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ORIGINAL ARTICLE

Comparison of Gaussian process regression, artificial neural network, and response surface methodology modeling approaches for predicting drying time of mosambi (*Citrus limetta*) peel

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Abstract

In this study, drying kinetics of mosambi peel was studied. The effect of three variables viz., temperature (50, 58, 70, 82, and 90 °C), salt concentration (2, 5, 8, and 10%), and thickness of drying bed (1, 2, 3, and 4 mm) on drying time was determined by the central composite design. Applicability of Gaussian process regression (GPR)-based approach for modeling drying kinetics was analyzed. GPR-based model was compared with the commonly used approaches like artificial neural network (ANN) and response surface methodology (RSM). The models were validated by comparing model simulations with observed values for unseen data. The models were compared based on performance indices like coefficient of determination, mean square error, root mean square error (*RMSE*), model predictive error, mean average deviation, goodness of fit, and chi-square analysis. All the three models fit both seen and unseen data excellently. *RMSE*, mean average deviation, and model predictive error for the unseen data of the GPR-based model were minimum (0.191, 0.285, 6.8%, respectively) followed by ANN (0.35, 0.298, 7.2%, respectively) and RSM (1.162, 0.905, 32.0%, respectively).

Practical applications

Modeling of the drying process is very important for control of industrial dryers. Several attempts have been made to model drying kinetics using RSM and ANN. This study shows the efficiency of GPR in modeling the drying kinetics of mosambi peel for the first time. GPR-based models were found to be a better alternative to RSM and ANN. This will help in developing more accurate models and increase the efficiency of drying.

1 | INTRODUCTION

Mosambi (*Citrus limetta)* belongs to Rutaceae family of genus Citrus. Mosambi fruit is mostly consumed in the form of juice because of the difficulty to separate the peel and slices from each other (Manthey & Grohmann, 2001). During the extraction of juice, the by-product which includes peel, pulp, and seeds is obtained and accounts for about half of the weight of whole fruit (Licandro & Odio, 2002). Peel of the fruit is quantitatively the top by-product obtained and despite possessing good nutritional value, has no direct use in human diets because of its bitter taste. The peel is usually discarded or used as fuel because of lack of processing facilities for the same.

Nowadays, the detrimental effects on health due to the changes in eating habits and lifestyle have created a huge pressure on the food scientists to develop the new healthy or functional foods. Our diets are deficient in dietary fiber content and are high in sugar, salt, and spices, posing ill consequences on our health. Mosambi peel is rich in dietary fiber and has been successfully incorporated in different foods after removing its bitterness. Treatment with sodium chloride has been reported to successfully remove the bitterness of the peel

(Younis, Islam, Jahan, Yousuf, & Ray, 2015). The powder of debittered mosambi peel may act as a potential source of dietary fiber in low fiber foods. The addition of mosambi peel results in increased dietary fiber content in food products (Younis, Islam, Jahan, Kundu, & Ray, 2016). Besides enhanced fiber contents, the incorporation of peel may affect other sensory properties of food as well. In a study conducted by Younis et al. (2015), the use of mosambi peel powder significantly improved quality parameters of jam.

Drying provides many advantages, for instance, reduction in bulk, long shelf life, least packaging requirements among others (Qadri & Srivastava, 2017). Drying is an important step in the preparation of powder. Proper drying is required to bring the moisture content of peel to the required concentration. The particle size of the powder and ease of grinding is dependent on the moisture content of peel (Larrauri, 1999). Drying of the foods usually affects the overall quality and over drying of the food may reduce the nutritional value of the powder (Mphahlele, Fawole, Makunga, & Opara, 2016). For accurate control of the drying process in industrial driers, it is important to have a good understanding of the process. Therefore, it is important to develop models of the drying process. Models are important for gathering insight into the process as well as for predicting future outcomes. They are essentially an approximation of the reality. There is no single model which is a true representation of the reality. The purpose of modeling is to understand the process in question. But every model is only an approximation of reality and not a full reality (Renshaw, 1993). Different approaches are present for modeling in food engineering. RSM and ANN have been used and proved to be an efficient tool for modeling and optimization of drying kinetics of food products (Maran, Sivakumar, Thirugnanasambandham, & Sridhar, 2013). ANN modeling to predict drying kinetics of different foods has been undertaken recently by different researchers, for instance, cassava and mango (Hernandez-Perez, Garcıa-Alvarado, Trystram, & Heyd, 2004), carrot (Kerdpiboon et al., 2006), and *Echinacea angustifolia* (Erenturk & Erenturk, 2007). Similarly, RSM has been used to model and optimize the drying of various products (Erbay & Icier, 2009; Varnalis, Brennan, MacDougall, & Gilmour, 2004). RSM has been found to overpredict the results occasionally resulting in errors, especially for complex models. ANNs have been reported to be better than RSM in modeling complex data (Desai, Survase, Saudagar, Lele, & Singhal, 2008).

