying allows food products to be preserved for a long time.² It is a technique used worldwide; it allows storing and enhancing agricultural production surpluses in order to market them in times of scarcity. Given the diversity of the products to be dried and industrial processes, each with its specific constraints, the multiplicity of industrial drying techniques has been developed.^{3–6} Several models of thin-layer drying kinetics of agricultural products have been proposed in literature⁷ based on their behaviour, as well as the laws that govern energy and mass conservation, adsorption and desorption rates, heat transfer, and humidity.^{8,9}

The goal of our work was to develop two models, fractional and semi-empirical models. The performance of these models has been investigated based on experimental dataset collected from previously published scientific papers of 15 experimental drying kinetics of apples of different layer thickness (2, 4, and 6 mm), and diverse temperatures (40, 50, 60, 70, and 80 °C). The accuracy of these models has been compared with 64 models from literature for thin-layer drying kinetics.

2 Modelling of the phenomenon of solar drying

Several mathematical models are proposed in the literature to model the drying kinetics of different products, in particular the semi-empirical models, which come from the drying phenomenology.¹⁰ Table 1 presents 64 models published in the literature and tested on the drying of agricultural products. The moisture content evolution in agricultural products is directly proportional to its own moisture content¹¹ (see Eq. 1).

$$\frac{d^\alpha X(t)}{d^\alpha t} = D_t^\alpha X(t) = -k_n (X(t) - X_e)^n \quad (1)$$

where $X(0) = X_0$, k is the kinetic constant of the model, X_0 the initial moisture content, X_e is the equilibrium moisture content, and α is the fractional time index where $0 < \alpha < 1$ with $\alpha \in R$.¹² The moisture ratio can be expressed and simplified into the following formula and after considering that X_e is too small compared to $X(t)$ and X_0 .

$$MR(t) = \frac{X(t) - X_e}{X_0 - X_e} \approx \frac{X_t}{X_0} \quad (2)$$

$X(t)$ is the moisture content at time t , which is given by $X(t) = \frac{m_h - m_s}{m}$, m_h is the successive weightings change of the wet product until it becomes stationary, m_s is the dry mass of the product and was determined by drying the samples at 105 °C until the weight became constant.^{13,14}

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Eq. 1 can be expressed in terms of moisture by Eq. 3:

$$\frac{\partial^\alpha MR(t)}{\partial^\alpha t} = -K_\alpha MR(t)^n \tag{3}$$

$$MR(t) = \left[\frac{1}{\frac{(n-1)K_\alpha t^\alpha}{(\alpha+1)} + \frac{1}{C_0^{n-1}}} \right]^{\frac{1}{n-1}} \tag{4}$$

with $K_\alpha = \frac{k_\alpha X_0^\alpha}{X_0^n}$, the solution of Eq. (3) gives the fractional model. See Eq. (4):

with α as the whole order between $1 < \alpha < 2$, K_α as the fractional rate constant, and n as the order of the reaction. These models were tested on 15 solar drying kinetics taken from the literature, of apple in a thin layer under the effect of 3 different thicknesses {2, 4, and 6 mm}, and 5 different temperatures {40, 50, 60, 70, and 80 °C}.¹⁵ The second developed model in this work is a semi-empirical model.

Table 1 – Thin-layer drying models tested in this work

Model Name	Equations	Code	Ref.
Lewis	$MR = \exp(-kt)$	MR1	7
Page	$MR = \exp(-kt^n)$	MR2	7
Modifie Page I	$MR = \exp[-(kt^n)]$	MR3	7
Modifie Page II	$MR = \exp[-(kt^n)]$	MR4	7
Modifie Page III	$MR = \exp[-(kt^n)]$	MR5	7
Modifie Page IV	$MR = a \exp[-(kt^n)]$	MR6	7
Modifie Page V	$MR = \exp[-(kt^n)]$	MR7	7
Modifie Page VI	$MR = \exp(kt^n)$	MR8	7
Modifie Page VII	$MR = \exp\left[-k\left(\frac{t}{L^2}\right)^n\right]$	MR9	7
Modifie Page IX	$MR = k \exp\left[\left(\frac{-t}{L^2}\right)^n\right]$	MR10	7
Otsura et al.	$MR = 1 - \exp[-(kt^n)]$	MR11	7
Fick Simplifie	$MR = k \exp\left[-c\left(\frac{t}{L^2}\right)\right]$	MR12	7
Henderson and Pabis	$MR = a \exp(-kt)$	MR13	7
Modifie Henderson and Pabis – I	$MR = a \exp(-k_0t) + b \exp(-k_1t) + c \exp(-k_2t)$	MR14	7
Modifie Henderson and Pabis – II	$MR = a \exp(-kt^n) + b \exp(-gt) + c \exp(-ht)$	MR15	7
Logaritmik	$MR = a \exp(-kt) + c$	MR16	7
TwoTerm	$MR = a \exp(-k_0t) + b \exp(-k_1t)$	MR17	7
Modifie TwoTerm – I	$MR = a \exp(k_0t) + (1-a) \exp(-k_1t)$	MR18	7
Modifie TwoTerm – II	$MR = a \exp(k_0t) + (1-a) \exp(k_1t)$	MR19	7
Modifie TwoTerm – III	$MR = a \exp(-k_0t) + a \exp(-k_1t)$	MR20	7

Table 1 – (continued)

