An artificial neural network model for predicting characteristic input parameters for physics based modelling of drying process

(Full title: An artificial neural network model for predicting characteristic input parameters for physics based modelling of drying process)

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Abstract

Drying is crucial in the quality preservation of food materials. Physics-based models are effective tools to optimally control the drying process. However, these models require accurate thermo-physical properties; unavailability or uncertainty in the values of these properties increases the possibility of error. Property estimation methods are not standardized, and usually involve the use of many instruments and are time-consuming. In this work, we have developed an experimentally validated deep learning-based artificial neural network model that estimates sensitive input parameters of food materials using temperature and moisture data from a set of simple experiments. This model predicts input parameters with error less than 1%. Further, using input parameters, physics-based model predicts temperature and moisture to within 5% accuracy of experiments. The proposed work when interfaced with food machinery could play a significant role in process optimization in food processing industries.

Keywords: Drying, Food properties, Food parameters, Modelling, Artificial Neural Network, Deep learning

Nomenclature

t	time (s)
ρ	density (kg/m^3)
ϕ	porosity (unit-less)
S	saturation
M	moisture content(dry basis, kg/kg)
T	temperature (^oC)
subscripts	
w	water
s	solid
o	initial
av	average
∞	ambient condition
min	minimum value
max	maximum value
$pred$	predicted value
superscripts	
*	normalised parameter
Abbreviations	
ANN	artificial neural network
RMSE	root mean square error

1. Introduction

Artificial neural network (ANN) is an effective tool for prediction modelling. In recent years, it has been implemented in various aspects of food processing and handling such as food quality, microbial growth, processing methodologies, properties estimation, transport processes etc.(Chen, Ramaswamy, & Marcotte, 2007; Huang, Kangas, & Rasco, 2007). Various quality measures such as ripeness of fruits (Brezmes, Llobet, Vilanova, Saiz, & Correig, 2000), shape attributes (Morimoto, Takeuchi, Miyata, & Hashimoto, 2000), their sugar contents(Kondo, Ahmad, Monta, & Murase, 2000), sensory properties (Di Natale, Macagnano, Martinelli, Proietti, et al., 2001; Haddi et al., 2014), harvesting and post-harvesting defects (Di Natale, Macagnano, Martinelli, Paolesse, et al., 2001; Guyer & Yang, 2000) have been predicted quantitatively using different ANN techniques. Image-based classification using artificial neural networks for cultivar detection(Liu, Zhao, Jia, Ji, & Sun, 2019; Parpinello et al., 2007), quality inspection (Shrestha, Kang, Yu, & Baik, 2016), size-based classification (Shahin, Symons, & Poysa, 2006), varietal classification(Kozłowski Michałand Górecki & Szczypiński, 2019; Ni, Wang, Vinson, Holmes, & Tao, 2019) and colour and morphology-based classification (Douik & Abdellaoui, 2010; Majumdar & Jayas, 2000a, 2000b) has also been performed. Another application is microbial growth analysis, their activity and associated food-safety assessments (Cheroutre-Vialette & Lebert, 2000; Jeyamkondan, Jayas, & Holley, 2001; Timsorn, Thoopboochagorn, Lertwattanasakul, & Wongchoosuk, 2016). These models also find their applications include food extrusion processes (Cubeddu, Rauh, & Delgado, 2014; Popescu, Popescu, Wilder, & Karwe, 2001). Besides, artificial neural network tools for predicting transport phenomena and shrinkage behaviour have also been proposed (Hernández, 2009; Kerdpiboon, Kerr, & Devahastin, 2006; Lertworasirikul & Tipsuwan, 2008; Mercier & Uysal, 2018; Mittal & Zhang, 2000; Reza, Mohebbi, & Khodaiyan, 2014; Tripathy & Kumar, 2009; Turker & others, 2008). Similarly, models to predict texture characteristics using properties data have been developed(Fan et al., 2013).

An important application of artificial neural networks in the field of food processing is properties estimation. Various researchers have analysed change in different engineering properties such as thermal conductivity (Mohamed Azlan Hussain & Rahman, 1999), porosity (M A Hussain, Rahman, & Ng, 2002), and diffusivity(Jena & Sahoo, 2013) for various food materials for their raw state and during drying. However, most of these studies focus on estimation of one or two properties and thus, exhibit limited contribution to physics-based modelling. Further, since the predictions are mostly based on experiments, the datasets used in model development are small leading to performance limitations. The importance and applicability of these properties' predictions in physics-based modelling is not well addressed and artificial neural network studies that focus on comprehensive modelling of thermal drying processes are limited.

Physics-based models have emerged as powerful tool in prediction of thermo-physical behaviour of food materials under different operating conditions. However, the prediction accuracy of these models is limited by the accuracy of input parameters. Due to organic nature of food materials, input properties such as moisture content, water saturation, porosity, etc. vary among different varieties of the same cultivar owing to the variation in geographical locations, climatic conditions and harvesting techniques and time etc. leading to erroneous predictions by physics-based models. We have found a well-defined methodology to predict all sensitive input parameters for drying modelling thus far. Further, the present work proposes a novel hybrid modelling approach that combines the advantages of experiments, artificial neural network model and physics-based model to provide an effective prediction tool for drying process.