ANNs are machine learning approaches which mimic the function of the biological neural network (Osama, Somvanshi, & Mishra, 2015). They have the capability of learning complex and noisy data. Neural networks are complex models and may not always be friendly to work with. Gaussian process models are nonparametric techniques which are gaining popularity in the field of machine learning (Vapnik, 2013). They are simpler than neural networks and are easy to use. The Gaussian process models are flexible and conceptually simpler to understand. Unlike ANNs, which are deterministic models, Gaussian Process Regression (GPR)-based models are probabilistic models based on Gaussian distribution (Williams & Rasmussen, 1996).

RSM, ANN, and GPR are three very different approaches for modeling engineering processes. In this study, the usability of GPR in modeling of drying process was checked and the results were compared with commonly used methods like RSM and ANN. This study is one of the first of its kind, to the best of the knowledge of authors, in which GPR modeling of the drying of food products has been attempted.

The objective of the study was to analyze the effect of air temperature, salt concentration, and drying bed thickness on drying kinetics of mosambi peel. The drying process was modeled using RSM, ANN, and GPR. The comparison of the efficiency of modeling approaches viz., RSM, ANN, and GPR in understanding drying behavior was made. Performance of the models was analyzed on their ability to predict unseen data and other parameters.

2 | MATERIALS AND METHODS

Mosambi peel was collected from the juice vendors of Lucknow and was washed and blanched at 100 °C for 2 min to reduce its microbial load and to soften its texture for easy grinding. Grinding was done to break the large pieces of peel into coarse particles resulting in an increase in surface area for efficient debittering. A different concentration of sodium chloride (2, 5, 8, and 10% w/w) was added to the peel. Water was added in a proportion of 1:1 (v/w) to the peel and the slurry was kept overnight for the debittering treatment. The slurry was washed in running water to remove the salt and bitter compounds. The washed slurry was pressed and hanged for 2 hr in a muslin cloth to drain excess water and the final moisture content reached around 85%. The debittered slurry of different thickness (1, 2, 3, and 4 mm) was dried in hot air oven at different temperatures (50, 58, 70, 82, and 90 °C). All the samples were dried up to 10% final moisture content. The whole procedure is depicted in Figure 1.

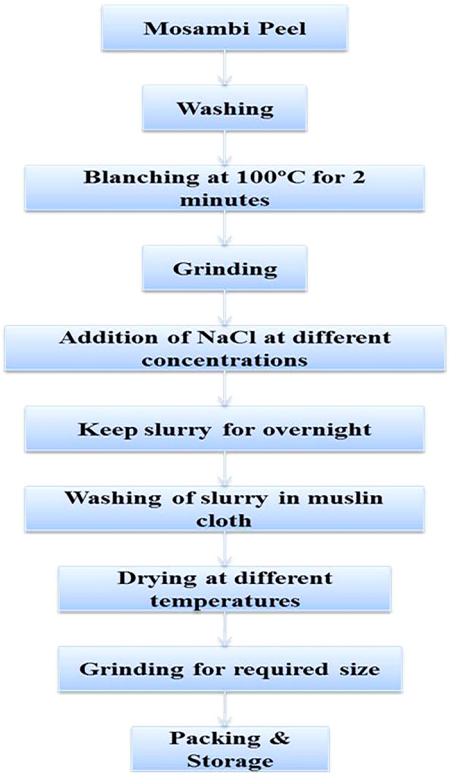

FIGURE 1 Preparation of mosambi peel powder

TABLE 1 Coded and un-coded values of independent variables

	Coded values				
Variables	**−1.6818**	**−1**	**0**	**1**	**1.6818**
Thickness (mm)	1	2	3	4	5
Temperature (°C)	50	58	70	82	90
Salt (%)	0	2	5	8	10