Model Name	Equations	Code	Ref.
Modifie TwoTerm – IV	$MR = a \exp(-k_0 t^n) + b \exp(-k_1 t)$	MR21	7
Modifie TwoTerm – V	$MR = a \exp(-k_0 t) + (1-a) \exp(-k_1 t)$	MR22	7
TwoTermExponential	$MR = a \exp(-kt) + (1-a) \exp(-kat)$	MR23	7
Verma et al.	$MR = a \exp(-kt) + (1-a) \exp(-gt)$	MR24	7
Diffusion Approximation	$MR = a \exp(-kt) + (1-a) \exp(-kbt)$	MR25	7
Midilli et al.	$MR = a \exp(-kt^n) + bt$	MR26	7
Modifie Midilli – I	$MR = \exp(-kt^n) + bt$	MR27	7
Modifie Midilli – II	$MR = \exp(-kt) + bt$	MR28	7
Modifie Midilli – III	$MR = a \exp(-kt) + bt$	MR29	7
Wang and Singh	$MR = 1 + at + bt^2$	MR30	7
Hii et al.	$MR = a \exp(-kt^n) + c \exp(-gt^n)$	MR31	7
Weibull Distribution – I	$MR = a - b \exp[-(kt^n)]$	MR32	7
Weibull Distribution – II	$MR = a - b \exp[-kt^n]$	MR33	7
Weibull Distribution – III	$MR = \exp[-(t/a)^n]$	MR34	7
Vega-Galvez et al. – I	$MR = n + k\sqrt{t}^n$	MR35	7
Vega-Galvez et al. – II	$MR = \exp(n + kt)$	MR36	7
Vega-Galvez et al. – III	$MR = (a + bt)^2$	MR37	7
Jena Das	$MR = a \exp(-kt + b\sqrt{t}) + c$	MR38	7
Wang et al. One Term	$MR = a \exp(bkt) + (1-a)$	MR39	7
Wang et al. Two Term	$MR = (1-a) \exp(bkt) + a \exp(ckt)$	MR40	7
Wang et al. Three Term	$MR = (1-a-b) \exp(ckt) + a \exp(dkt) + b \exp(fkt)$	MR41	7
Demir et al.	$MR = a \exp[-(kt)^n] + b$	MR42	7
Haghi and Angiz – I	$MR = a \exp(-bt^c) + dt^2 + et + f$	MR43	7
Haghi and Angiz – II	$MR = a + bt + ct^2 + dt^3$	MR44	7
Haghi and Angiz – III	$MR = \frac{a + bt}{1 + ct + ct^2}$	MR45	7
Haghi and Angiz – IV	$MR = a \exp\left[\frac{-(t-b)^2}{2c^2}\right]$	MR46	7
Sripinyowanich and Noomhorm	$MR = \exp(-kt^n) + bt + c$	MR47	7
Noomhorm and Verma	$MR = a \exp(-kt) + b \exp(-gt) + c$	MR48	7
Hasibuan and Daud	$MR = 1 - at^n \exp(-kt^m)$	MR49	7
SharefEldeen et al.	$MR = a \exp(kt) + [1 - a \exp(-bkt)]$	MR50	7

Table 1 – (continued)

Model Name	Equations	Code	Ref.
Henderson and Henderson I	$MR = c \left[\exp(-kt) + \frac{1}{9} \exp(-9kt) \right]$	MR51	7
Henderson and Henderson II	$MR = c \exp(-kt) + \frac{1}{9} \exp(-9kt)$	MR52	7
Parabolic	$MR = a + bt + ct^2$	MR53	7
Geometric	$MR = at^{-n}$	MR54	7
Logistic	$MR = \frac{a_0}{[1 + a \exp(kt)]}$	MR55	7
Power Law	$MR = at^b$	MR56	7
Regression – I	$MR = \exp[-(at^2 + bt)]$	MR57	7
Chavez-Mendez et al.	$MR = a + b \ln(t)$	MR58	7
Aghbashlo	$MR = \exp \left[-\frac{k_1 t}{(1 + k_2 t)} \right]$	MR59	7
Modifie Henderson and Perry	$MR = a \exp(-kt^n)$	MR60	7
Three Parameter	$MR = a \exp[-(kt)^n]$	MR61	7
Asymptotic	$MR = a_0 + a \exp(-kt)$	MR62	7
Khazaei and Daneshmandi	$MR = a + \exp(-bt) - ct$	MR63	7
Proposed model I	$MR = \exp[-(at^n + bt)]$	MR64	This study
Kaleemullah 2006	$MR = \exp(-(at + b)t^{(ct+d)})$	MR65	16
Proposed model II	$MR = \left[\frac{1}{\frac{(n-1)K_\alpha t^\alpha}{(\alpha+1)} + \frac{1}{C_0^{n-1}}} \right]^{\frac{1}{n-1}}$	MR66	This study

3 Results and discussion

3.1 Results of semi-empirical modelling

Parameter adjustments of selected models from literature (64 models), as well as the proposed model were performed using dragonfly and swarm algorithms (DA MATLAB function). To avoid convergence to local minima, optimisation using dragonfly and swarm algorithms was performed 20 times. The optimised parameters of each model were used to estimate the moisture ratio and compare it with the experimental moisture ratio. The performance of each model was measured using different statistical parameters, like root mean square error (RMSE), reduced chi-squared (X^2), modelling efficiency (EF), and determination coefficient (R^2) for each kinetic and for each model. The average of these parameters for about 276 experimental points covering the

15 kinetics are presented in Table 2. The best performing model was selected based on the smallest average error (≈ 0) and the largest coefficient of determination (≈ 1). The mathematical formulas of these errors are presented in the articles cited in these references.¹⁷⁻²³

In order to simplify the comparison, the performances of the best 16 models are shown in Table 3 and Fig. 1, after having classified them from the smallest value to the largest value of MRMSE. The comparison between the performances of the different models indicates that the model proposed in this work MR64 provides the best correlation performance, where the value of MRMSE is ($\approx 0.43\%$). The second best correlation performance is given by the coded model MR57, where the MRMSE has a value of ($\approx 0.61\%$).