The objective of the present work is to develop a framework for predictive modelling of food drying process utilizing artificial neural network. A methodology is proposed that predicts characteristic input parameters for food materials using an artificial neural network model applied over a developed control experiment. Then, the predicted parameters are implemented in physics based models for prediction of transport behaviour of food materials and the results are validated with experiments.

2. Modelling methodology

In order to train neural network model, a large data set of input vectors and corresponding output is needed. Since carrying out such large number of experiments is not practical, an experimentally validated physics-based model taken from our earlier work (Sinha & Bhargav, 2019) was used for data generation. Fig. 1 reproduces the modelling framework. This model also helped in focusing attention on a subset of sensitive parameters, which were determined through a sensitivity analysis. These sensitive parameters include initial porosity ($\emptyset_{wo}$), initial water content (S_{wo}) and solid density (ρ_s). These parameters are referred hereafter as characteristic input parameters. Here $\emptyset_{wo}$ is the ratio of initial void volume to the initial total volume, S_{wo} is the ratio of initial water volume to the initial total volume and ρ_s is the ratio of mass of solids to volume of solids.

It is worth noting that variation in geographic location, climatic condition, method and time of harvests etc. impacts the sensitive parameters values and consequently alter the transport and deformation behaviour. This was accounted by generating various combination of these characteristic input parameters. Each combination would result in a different transport-deformation behaviour.

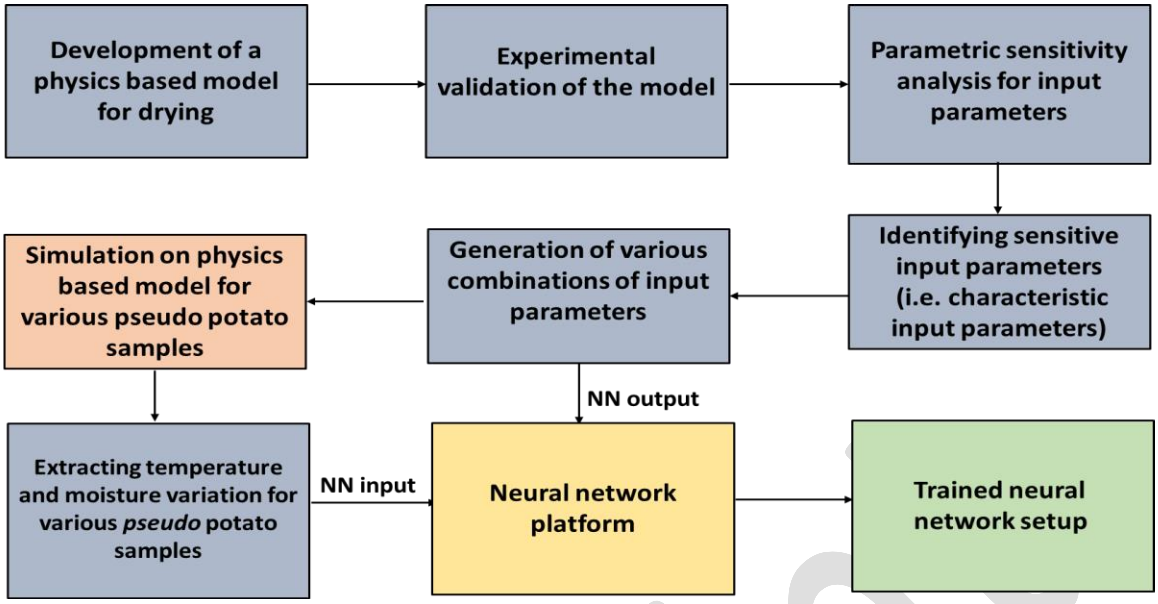


Fig. 1- Schematic representation of pathway followed in setting up the deep neural network model

Potato was selected as the subject of study. For each sensitive parameter, a range of variation was identified (Table 1). In total, 12 values were selected through randomized selection from a uniform distribution in the specified range. Then, all the possible combinations were created leading to the development of a total of 1728 (12^3) pseudo-varieties of potato. The values selected using uniform distribution are shown in Fig. 2. Physics-based model was used to simulate the transport behaviour of each of the developed variety for a particular set of operating conditions as discussed in the later sections.