2.1 | Modeling drying kinetics

Response Surface Models are multivariate polynomial models used to optimize processes. In this study, effect of temperature, salt concentration, and thickness of the bed on the drying time was modeled. A five-level circumscribed central composite design (CCD) containing 15 experiments was developed. The summaries of coded and uncoded values are given in Table 1. The design was developed using "ccdesign" function of the Statistics and Machine learning toolbox of MATLAB 8.6.0 (R2015b) (The MathWorks Inc., Massachusetts, U.S.). Drying experiments were performed thrice for each combination and the intermittent weight of the sample was recorded after every 30 min till the final moisture content reached 10%. The time of drying was then modeled based on salt concentration, temperature, and thickness of bed. A quadratic model was developed using "regstats" function of Statistics and Machine learning toolbox of MATLAB 8.6.0. The model was then used to predict the time of drying for unseen data to validate the robustness of the model.

$$Y = K_0 + K_1X_1 + K_2X_2 + K_3X_3 + K_4X_1{}^*X_2 + K_5X_1{}^*X_3 + K_6X_2{}^*X_3 + K_7X_1\hat{2} + K_8X_2\hat{2} + K_9X_3\hat{2}$$

Where Y is the time of drying, X_1 is the thickness of bed in millimeters, X_2 is the temperature in degree Centigrade, and X_3 salt concentration in %. K values are coefficients of individual, interaction, and square effects.

GPR was also used to model the effect of temperature, the thickness of bed, and salt concentration at the time of drying. A Gaussian Process is a collection of random variables, such that when these variables are collected in a finite number they represent a Gaussian distribution. Regression models based on Gaussian processes are simple to implement, flexible, fully probabilistic, and thus, a powerful tool in many areas of application (Rasmussen, 2004). For large training data, however, GPR requires more memory and computational power. This limits its application to problems with more than a few thousand cases in a data set. They have gained popularity because they allow the exact Bayesian analysis with simple matrix manipulation and still provide a good approximation. Like support vector machine they allow the direct specification of the smoothness and properties of the class of functions under consideration (Smola & Bartlett, 2001).

The model was developed using "fitrgp" function of statistics and machine learning toolbox of MATLAB 8.6.0. The CCD design data was used to train the GPR model. Different combinations of basis function, Kernel (Covariance) function, and fit method (method to estimate the parameters of the GPR model) were tested. The model was then evaluated on its ability to predict the training data set and the validation data set.

Additionally, the Neural Network model was also prepared to model drying kinetics. Neural network toolbox of MATLAB 8.6.0 was used to design feed forward neural network. Different architectures of neural network were designed and trained to find the best architecture. The networks were trained using different transfer and training functions. The performance of the trained networks was then analyzed based on their capability of predicting both seen and unseen data. The networks were trained using the CCD design and were then tested using additional experimental data which was not presented to the network during training.

2.2 | Model comparison

The tree models developed were then compared, based on their capability to predict the effect of different parameters that is, temperature, thickness of bed, and salt concentration at the time of drying. Different parameters like coefficient of determination, mean square error, root mean square error (*RMSE*), model predictive error, mean average deviation, goodness of fit, and chi-square analysis (Table 2) were determined to analyze the model efficiency in predicting seen and unseen data. The null hypothesis in the Chi-square test for goodness of fit was that there is no significant difference between observed values and model prediction. While the alternate hypothesis was that the model predictions and the observed values differ significantly.

3 | RESULTS AND DISCUSSION

The mosambi peel was dried to 10% moisture content. The time of drying was observed for different combinations of temperature, salt concentration, and bed thickness. It was observed that the time of drying decreased on decreasing the bed thickness and increasing temperature. The mosambi peel was pre-treated with sodium chloride to reduce the bitter taste. The effect of salt pretreatment on the time of drying was observed. It was found that the minimum time required to dry the mosambi peel was at a thickness of 1 mm, drying temperature of 70 °C, and sodium chloride concentration of 5% (Table 3).