Table 2 – Results of calculation of the means of the statistical parameters

Model code	MRMSE	MX ²	MR ²	MEF	Model code	MRMSE	MX ²	MR ²	MEF
MR1	0.02470	0.00439	0.995315	0.99192	MR34	0.00632	0.15171	0.996306	0.99949
MR2	0.00632	0.00038	0.993841	0.99949	MR35	0.05906	0.00006	0.983223	0.96395
MR3	0.70613	0.03676	0.989492	-3.94113	MR36	0.02058	0.00268	0.99675	0.99460
MR4	0.00632	0.03050	0.999572	0.99949	MR37	0.02667	0.00006	0.994811	0.99221
MR5	0.23524	0.00614	0.924816	-0.10991	MR38	0.11913	0.00167	0.888276	0.76815
MR6	0.03687	0.00392	0.98012	0.96187	MR39	0.03493	0.00267	0.965836	0.95844
MR7	0.00632	0.00138	0.999661	0.99949	MR40	0.01623	0.01290	0.997865	0.99598
MR8	0.00632	0.00140	0.988855	0.99949	MR41	0.00957	0.00400	0.991579	0.99876
MR9	0.37653	0.02497	0.24018	-0.53374	MR42	0.27060	0.00030	0.68628	0.17489
MR10	0.42449	0.15176	0.240178	-0.78284	MR43	0.41069	0.00573	0.467703	-3.97645
MR11	0.05268	0.00178	0.987291	0.97250	MR44	1.33998	0.00772	0.771128	-43.16799
MR12	0.34640	0.15171	0.377639	-0.27247	MR45	0.05469	0.00439	0.96633	0.96772
MR13	0.02058	0.00006	0.996043	0.99460	MR46	0.01647	0.00038	0.992901	0.99692
MR14	0.02001	0.00268	0.990786	0.99313	MR47	0.14314	0.03676	0.828988	0.72248
MR15	0.04604	0.00006	0.952705	0.95388	MR48	0.10609	0.03050	0.937033	0.78844
MR16	0.03987	0.00167	0.935228	0.94958	MR49	0.04610	0.00614	0.848811	0.95346
MR17	0.01830	0.00267	0.947923	0.99249	MR50	0.03360	0.00392	0.956268	0.97026
MR18	0.00809	0.01290	0.999281	0.99914	MR51	0.03334	0.00138	0.993357	0.98753
MR19	0.00678	0.00400	0.998558	0.99933	MR52	0.03373	0.00140	0.993219	0.98737
MR20	0.04672	0.00030	0.97757	0.96264	MR53	0.08623	0.02497	0.736838	0.80391
MR21	0.02446	0.00573	0.956404	0.98815	MR54	0.36640	0.15176	0.394482	-0.31502
MR22	0.00809	0.00772	0.999225	0.99918	MR55	0.03102	0.00178	0.994644	0.98602
MR23	0.02016	0.00439	0.997007	0.99488	MR56	0.36634	0.15171	0.434155	-0.31463
MR24	0.00824	0.00038	0.999091	0.99912	MR57	0.00609	0.00062	0.999681	0.99949
MR25	0.00681	0.03676	0.999158	0.99925	MR58	0.04635	0.00268	0.985938	0.97258
MR26	0.18126	0.03050	0.536473	0.51637	MR59	0.00701	0.00006	0.999353	0.99930
MR27	0.10073	0.00614	0.737014	0.79737	MR60	0.01387	0.00167	0.95625	0.98627
MR28	0.01949	0.00392	0.930226	0.99312	MR61	0.03375	0.00267	0.983897	0.97329
MR29	0.14617	0.00138	0.780538	0.58332	MR62	0.05857	0.01290	0.952211	0.87420
MR30	0.03535	0.00140	0.890798	0.97863	MR63	0.04689	0.00400	0.971614	0.96073
MR31	0.07696	0.02497	0.830475	0.89322	MR64	0.00429	0.00030	0.999814	0.99967
MR32	0.07730	0.15176	0.912332	0.91464	MR65	0.04619	0.00573	0.919098	0.95821
MR33	0.09243	0.00178	0.898699	0.85327					

Table 3 – Comparative table of the 16 models considered

Model index	MRMSE/%	MX ²	MR ²	MEF	Model index	MRMSE/%	MX ²	MR ²	MEF
MR64	0.43	0.00030	0.999814	0.99967	MR25	0.68	0.03676	0.999158	0.99925
MR57	0.61	0.00006	0.999681	0.99949	MR59	0.70	0.00006	0.999353	0.9993
MR7	0.63	0.00138	0.999661	0.99949	MR22	0.81	0.00772	0.999225	0.99918
MR4	0.63	0.03050	0.999572	0.99949	MR18	0.81	0.01290	0.999281	0.99914
MR8	0.63	0.00140	0.988855	0.99949	MR24	0.82	0.00038	0.999091	0.99912
MR2	0.63	0.00038	0.993841	0.99949	MR41	0.96	0.00400	0.991579	0.99876
MR34	0.63	0.15171	0.996306	0.99949	MR60	1.39	0.00167	0.95625	0.98627
MR19	0.68	0.00400	0.998558	0.99933	MR40	1.62	0.01290	0.997865	0.99598

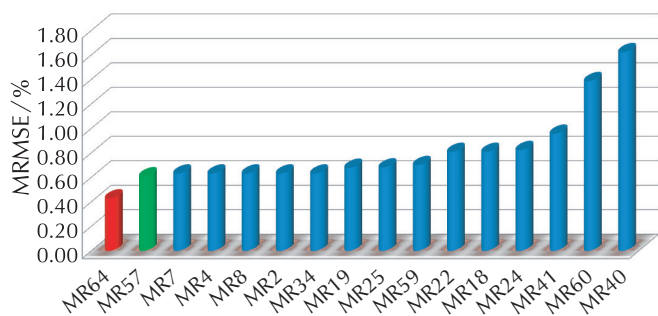


Fig. 1 – Classification of the 16 models considered for solar drying of the apple thin layer

3.2 Comparison of the performance of the two selected models

The comparison between the two selected models (MR64 and MR57) is presented in the form of kinetics curves in which the moisture content (MR) is plotted against time. Figs. 2–4 represent the modelling results by the two models of the fifteen drying kinetics of a thin layer of apple at different thicknesses and drying temperatures. Results

show a slight superiority of the MR64 model compared to the MR57 model when modelling the experimental data of apple drying. Another comparison was made in terms of linear regression between the predicted and experimental rate of humidity (MR) to assess the ability of both models MR64 and MR57 to model solar drying kinetics. Figs 5–7 show the juxtaposition of the first bisector and the line of the best linear fit of the output with the target, as well as the distribution of the experimental points confirming the excellent agreement between the moisture rate calculated by the two models and that of the experiment under different thicknesses and different temperatures for the entire database. Table 4 summarizes the errors and the linear regression vectors that are very close to ideal for all kinetics.