Table 1 Sensitive system parameters and their range

Property	**Symbol**	**Value range**
Initial porosity	$\emptyset_o$	0.68-0.88
Initial water saturation	S_{wo}	0.49-0.99
Density of solids	ρ_s	1100-2700 kg/m^3

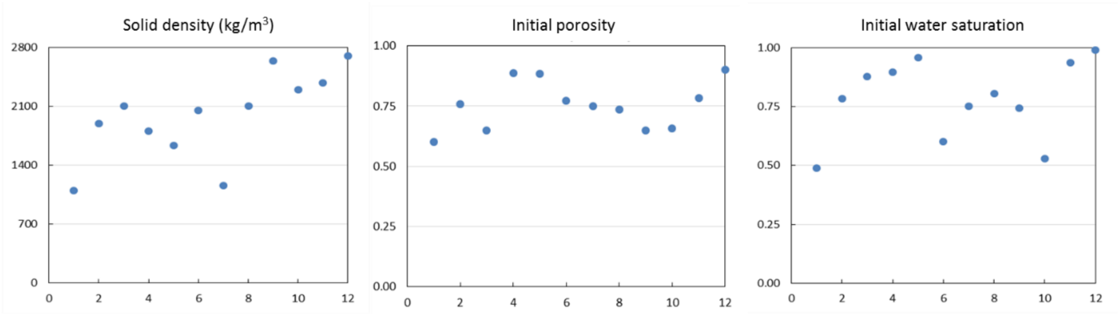


Fig. 2 - Selected dataset for characteristic input parameters

3. Artificial neural network (ANN) model

3.1 Input and output vectors

The objective of the neural network is to predict characteristic input parameters of any given potato sample. These characteristic input parameters form the output vector of neural network model. The input vector for the neural network needs to be some *in-situ* measurable characteristics for the utility of model. Therefore, temporal variation of surface temperature, centre temperature and average moisture content measure at a pre-defined set of operating condition was used as the input for the neural network model. This set of operating condition is hereafter referred as the control experiment (discussed in detail in section 4). For the considered control experiment, the maximum gradient in temperature and moisture content was observed in first 20 minute of process. Therefore, only 20-minute data of temperature and moisture is sufficient to be fed as input for neural network.

All the input parameters (centre temperature, surface temperature and average moisture content) were normalised using equation 1 and 2. A concatenated matrix of these vectors is then generated, in which each row corresponds to a time step. The matrix is then transposed and then finally converted to a column vector. The column vector is then fed as an input vector for the neural network model. The corresponding output comprises of a column vector with normalised initial porosity, initial water saturation and solid density as its elements. These properties were then converted to dimensional form using equation 3, 4 and 5 respectively.

Equations for normalisation:

$$T^* = \frac{T - T_O}{T_\infty - T_O} \tag{1}$$

$$M_{av}^* = \frac{M_{av}}{M_O} \tag{2}$$

$$\rho_s^* = \frac{\rho_s - \rho_{s,min}}{\rho_{s,max} - \rho_{s,min}} \tag{3}$$

$$\phi_O^* = \phi_O \tag{4}$$

$$S_{wO}^* = S_{wO} \tag{5}$$

3.1.1 Input and output vectors formulation

Neural network input:

$$\underset{\text{Actual data}}{[T_c]_{t\times1}\ [T_s]_{t\times1}\ [M_{av}]_{t\times1}} \longrightarrow \left[[T_c^*]_{t\times1}\ [T_s^*]_{t\times1}\ [M_{av}^*]_{t\times1}\right]_{3t\times1} \longrightarrow \underset{\text{ANN input}}{\begin{bmatrix} T_c^* \\ T_s^* \\ M_{av}^* \end{bmatrix}_{3t\times1}}$$

Neural network output:

$$\underset{\text{ANN output}}{\begin{bmatrix} \emptyset_O^* \\ S_{wO}^* \\ \rho_O^* \end{bmatrix}_{3\times1}} \longrightarrow \underset{\text{Actual properties}}{\begin{bmatrix} [\emptyset_O \\ S_{wO} \\ \rho_s \end{bmatrix}_{3\times1}}$$

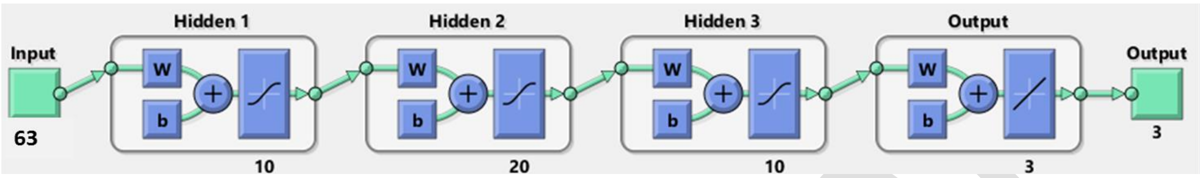
here t is the number of time-steps and equals to 21 for the present study.

3.2 Model development

The neural network model was developed using deep learning toolbox of a commercial software MATLAB R2017a. The curve fitting model was implemented for developing the prediction model. Levenberg-Marquardt optimization algorithm was used for backpropagation while training the model and tan-sigmoid and linear functions were used as transfer functions in the neural network. The data fed to the model was divided into training, validation and testing in the ratio 65:20:15. Data division was performed randomly.