Different computational techniques were compared for their efficiency in modeling the drying process. In the present study, three different approaches commonly used for modeling food engineering processes were compared to find the better approach. Around 70% of the experimental data was used for training the models and 30% data was used to validate the model performance. The models were used

TABLE 2 Error functions

Error function	Equation	Reference
RMSE	$RMSE = \sqrt{\sum_{i=}^{n}\left(Y_{i,e} - Y_{i,p}\right)^2 \Big/ n}$	Youssefi et al. (2009)
Mean absolute deviation	$MAE = \frac{1}{n}\sum_{i=1}^{n}\left\|Y_{i,e} - Y_{i,p}\right\|$	Youssefi et al. (2009)
Model predictive error	$MPE = \frac{100}{n}\sum_{i=1}^{n}\left\|\frac{Y_{i,e} - Y_{i,p}}{Y_{i,p}}\right\|$	Maran et al. (2013)
Chi-square statistic	$\chi^2 = \sum_{i=1}^{n}\frac{\left(Y_{i,p} - Y_{i,e}\right)^2}{Y_{i,p}}$	Çelekli and Geyik (2011)
Correlation coefficient	$R^2 = \frac{\sum_{i=1}^{n}\left(Y_{i,p} - Y_{i,e}\right)}{\sum_{i=1}^{n}\left(Y_{i,p} - Y_e\right)^2}$	Sinha et al. (2013)

TABLE 3 Comparative response of different models for seen data

Thickness (mm)	Temperature (°C)	Salt (g/L)	Total time	RSM predicted time	ANN predicted time	GPR predicted time
4	90	5	3.5833	4.2600	3.9541	3.5877
2	82	2	3	3.8264	3.4213	2.9371
2	82	8	3	3.7374	3.5124	3.0446
3	82	2	4.8333	3.4787	4.0125	4.7851
3	82	8	4.8333	3.5526	4.1254	4.8926
1	70	5	1	0.7186	0.8954	0.9824
4	70	5	6	6.0619	5.9547	6.0174
4	70	0	6.6167	6.5569	6.2147	6.6743
4	70	10	7.1667	7.1251	7.2458	7.1090
5	70	5	9	9.1407	8.9574	9.0001
2	58	2	5	4.5101	4.8974	4.9373
3	58	8	7.5	8.5394	8.0147	7.3586
3	58	2	7.0833	8.2571	7.8541	7.1612
2	58	8	5	4.6295	5.0124	5.1337
4	50	5	20	19.222	20.1354	19.9956

to predict both seen and unseen data (Table 4). The performance of models was evaluated, based on different parameters.

Multivariate Regression of the drying data was done using a statistical toolbox of MATLAB. The quadratic Response Surface Model showing a relationship between the independent variables (temperature, salt concentration, and bed thickness) and the time of drying was obtained as shown in the equation.

$$Y = 48.7478 + 11.9662^{*}X_1 - 1.6721^{*}X_2 - 0.2621^{*}X_3 + 0.3244^{*}X_1{}^2 + \ + 0.0142^{*}X_2{}^2 + 0.0312^{*}X_3{}^2 - 0.1706^{*}X_1{}^{*}X_2 + 0.0271^{*}X_1{}^{*}X_3 - 0.0014^{*}X_2{}^{*}X_3$$

Where, Y is the response that is, the time of drying in hours and X_1, X_2, and X_3 are the uncoded values of the independent variables bed thickness, air temperature, and salt concentration, respectively. The goodness of fit of the model predicted data with experimental results was evaluated using a statistical toolbox of MATLAB. The "goodness of fit" function of MATLAB tests the model prediction with target data, based on the specified cost function. The cost function used in this study was normalized root mean square error. The regression model showed a very good fit with the target data with a value of 0.8180. Normalized root mean square error cost vary from -∞ for very bad fit to 1 for a perfect fit. The coefficient of determination (R^2) for the regression model was 0.967 and the adjusted R^2 was 0.964 for the seen data (Figure 2). This indicated that the model was able to explain 96% of the variations in the target data. However, to validate the model, prediction of unseen data by the model was made. Six experiments were performed on random combinations of independent variables and time of drying was observed. These combinations were not present in the design of the experiment used to develop the model. The regression model was then used to predict the time of drying for these combinations. The regression model was able to predict 60% of the variations in the unseen data set (R^2 = 0.66 and adjusted R^2 = 0.57). RSM has been extensively used as an optimization tool in drying studies (Jangam & Thorat, 2010; Šumić et al., 2016).