Table 4 – Errors and linear regression vectors obtained for the two models

Model	A	β	R	MRMSE
MR64	1	$-4.3 \cdot 10^{-05}$	0.99981	0.00429
MR57	1	0.0014	0.99974	0.00609

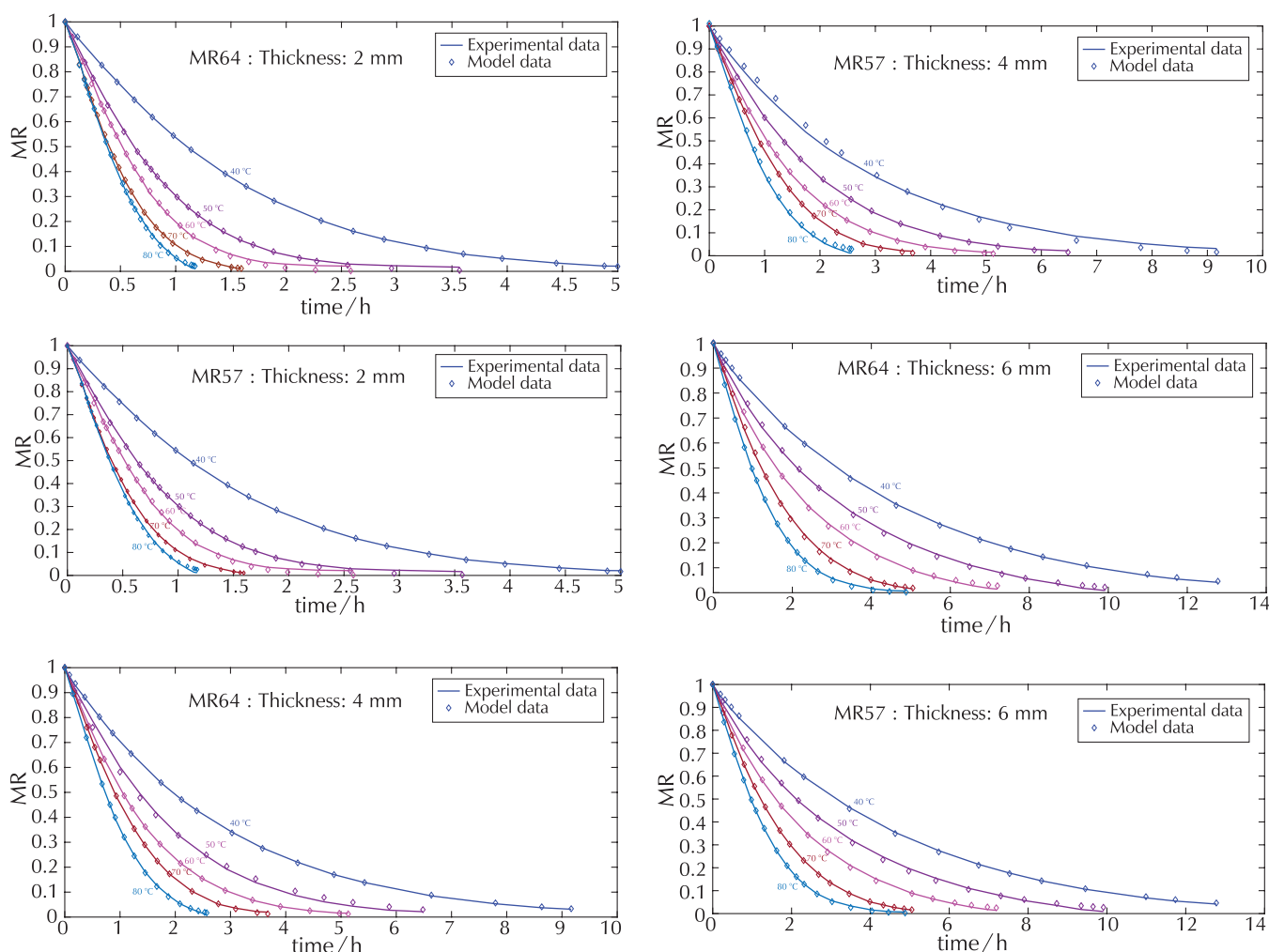


Fig. 2 – Performance of each MR57 and MR64 model to predict drying kinetics