Further details of the toolbox are given in its user-guide(Beale, Hagan, & Demuth, 1992) whereas details about neural networks, Levenberg-Marquardt optimization algorithm and backpropagation technique can be referred in the literature (Demuth, Beale, De Jess, & Hagan, 2014)

The accuracy of the model was very poor for single layer. Therefore, additional modifications in the code were performed to add hidden layers so as to implement deep learning in the neural network. In order to improve accuracy, various combinations of number of neurons and number of hidden layers were tried. For each tried case, model was run 15 times so as to ensure that accuracy sustains and the most suitable neural network was selected (shown in Fig. 3).



63-10-20-10-3 neural network

Fig. 3 - Selected deep learning-based neural network

Further to ensure the accuracy of the model for future runs, following selection criteria for output prediction were added in the neural network code:

1. Additional validation samples: While training the neural network model, an additional validation was performed on the unseen datasets that were not fed to the neural network model.
2. Termination criteria: While training, the developed neural network was made to run till the root mean square error of the predicted output for the fed data as well as additional validation data became less than 1%.

$$RMSE < 1\% \tag{6}$$

3. Range of predicted output: While training and application of model, the developed code checks if the predicted output meet following conditions:

$$0 < \phi_o < 1 \tag{7}$$

$$0 < S_{wo} < 1 \tag{8}$$

4. Initial moisture content criteria: While training and application of model, it is ensured that the predicted output values are consistent with the experimental value of initial moisture

content. This condition is put because initial moisture content is a combination of the characteristic input parameters and thus transport and deformation phenomena are sensitive to it.

$$\frac{\emptyset_o S_{wo} \rho_w}{(1-\emptyset_o)\rho_s} = M_{o,pred} \approx M_{o,experiment} \tag{9}$$

3.3 User approach

The developed neural network along with physics-based model could be implemented for prediction of drying process. The methodology is shown in Fig. 4. Firstly, a control experiment is performed for obtaining the neural network input data. Details of the control experiment is given in section 4. Neural network model predicts the characteristic input parameters which are then fed to physics-based model. The physics-based model then could be run for any desired condition by providing appropriate initial and boundary conditions.

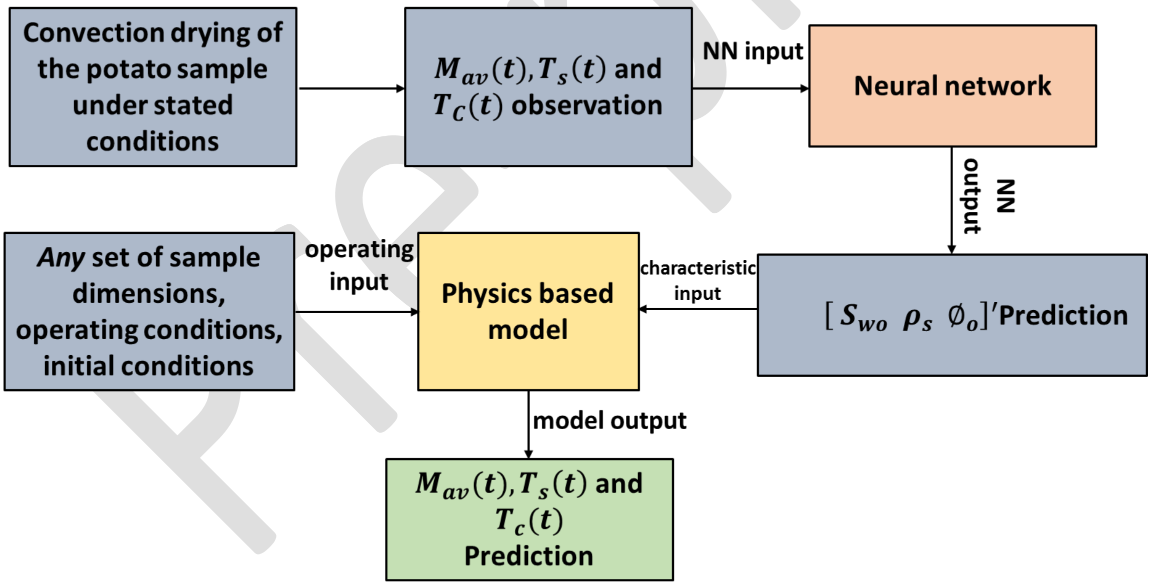


Fig. 4 - User approach for the model implementation

4. Materials and methods (Experiments' details)

In order to implement the developed neural network, a control experiment has to be performed first. The details of the controlled experiment performed during the validation of model is given below. For the application of the developed neural network in any commercial space or for research purpose, the similar control experiment is required to be performed.

Potato (*Solanum tuberosum*) were bought from a local market and were kept in cold storage. For each of the experiments, potatoes were bought to room temperature, washed, peeled and cut into cubes with each side measuring 14 mm. The excess moisture on the surface was wiped out gently using dry paper napkins.

Initial moisture content was measured using gravimetric method. The initial weight of the sample was measured and then it was dried in the oven at a temperature of $103^{o}C$ for 24 hours and then weighed again. Dry basis moisture content was measured as the ratio of difference of initial and final weight to the final weight of the sample. The experiment was repeated thrice so as to ensure replicability and the mean value was used as initial moisture content.