3.1 | Development of an ANN-based model

A three-layered feedforward ANN was used to model the drying kinetics of the mosambi peel. To find the best architecture of ANN the number of hidden layers in the network was varied from 2 to 10. Increasing the number of nodes in the hidden layer increases the complexity of the model and the chances of network overfitting the training data. The best performing network was found to have three nodes in the hidden layer. The final network had three nodes in input and hidden layer and one node in the output layer. The transfer function for input and output layer was linear while in hidden layer hyperbolic tangent sigmoidal transfer function was found to be the most efficient. The network was trained using Lavenberg–Marquardt training function. The training data was same as that of the regression model. The network showed a good fit for the target data with the goodness of fit value of 0.8964 using normalized root mean square error cost function for the training data set. The R^2 for the training data set was 0.99 and the adjusted R^2 was 0.99 (Figure 2). This shows that the neural network model was highly effective and could explain 99% of the

TABLE 4 Comparative response of different models for unseen data

Thickness (mm)	Temperature (°C)	SALT (g/L)	Total time	RSM predicted time	ANN predicted time	GPR predicted time
3	80	5	4.833	3.05	4.223	2.738
2	70	2	4	2.1398	4.238	2.2020
4	70	2	6.23	6.1894	6.164	6.2017
4	80	5	4.833	3.7745	5.035	5.2675
2	80	5	3	2.9743	3.524	0.8450
3	70	2	4.5	3.8402	4.354	3.8769