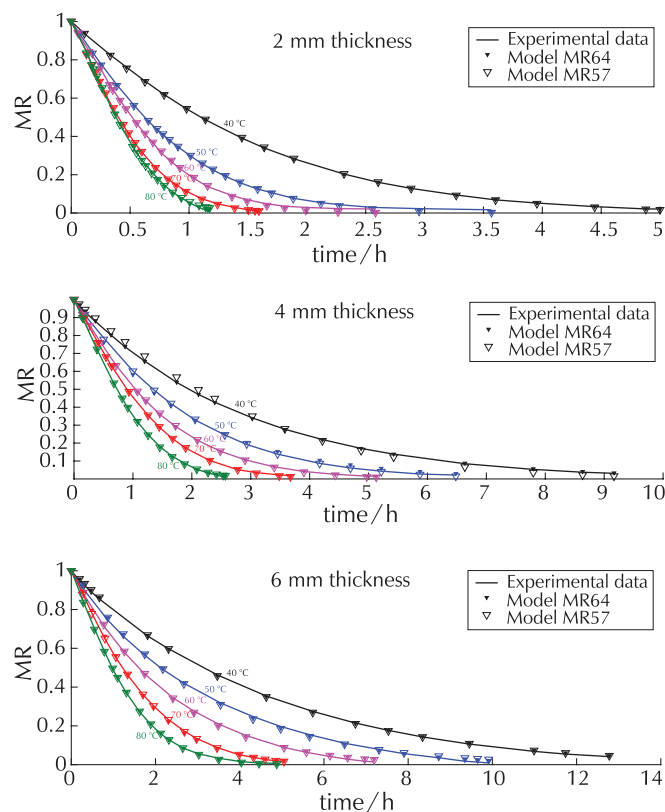


Fig. 3 – Comparison between the two models to predict the drying kinetics vs temperature at different thicknesses

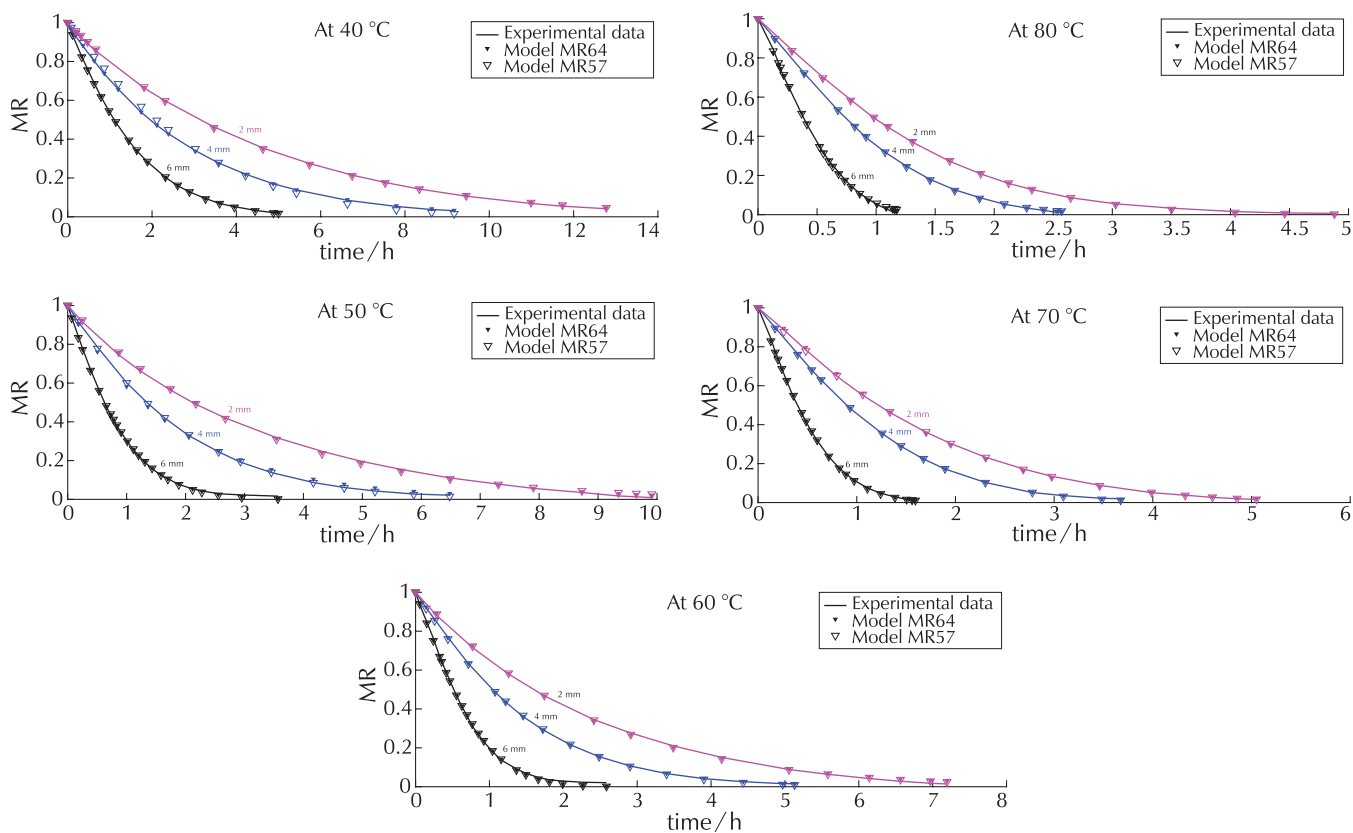


Fig. 4 – Comparison between the two models to predict the drying kinetics vs thicknesses at different temperatures