For conducting drying experiment (control experiment), the convection oven was maintained at a temperature of $60^{o}C$ by passing dry hot air (zero relative humidity) at a velocity of 1 m s^{-1}.

For measuring variation in temperature during drying, sample was kept in convection oven and thermocouples were attached at the surface and centre of the sample. The drying was performed for 20 minute and surface and centre temperature were recorded. The experiment was repeated thrice, each time with a fresh sample.

For average moisture content measurement, the sample was weighed and then put in convection oven for 1 minute. The sample was then taken out and weighed again. On the basis of initial moisture content and difference in sample weight, the moisture content of the dried sample was estimated. The experiment was repeated thrice. Same set of experiment is then repeated with an interval of 1 minute (i.e. drying for 2 minutes, 3 minutes etc.) for drying time up to 20 minutes.

In each of the above-mentioned experiments, sample once used was discarded and not used for other trial or other set of experiment.

5. Results and discussions

Results are presented in the following order. First, the performance of developed deep ANN model is discussed. Secondly, the developed neural network is further validated with new datasets that were not used in model development. Effect of changing neural network input variables and number of training datasets on the model performance is also described. Finally, the developed neural network is validated with experiments and the associated methodology and obtained results are discussed.

5.1 Performance of the developed deep neural network

Fig. 5 shows mean square error and error histogram. Error of less than 1e-2 for test data and less than 1e-6 for training and validation data was achieved in 250 epochs (Fig. 5(a)). Similarly, error histogram (Fig. 5(b)) shows that for maximum number of instances, difference between target and obtained output values was less than 0.0005. Thus, the model is in well agreement with the actual data.

5.1.1 Effect of number of datasets:

In order to analyse the effect of number of modelling datasets on the performance of model, another model with only 64 datasets (4 values for each of the 3 parameters) was developed. Fig. 6 show mean square error and error histogram for 64 datasets based model. Comparison of the plots show that though error while training is very less for small datasets, the model doesn’t achieve high accuracy during validation and test with small dataset. This is due to the overfitting that occurs when neural network model is developed with small datasets. The error increases further when the model is tested with data completely unseen to the model (not t used in training, validation or test while model development). This is further explained in the next section.

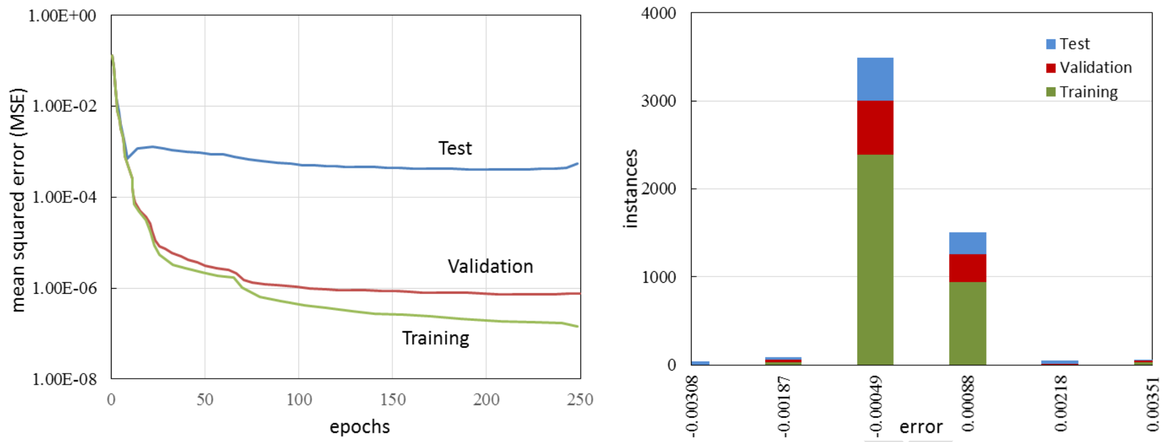


Fig. 5 - Performance plots for the neural network model with 1728 modelling dataset: (a) Mean square error (b) error histogram