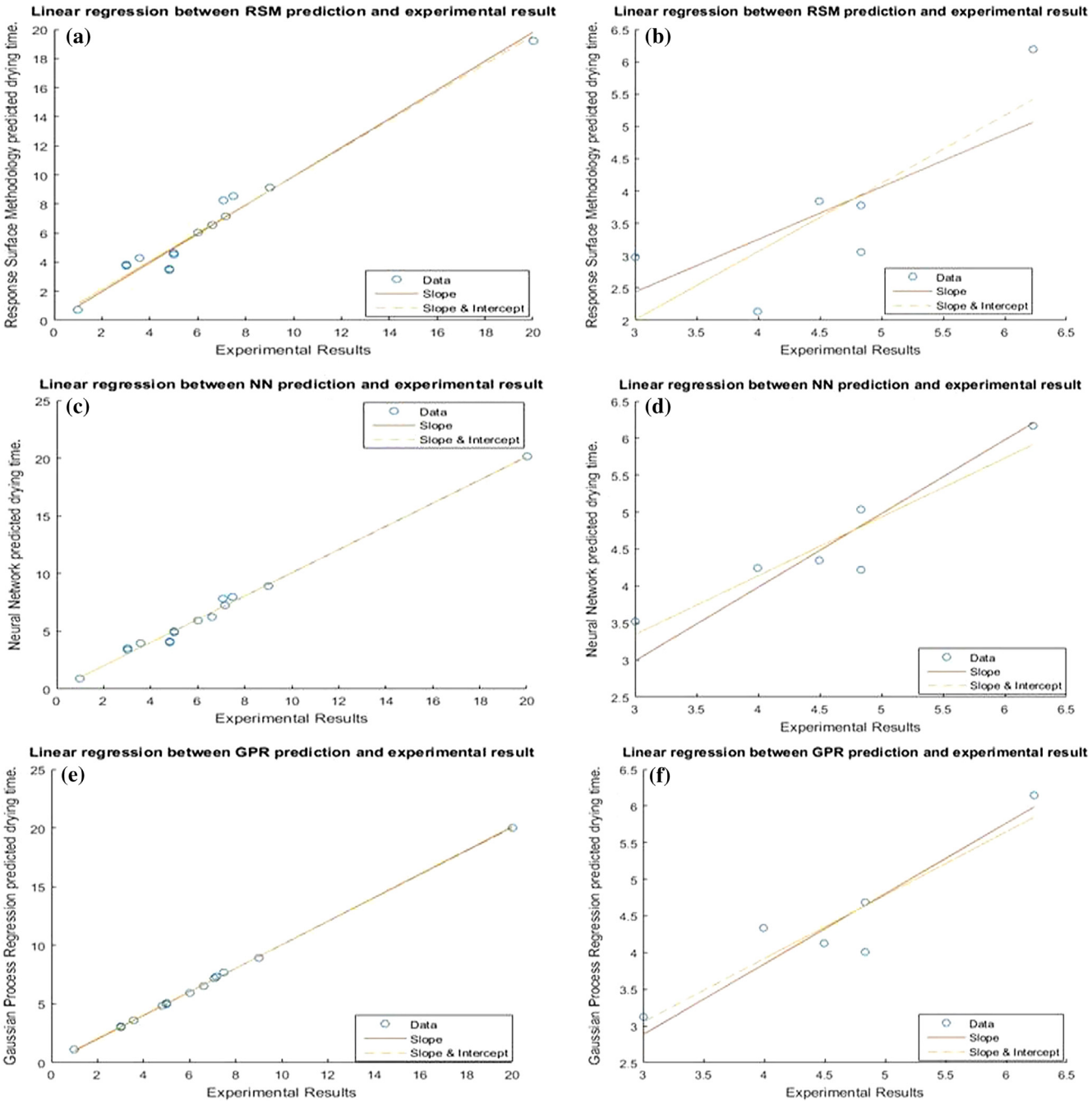

FIGURE 2 Linear regression of models. (a) Linear regression of response surface methodology for seen data. (b) Linear regression of response surface methodology for unseen data. (c) Linear regression of artificial neural network for seen data. (d) Linear regression of artificial neural network for unseen data. (e) Linear regression of Gaussian process regression for seen data. (f) Linear regression of Gaussian process regression for unseen data

variations in the training data set. To check the model's capability and predict unseen data it was validated with a test data set containing six data. The neural network model was able to predict unseen data with good efficiency. The R^2 for the test data was 0.87, that is, the model was able to predict the test data set with 87% accuracy.

3.2 | Development of GPR-based model

Gaussian Process-based models are flexible and more practical than parametric models like feed-forward neural networks. In this study, a Gaussian Process-based regression model was developed and trained using Statistics and Machine Learning Toolbox of MATLAB 8.6.0. The covariance (Kernel) function used for defining the Gaussian Process model was "ARD Squared Exponential Kernel" function. This covariance function is the exponential kernel function, with a separate length scale for each predictor. It is defined as

$$(x_i, x_j \mid \theta) = \sigma_f^2 exp\left(- \sqrt{\sum_{m=1}^{d} \frac{(x_{im} - x_{jm})^2}{\sigma_m^2}} \right)$$

Where, x_i, x_j are response variables, $f2$ is standard deviation, θ is Kernel vector.