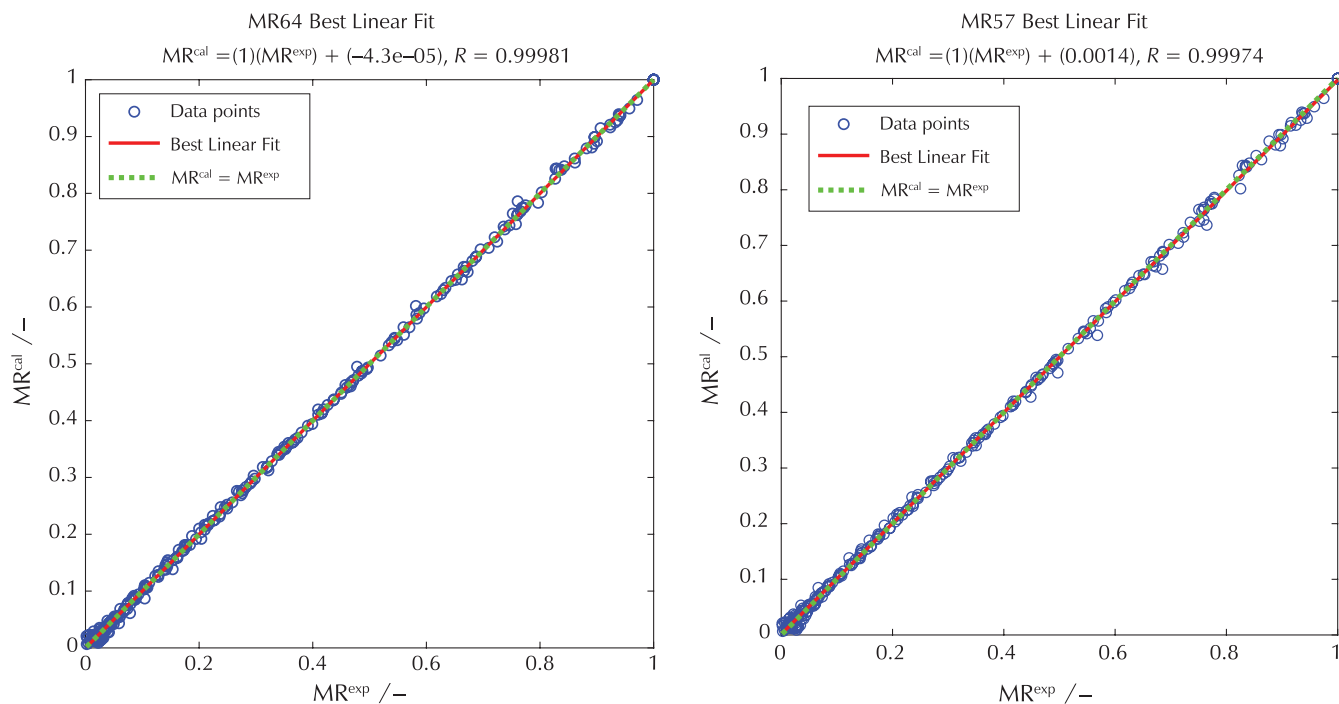


Fig. 5 – Linear regression between the experimental and the calculated moisture ratio using the proposed model (MR64) and the regression I model (MR57)

3.3 Fractional modelling results

This methodology was applied to fifteen drying kinetics of apple pieces in a thin layer under the effect of different temperatures and thicknesses. The results of the fractional modelling were then compared to those of the two best performing models found. The comparison was made

using the mean statistical parameters and in the form of graphical illustrations and tables. The parameters of the fractional model were optimised using the “dragonfly” optimisation method programmed in the MATLAB software. Optimisation results are presented in Table 5. In order to avoid local minima caused by the optimisation method, each optimisation operation was repeated 20 times.

Table 5 – Statistical parameters optimised by fractional model

T/C°	Thickness/mm	Statistical parameters			Coefficients		
		RMSE	χ^2	R^2	k	α	n
40	2	0.00238	0.00001	1.0000	0.641	1.091	0.954
	4	0.00421	0.00002	0.9999	1.260	1.139	0.972
	6	0.02233	0.00057	0.9996	1.000	0.887	0.497
50	2	0.01428	0.00024	0.9998	1.000	0.769	0.286
	4	0.00651	0.00005	0.9988	1.000	0.772	0.127
	6	0.00192	0.00000	1.0000	0.346	0.979	0.918
60	2	0.00241	0.00001	1.0000	0.513	1.058	0.941
	4	0.00559	0.00004	1.0000	0.755	1.181	1.086
	6	0.00958	0.00011	0.9999	1.000	1.302	1.119
70	2	0.00413	0.00002	0.9998	0.896	1.068	0.672
	4	0.00120	0.00000	1.0000	0.220	0.937	0.828
	6	0.00461	0.00003	0.9999	0.306	0.865	0.695
80	2	0.00285	0.00001	1.0000	0.399	0.923	0.752
	4	0.00170	0.00000	0.9998	0.553	1.087	0.854
	6	0.00419	0.00002	0.9998	0.804	1.216	0.987
Average		0.59 %	0.00008	0.99981	–	–	–