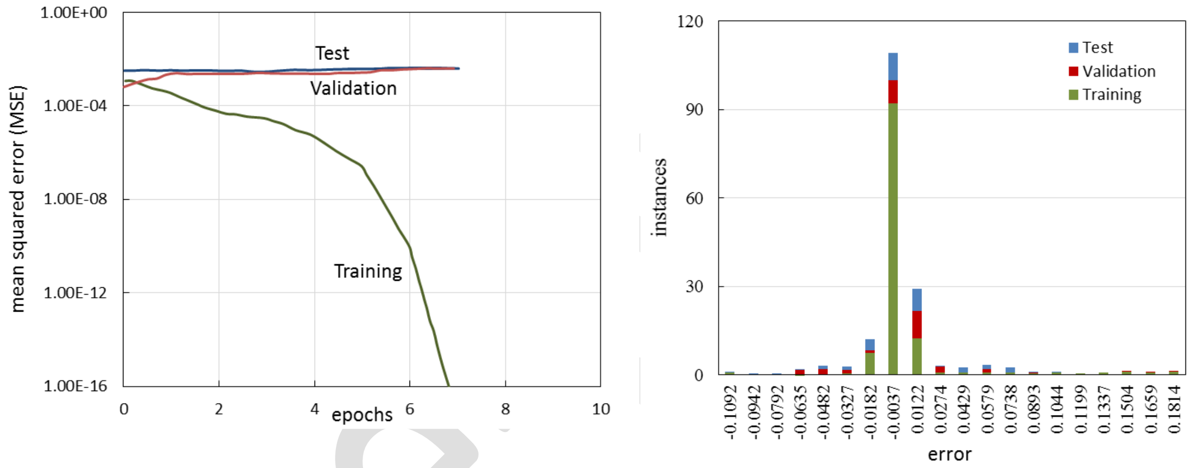


Fig. 6 - Performance plots for neural network model with 64 modelling datasets: (a) Mean square error (b) error histogram

5.2 Post-modelling tests

Six datasets were used to test the developed neural network model. None of these datasets were used during model development. Table 2 shows the error obtained for each of the fed input dataset. The model fits well for these unknown datasets as error less than 1% is observed for each case. Further, these six datasets were then tested on model developed with 64 datasets as described in previous section. The root mean square in this case increased up to 6% whereas true error increased up to 8% approximately as shown in Table 3. It is important to note that while the performance plots developed during the model development depicted very less error even for small datasets, the error actually amplified when tested for unknown datasets. This might happen due to the overfitting. Since a large number of independent variables (called as weights) are involved in neural network models, neural network tend to overfit the data for small datasets (Huang et al., 2007; Knight, 1990; Wythoff, 1993).

Table 2 Post-modelling test for the model trained with 1728 datasets, input variables: average moisture content, centre temperature and surface temperature, drying time: 20 min

Table 3 Post-modelling test for the model trained with 64 datasets, input variables: average moisture content, centre temperature and surface temperature, drying time: 20min

Dataset	$\emptyset_o$			ρ_s			S_{wo}			% RMSE
	actual value	ANN prediction	%error	actual value	ANN prediction	%error	actual value	ANN prediction	%error	
1	0.40	0.40	**-0.91**	1896.00	1893.88	0.11	0.65	0.65	0.19	**0.54**
2	0.88	0.88	0.01	1896.00	1895.25	0.04	0.66	0.66	-0.03	0.03
3	0.96	0.96	-0.03	2380.00	2380.85	-0.04	0.75	0.75	-0.03	0.03
4	0.74	0.74	0.00	1896.00	1896.08	0.00	0.78	0.78	0.00	0.00
5	0.94	0.94	-0.04	2700.00	2700.56	-0.02	0.89	0.89	-0.05	0.04
6	0.99	0.99	-0.05	1896.00	1897.03	-0.05	0.65	0.65	0.01	0.04

Dataset	$\emptyset_o$			ρ_s			S_{wo}			% RMSE
	actual value	ANN prediction	%error	actual value	ANN prediction	%error	actual value	ANN prediction	%error	
1	0.49	0.48	2.75	2200.00	2210.96	-0.50	0.60	0.60	-0.44	4.16
2	0.55	0.55	-0.16	1600.00	1706.46	-6.65	0.85	0.85	-0.09	2.54
3	0.73	0.72	0.80	2200.00	2296.72	-4.40	0.78	0.78	-0.48	2.07
4	0.99	1.00	-0.82	1600.00	1655.53	-3.47	0.85	0.84	1.36	4.56
5	0.99	0.90	9.39	2700.00	2490.88	**7.75**	0.60	0.60	-0.71	**5.46**
6	0.55	0.55	0.43	1100.00	1090.45	0.87	0.78	0.77	1.07	0.67

5.2.1 *Effect of input variables*

When instead of average moisture content, centre and surface moisture content was used as input variable along with centre and surface temperature; then the observed error decreases. For model trained with larger datasets, the error reduced from 0.54 % to 0.15% as shown in Table 4. Similarly, for smaller datasets, it reduced from 5.46 % to 3.86%. This is shown in Table 5. It is important to note that while using large datasets, the RMSE is below 1% for both the cases. . Besides, techniques for measuring surface and centre moisture during drying experiments are not readily available. Therefore, model having average moisture content, centre temperature and surface temperature as input variables when trained with large datasets serve as suitable models for predicting characteristic parameters.

5.2.2 Effect of drying time

As mentioned in the modelling section, it was observed that maximum variation in temperature and moisture was observed within first 20 minutes of drying. In order to further validate that 20-minute data suffice for the development of neural network model, a 20-minute data-based modelling was compared with modelling using 100 min data. Post-modelling tests results are shown in Table 5 and

Table ***6*** respectively. It is evident that the order of error for both the cases remain same. To further ensure this, the model was run multiple times and no significant variation in the order for both the cases model was observed. Although, using 100 min drying data increases the number of variables in the model and thus often led to overfitting and thus error incurred in post modelling test was higher.