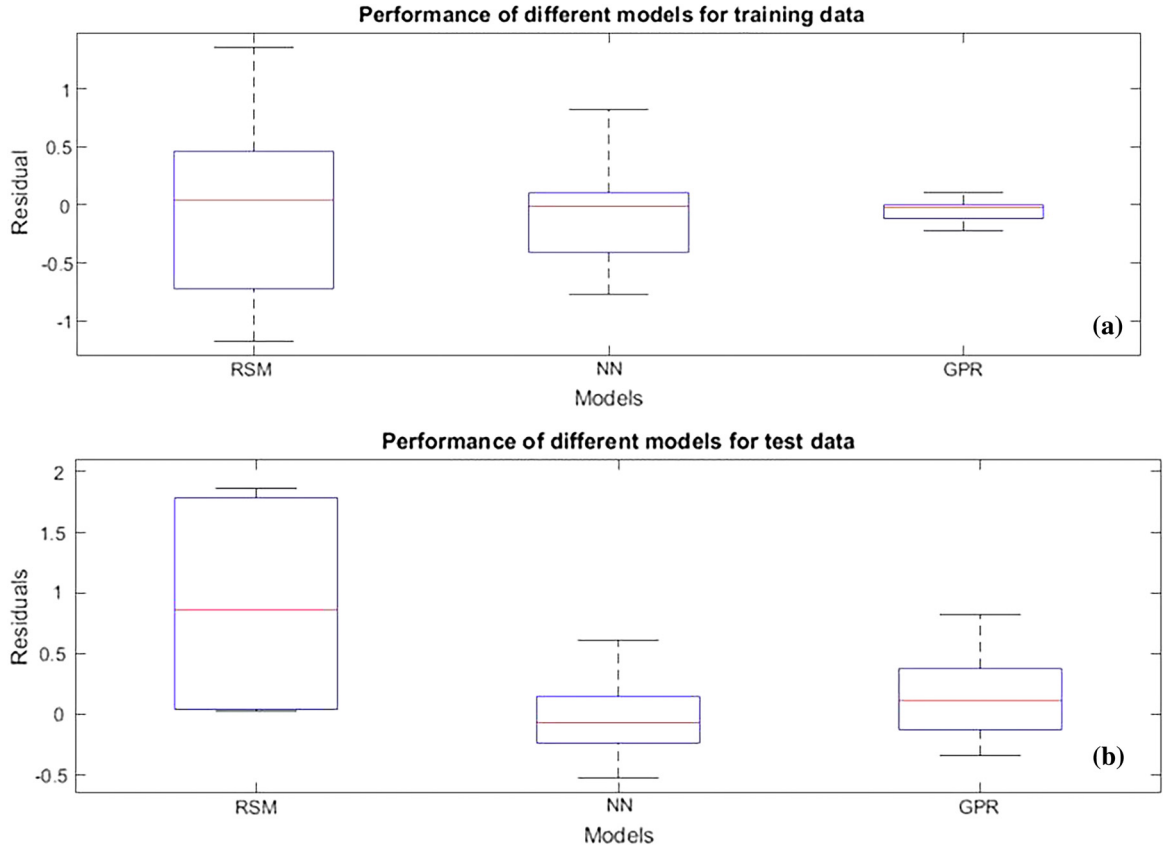

FIGURE 3 Comparison of box plot of residuals of response surface methodology, artificial neural network, and Gaussian process regression for seen (a) and unseen (b) data

The GPR model was very efficient and it predicted the training data set with excellent efficiency. The goodness of fit was 0.9747 using normalized root mean square error-based cost function. The model was able to predict the training data with 99.9% efficiency (R^2 = 0.9998 and adjusted R^2 = 0.9997). The model was also able to predict the unseen data with good efficiency. The R^2 for the unseen data was 0.82 and adjusted R^2 was 0.77 (Figure 2).

3.3 | Comparison of models

All the three models tested in this study fit the observed values. Chi-square test revealed that the null hypothesis was accepted in all the three cases. The GPR model was found to be a better predictor of both seen and unseen data (Figure 3). Error in prediction was least in GPR followed by ANN and RSM (Figure 4). The *RMSE* of the GPR model for seen data was 0.067 while that of RSM and ANN was 0.762 and 0.434. Similarly, the mean average deviation (MAD) of both seen and unseen data was calculated. The MAD values ranged between 0.0527 and 0.621 where the minimum value (0.0527) was obtained for the GPR model for seen data and the maximum MAD value (0.621) was obtained for RSM for seen data. For unseen data, GPR model produced minimum *RMSE* of 0.191 while RSM produced maximum *RMSE* of 1.36. ANN was found to be a better predictor than RSM with *RMSE* of 0.188 for the seen data and 0.358 for the unseen data. Mean absolute percentage error (MAPE) was calculated and GPR produced minimum MAPE of 1.1% for seen data and 3.4% for unseen data. Mean absolute percentage error of RSM for seen data was 13.95% and for unseen data was 32.023%. GPR was also found best in terms of R^2 with a value of 0.99 for the seen data and 0.82 for the unseen data (Table 5). So, GPR proved to be an efficient technique for modeling of the drying kinetics of mosambi peel.

The objective of this study was to establish the usability of GPR in modeling drying process and to compare it with existing methods. Therefore, only three independent variables were chosen during the experiment. However, there are various other parameters that affect the rate of drying like the size of a particle of mosambi peel, air velocity, relative humidity, the composition of peel, etc. These factors were not considered in this study. This lack of predictors has affected the predictive capability of the models and that is evident from the low values of R^2. R^2 is dependent on the number of independent variables and the value improves on adding more number of variables. The value of R^2 and the adjusted R^2 using GPR approach is slightly lower than that using ANN. However, other indices like *RMSE*, MAD, MPE were better in case of GPR compared to ANN. Also, the deviation of the residuals was small in the case of GPR followed by ANN and RSM for both seen and unseen data (Figure 3). So, GPR can be considered as a better technique compared to RSM and ANN.

There are several studies that have compared RSM and ANN for modeling of different processes (Desai et al., 2008; Gomes & Awruch, 2004; Pathak et al., 2015; Youssefi, Emam-Djomeh, & Mousavi, 2009). Both models were compared based on their capability of predicting both seen and unseen data. The parameters used for this comparison included the R^2, *RMSE*, Mean Square