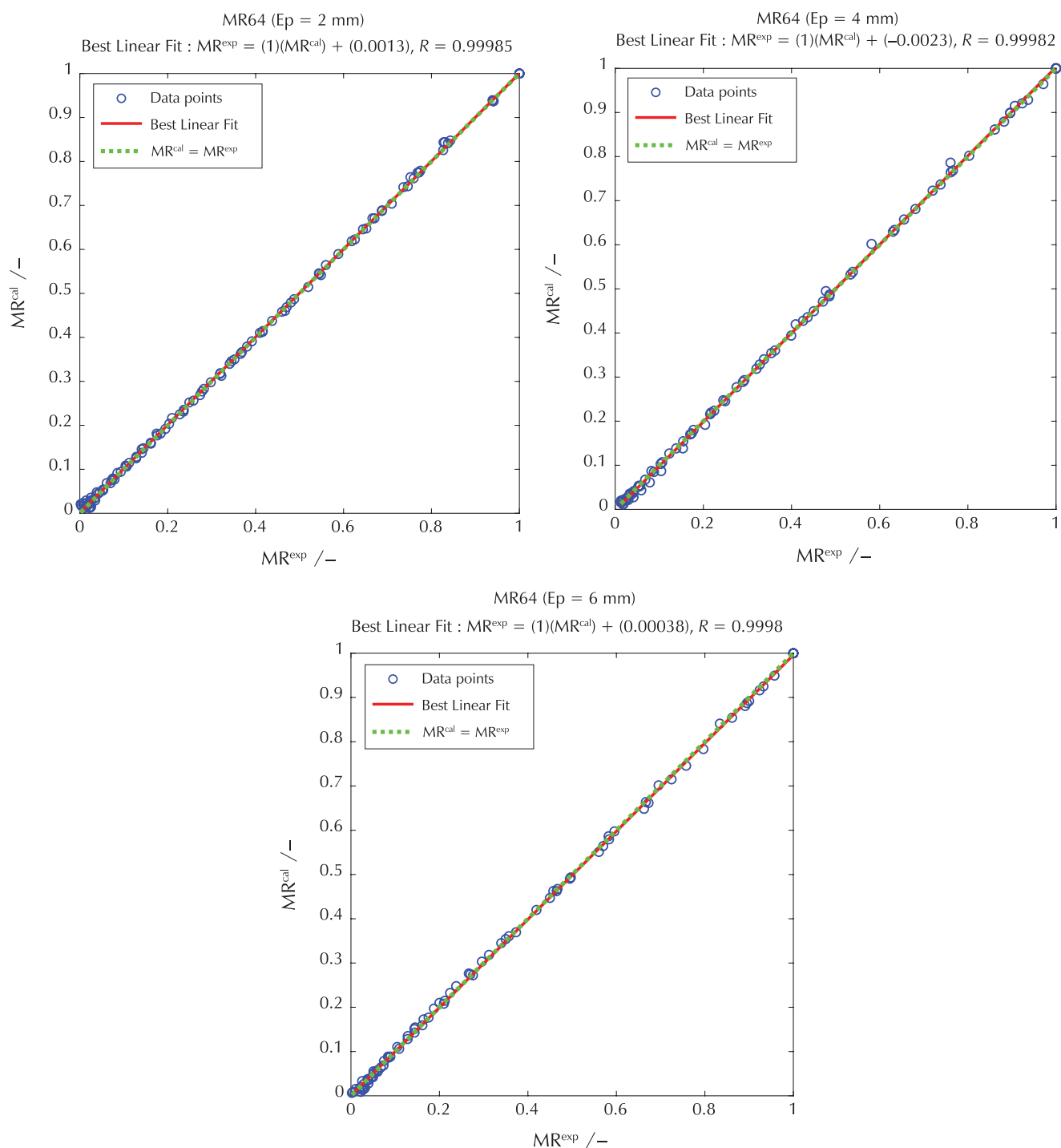


Fig. 6 – Linear regression between the experimental and the calculated moisture ratio using the proposed model (MR64) at different thicknesses (Ep) of the 15 selected kinetics

A comparison in terms of histograms between the three best models was made by the overall coefficient of determination and the average of the mean absolute relative errors of the 15 drying kinetics of the apple in a thin layer (see Table 6).

Table 6 – Comparison between the three models

Model	MRMSE / %	χ^2	R^2	EFM
Fractional	0.59	0.00008	0.99981	0.99934
MR57	0.61	0.00062	0.99968	0.99949
MR64	0.43	0.00030	0.99981	0.99967

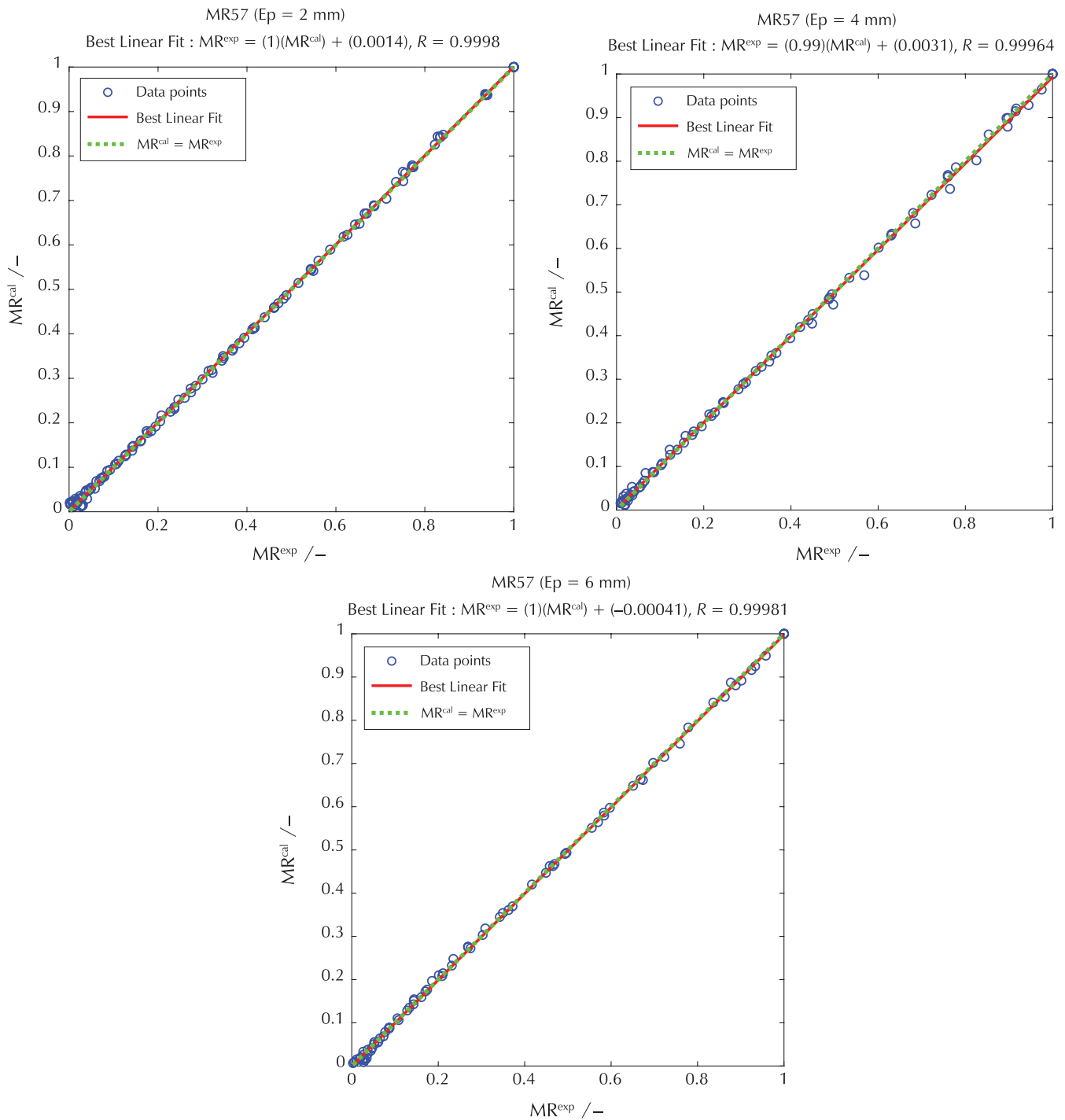


Fig. 7 – Linear regression between the experimental and the calculated moisture ratio using the proposed model (MR57) at different thicknesses (Ep) of the 15 selected kinetics