Table 4 Post-modelling test for the model trained with 1728 datasets, input variables: centre moisture content, surface moisture content, centre temperature and surface temperature, drying time: 20min

Dataset	$\emptyset_o$			ρ_s			S_{wo}			% RMSE
	actual value	ANN prediction	%error	actual value	ANN prediction	%error	actual value	ANN prediction	%error	
1	0.40	0.40	-0.13	1896.00	1894.72	0.07	0.65	0.65	**0.21**	**0.15**
2	0.88	0.88	0.08	1896.00	1895.92	0.00	0.76	0.76	0.00	0.04
3	0.96	0.96	-0.03	2380.00	2380.36	-0.02	0.75	0.75	0.03	0.03
4	0.74	0.74	0.00	1896.00	1895.78	0.01	0.78	0.78	-0.01	0.01
5	0.94	0.94	0.04	2700.00	2698.82	0.04	0.89	0.89	-0.03	0.04
6	0.99	0.99	-0.01	1896.00	1896.16	-0.01	0.65	0.65	-0.01	0.01

Table 5 Post-modelling test for the model trained with 64 datasets, input variables: centre moisture content, surface moisture content, centre temperature and surface temperature, drying time: 20min

Dataset	$\emptyset_o$			ρ_s			S_{wo}			% RMSE
	actual value	ANN prediction	%error	actual value	ANN prediction	%error	actual value	ANN prediction	%error	
1	0.49	0.49	-0.29	2200.00	2200.30	-0.01	0.60	0.59	0.85	0.52
2	0.55	0.55	-0.81	1600.00	1586.12	0.87	0.85	0.85	-0.11	0.69
3	0.73	0.73	0.18	2200.00	2229.61	-1.35	0.78	0.78	0.23	0.80
4	0.99	0.99	0.41	1600.00	1612.83	-0.80	0.85	0.85	-0.23	0.54
5	0.99	1.00	-1.42	2700.00	2719.78	-0.73	0.60	0.64	**-6.50**	**3.86**
6	0.55	0.57	-3.80	1100.00	1127.81	-2.53	0.78	0.80	-2.32	2.96

Table 6 Post-modelling test for the model trained with 64 datasets, input variables: centre moisture content, surface moisture content, centre temperature and surface temperature, drying time: 20min

Dataset	$\emptyset_o$			ρ_s			S_w			% RMSE
	actual value	ANN prediction	%error	actual value	ANN prediction	%error	actual value	ANN prediction	%error	
1	0.49	0.48	3.00	1600.00	1571.21	1.80	0.85	0.86	-0.61	2.05
2	0.55	0.55	-0.29	2200.00	2140.75	2.69	0.60	0.60	-0.61	1.60
3	0.55	0.53	4.35	2700.00	2526.89	6.41	0.60	0.62	-3.22	**4.84**
4	0.55	0.55	0.56	2700.00	2669.00	1.15	0.78	0.78	-0.18	0.75
5	0.73	0.73	-0.13	2700.00	2620.11	2.96	0.90	0.89	1.09	1.82
6	0.99	1.01	-2.07	1100.00	1142.39	**-3.85**	0.60	0.62	-2.98	3.06

5.3 Experimental validation

The developed methodology was validated with experiments. Steps involved in the procedure are shown in Fig. 7. Table 7 shows the estimated characteristic input parameters. In order to check the accuracy of parameters, a physics-based simulation was performed using these parameters. Comparison of the predicted behaviour and experimental observations is shown in Fig. 8. The observed absolute error was up to 15% whereas the overall root mean square error was less than 5%. Various possible sources of error in the experiments include moisture susceptibility while taking out and weighing the sample, displacement of the thermocouple due to sample shrinkage, varied initial temperature, temperature fluctuations in convection oven, instrumentation error and other human error.

Table 7 Estimated characteristic input parameters

Property	Symbol	Value
Initial porosity	$\emptyset_0$	0.909
Initial water saturation	S_{w0}	0.9538
Density of solids	ρ_s	2995.84 kg/m^3