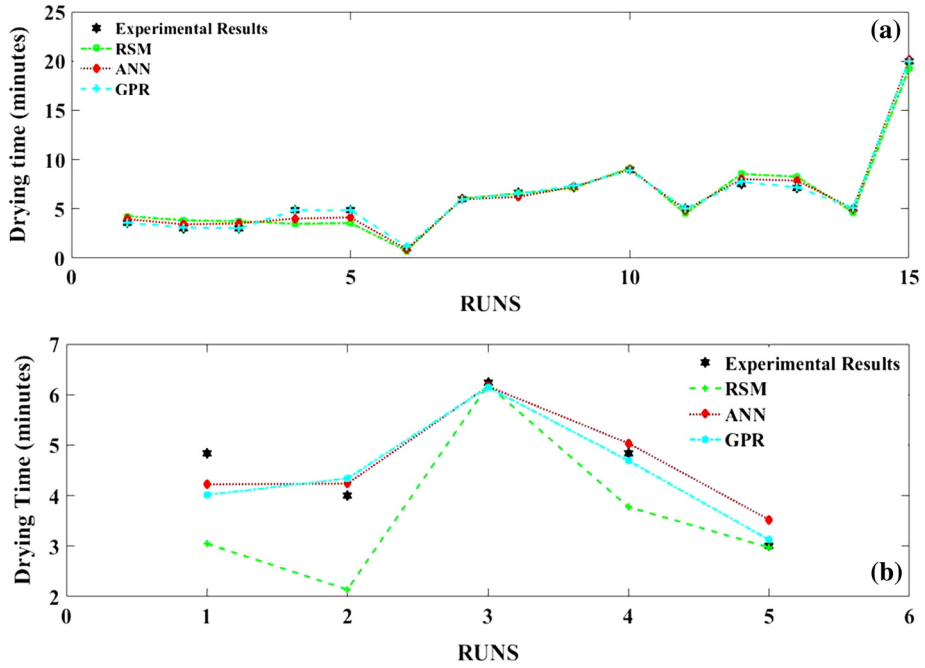

FIGURE 4 Comparison of the predictive capability of response surface methodology, artificial neural network, and Gaussian process regression for seen (a) and unseen (b) data

TABLE 5 Model comparison

	Response surface methodology		Artificial neural network		Gaussian process regression	
Statistical parameter	Seen data	Unseen data	Seen data	Unseen data	Seen data	Unseen data
RMSE	0.762	1.169	0.434	0.358	0.106	0.191
Mean absolute deviation	0.621	0.905	0.336	0.298	0.081	0.285
Model predictive error (%)	14.981	32.023	7.575	7.228	2.101	6.816
Chi square statistic	1.942	3.070	0.602	0.193	0.044	0.000
Correlation coefficient	0.983	0.812	0.995	0.934	1.000	0.923

Error, Average Deviation, etc. ANN proved to be a better approach when compared with RSM. In a study conducted by Youssefi et al. (2009), on comparison of RSM and ANN models for prediction of quality parameters of spray-dried pomegranate juice, the authors found that ANN model was able to predict the quality parameters of juice during drying more accurately compared to RSM. ANN has an advantage over RSM where one has to develop multiple response models. RSM comprises of only quadratic models limiting its ability to explain complex data sets. ANNs can learn complex nonlinear data sets with good accuracy (Osama, Somvanshi, Pandey, & Mishra, 2013).

There are currently no reports on the application of GPR in modeling drying kinetics in food engineering. Although, neural networks are accurate and provide a good approximation, they are difficult to tune with structural parameters. The convergence of the neural network model, as well as the accuracy, greatly depends on the initialization of the weights (Yuan, Wang, Yu, & Fang, 2008). Neural network models occasionally lead to overfitting while minimizing the training cost function. In addition to that, they require prior data of the process. The quality of network prediction largely depends on the quality and quantity of the training data.

Although, ANN and GPR are both heuristic approaches, conceptually they are very different. GPR requires fewer data compared to ANN and is easy to use. There is no concern of overfitting in GPR compared to ANN. However, GPR approach is not recommended for large training data set. The computational cost of using GPR escalates rapidly with an increase in number of the data set. Therefore, ANN should be preferred over GPR for data sets larger than 1,000. For smaller data set GPR gives better prediction than ANN. In a recent study, GPR was compared with ANN for representing potential energy surfaces in molecules and the authors concluded that GPR proved to be better predictor than ANN with *RMSE* of 0.62 compared to 0.86 of ANN (Kamath, Vargas-Hernandez, Krems, Carrington, & Manzhos, 2018). The results are in agreement with our study, although, in a different domain.

4 | CONCLUSION

This study introduced Gaussian process-based models for modeling of drying kinetics. The Gaussian process models were compared with RSM and ANNs. GPR-based models proved to be more accurate than the other models and these models were simple to handle and easy to understand. ANN also showed good accuracy in predicting both

seen and unseen data, but neural network-based models are complex and use many parameters. Therefore, this study concludes that regression-based models of the Gaussian process are efficient in modeling drying kinetics and have better prediction capability than RSM and ANN.

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