From Fig. 8, the proposed empirical model MR64 shows to be the best in terms of MRMSE and R^2 ; followed by the fractional model and the MR57 model.

4 Conclusion

The aim of this work was to model the phenomenon of apple drying in a thin layer using empirical and fractional methods. For this purpose, a dataset of 15 kinetics tak-

en from previously published papers was extracted from drying kinetics of apple using Digitizer software. Sixty-four semi-empirical models were tested firstly, and based on the structure and performance of the best model, a semi-empirical model was proposed and tested using the same dataset. In addition, a novel model has been proposed using fraction calculus based on Fick’s first law of n order.

The proposed semi-empirical model proves to be the most efficient by modelling the fifteen kinetics with MRMSE of 0.43 %, R^2 of 0.9998, followed by the fractional mod-

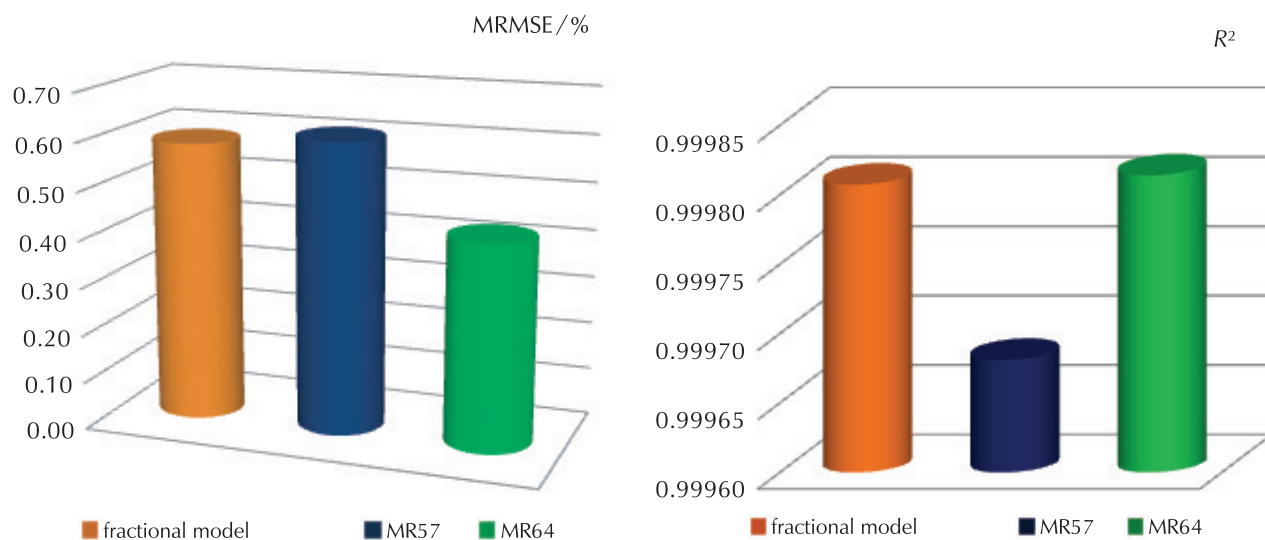


Fig. 8 – Comparison in terms of MRMSE (%) and R^2 between the fractional model and the two semi-empirical models MR57 and MR64 by modelling the 15 kinetics of solar drying thin layers of apple

el with MRMSE of 0.59 %, R^2 of 0.9998, and finally, the best model from literature (Regression I) with MRMSE of 0.61 %, R^2 of 0.9997. The results show that the two proposed models can fit with accuracy the drying desorption kinetics during thin-layer apple drying in comparison with those models from literature.

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SAŽETAK

Modeliranje kinetike sušenja jabuke (sorta Golab): Frakcijski račun u odnosu na poluempirijske modele

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U ovom radu predložena su dva nova modela temeljena na poluempirijskom i frakcijskom računu koji uključuje necjelobrojne vremenske derivate u Fickovom prvom zakonu anomalne difuzije. Eksperimentalni podaci o 15 kinetika istraženih u konvektivnom sušioniku pod utjecajem temperatura u rasponu od 40 do 80 °C u razmaku od 10 °C i debljine kriški od 2 do 6 mm u razmaku od 2 mm prikupljeni su iz literature. Prikupljeni eksperimentalni skup podataka bio je na kriškama jabuke (sorta Golab). Rezultati ove studije uspoređivani su s nizom od 64 modela tankoslojnog sušenja koji su prethodno objavljeni u literaturi. Sposobnost uklapanja modela uspoređena je koristeći srednju vrijednost srednje kvadratne pogreške MRMSE (%) svih kinetika i globalni koeficijent određivanja R^2 . Konstante i koeficijenti svih modela optimizirani su algoritmom dragonfly programiranim u softveru MATLAB. Rezultati pokazuju da je frakcijski model visoko sposoban opisati krivulju sušenja kriški jabuke s koeficijentom utvrđivanja (R^2) 0,99981 i prosječnom srednjom kvadratnom pogreškom (MRMSE) 0,43 % u usporedbi s najboljim empirijskim modelima s R^2 0,99968 i MRMSE 0,61 %.

Ključne riječi

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