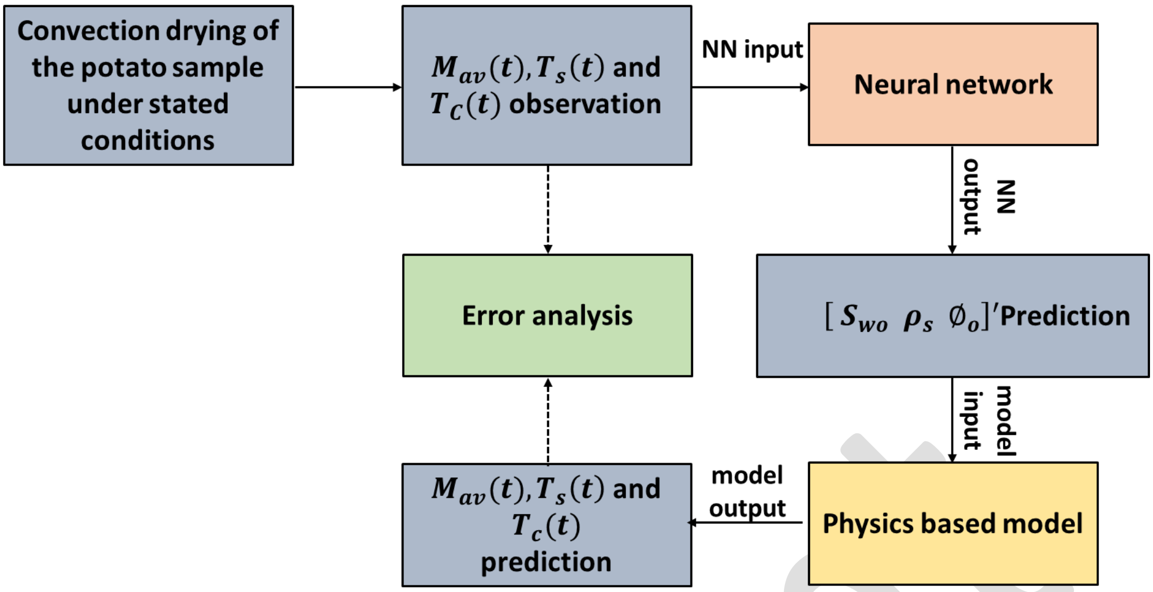


Fig. 7 - Schematic representation of steps involved in validation of the ANN model

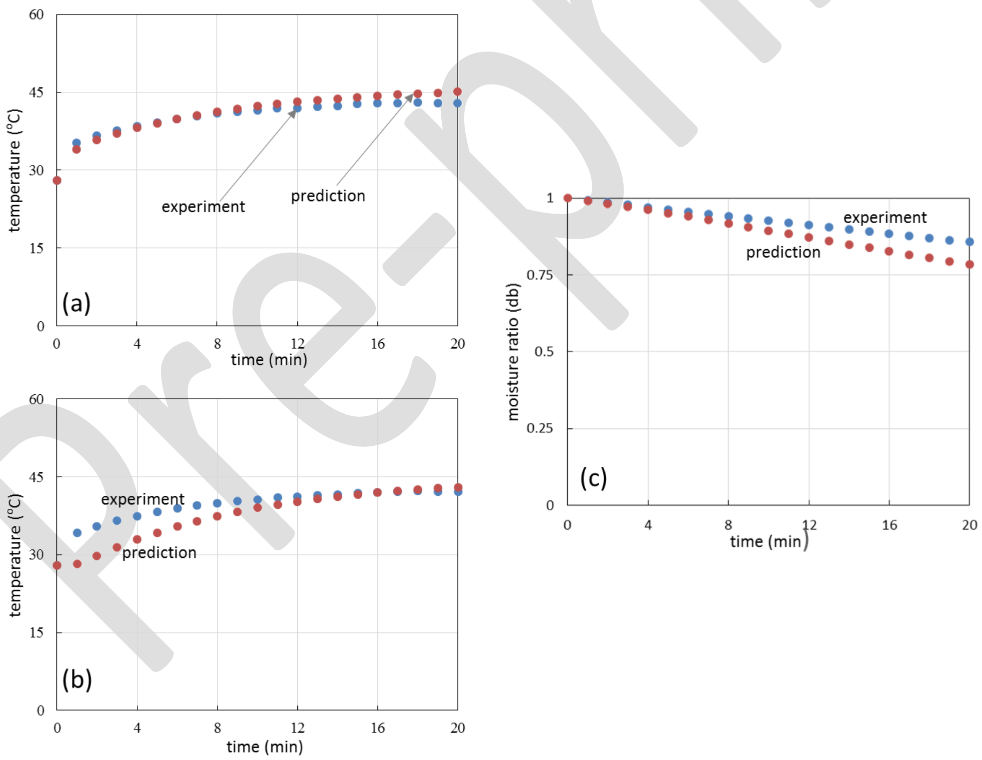


Fig. 8 - Prediction of transport behaviour using ANN and physics-based model and its comparison with experimental results: (a) variation in surface temperature with time (b) variation in centre temperature with time (c) variation in average moisture

6. Conclusions

A novel methodology for estimating sensitive input parameters for food materials has been developed and its utility in physics-based modelling is discussed. The major conclusions from the study are:

1. Neural network models could serve as an effective indirect method of properties estimation in food materials.
2. A small initial period data of a controlled drying experiment is sufficient to predict characteristic parameters accurately.
3. In case of the availability of large datasets, surface temperature, centre temperature and average moisture content are sufficient model inputs for neural network model development.
4. Artificial neural network when coupled with physics-based modelling altogether could serve as a promising methodology for prediction modelling of food processes.

This work could be extended further to develop a commercial interface for properties prediction as well prediction and optimization of transport and deformation behaviour in food materials, while processing. The applicability of neural network modelling in other aspects of food engineering could also be explored in future.

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Conflict of Interest

The authors declare that they do not have any conflict of interest.

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