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Mathematical Modeling in Drying and determination of effective moisture diffusivity of $CaSO_4$ ½ H_2O during Microwave drying

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Abstract : Mathematical modeling of the dehydration process is very useful in design and optimization of dryers. However, theoretical simulations of the drying process require a substantial amount of computing time because of the complexity of the diffusion equations governing the process. A number of complex theoretical models to describe the heat and mass transfer phenomena during drying are available. In particular, thin-layer equations contribute to the understanding of the heat and mass transfer phenomena, and computer simulations, for designing new processes and improving existing commercial operations. The objective of the study was to investigate the effect of microwave output power, initial moisture content on drying kinetics of plaster, to compare the experimental data found during drying with the predicted values obtained by using some drying models, to calculate the effective moisture diffusivity, to derive a relationship between the drying rate constant and the effective moisture diffusivity, to develop a new suitable model to represent the present experimental data, including combined effect of drying time and input power and to analyze the changes in porous structure for microwave drying of plaster of paris.

Key words : Mathematical modeling, Optimization, Simulation, Diffusivity.

Introduction :

Plaster of Paris (POP) is a dry, fine, white powdered building material similar to mortor or cement, based on calcium sulfate ($CaSO_4$ ½ H_2O). The microstructure of hardened gypsum pastes affects most of the physical and engineering properties particularly its rigidity. POP, is used as fire resistance on residential and other structures, casted into various shapes including sheets, sticks and molds. The conditions of moisture removal can be changed to adjust the porosity of the hemihydrate, resulting in the formation of alpha and beta hemihydrates, which are chemically identical. Several drying methods are commercially available and the selection of the optimal method for drying is determined by quality requirements, raw material characteristics, and economic factors. Advances in the drying of porous material have been increasingly stimulated over the past few years. The use of microwave rays in the drying of products has become widespread because it minimizes the decline in quality and provides rapid and, effective heat distribution in the material. Furthermore, high quality product is obtained via microwave drying in addition to the reduction in drying period and energy conservation during drying[1]**.** Therefore, microwave heating has shown advantages over the conventional heating method in terms of energy efficiency, higher reaction rates and shorten in reaction times. Mathematical models are necessary in analyzing, designing, simulating and conducting the drying process. Dynamic simulation requires more comprehensive models, while simple models meet the requirements of designing or presenting the technical calculation. Investigators show greater importance in developing new models particularly for food stuffs including the drying parameter like air velocity and drying temperature, for apricot, grape, rough rice, carrot, mushroom and pollen [2-4]. In general, these attempts are performed to obtain the best model from the basic models. Due to the limited amount of experimental work on microwave drying of POP, reported to date, it is therefore, the objective of this study, to investigate microwave drying of POP and create new suitable models including combine effect of drying time and input power.

Materials and methods :

Sample preparation :

The commercially available high purity POP, was made into paste with carrier water and molded to square (70 x 70 x 15 – L x B x H in mm), rectangle (80 x 70 x 13 – L x B x H **-** in mm) and cylinder (64 x 18 – D x H **-** in mm) approximately weighing 150grams. The freshly molded samples were initially tempered. Tempering is done for a period of 18 to 24 hours, so that the material becomes rigid and stable. The experiments were conducted with an initial moisture content of 70-80%, before exposing to microwave drying.

Microwave drying and procedure :

The microwave-drying oven employed for experimentation was a SAMSUNG C-103F model, with inbuilt bio-ceramic cavity. The microwave generator (352 x 220 x 300-W x H x D - in mm) used works at 2450 MHz and 900Watts of nominal power at controllable level with increments. As the commercially available microwave oven has its own limitation in that of monitoring the sample weight, an inbuilt weighing system was used. The amount of evaporated water during drying was determined directly from digital screen of drying equipment at about 10 sec intervals until the final moisture content of the sample was attained. Drying of POP was started with initial moisture content of approximately 70 to 80 % (wet basis), and continued for a period of time with constant power input. All experiments were conducted at three different initial moisture contents (70%, 75% and 80%), power ranges (180W, 360W and 540W), and geometry (square, rectangle and cylinder). The mass of the samples chosen for the runs was approximately 150 g. All experiments were performed in triplicate, the average values of these replications were used for further analysis of microwave drying parameters like drying rate, moisture content at various drying time.

Mathematical modeling of microwave drying curves :

The obtained microwave drying curves were analyzed with 9 different empirical and semi-empirical drying models (Table 1) through regression analyses. Average regression coefficient (r_{avg}) is found out to describe the current microwave drying curves of POP. The root mean square error (RMSE), residual sum of squares (RSS) and modeling efficiency (EF) were used as the primary criterion to select the best equation to account for variation in the drying curves of the dried samples[5,6]. These statistical values can be calculated as follows :

$$RMSE = \left[(1/2) \sum_{i=1}^{N} (MR_{\exp,i} - MR_{pred,i})^2 \right]^{0.5}$$

$$RSS = \sum_{i=1}^{N} (MR_{\exp,i} - MR_{pred,i})^2$$

$$EF = \frac{\sum_{i=1}^{N} \left(MR_{\exp,i} - MR_{\exp,avg}\right)^2 - \sum_{i=1}^{N} \left(MR_{pre,i} - MR_{\exp,i}\right)^2}{\sum_{i=1}^{N} \left(MR_{\exp,i} - MR_{\exp,avg}\right)^2}$$

These statistical parameters have been widely used as a primary criterion for the selection of the best equation to account for variation in the drying curves of dried samples [7].

Result of discussions :

Effect of intensity of microwave drying by varying power, moisture content and various shape :

The microwave power supplied to the system plays a major role in shaping the final moisture content, which explains the drying nature of samples[8]. It was observed from fig. 1, at high power (540watts), the continuous supply of microwave energy produces the sample temperature to attain a point in which the samples begin to crack, while lower power favors maximum drying of POP. The presence of maximum moisture content in sample responded quantitatively large to microwave which results immediate and complete drying of POP. Further it was noted (fig. 2) in all experiments (irrespective of shape and power), the drying rate was higher for samples with higher initial moisture content, which is impossible to achieve by other conventional drying methods. Though the curves obtained for rectangular samples were little deviated from that of square and cylindrical geometries, much change were not visible for the sample structure (fig. 3). The moisture removal was from 66.40 to 28.55% for rectangular samples and was from 70.07 to 33.06% and 68.99 to 39.10% for square and cylindrical geometries respectively. Based on the above results it was clear that maximum drying rate could be achieved in rectangular sample with a power input of P-20 (180 watt) and initial moisture content of 80%.

Mathematical modeling of microwave drying curves :

The results have shown that the highest values of EF and the lowest values of chi square and RMSE could be obtained with Midilli et al. equation (model 9) than values of the other model (fig. 4). Therefore, model 9 can be proposed to evaluate the moisture ratio of POP for interval of drying power and time in this study. Model 9 will be useful for the materials related with ceramics (table 2). Although modeling efficiency of all models are sufficient for modeling of drying curves of microwave dried POP, only Midillis model satisfactorily responded to the current system. Midillis model have better values of modeling efficiency values than the other models. When we examined the effect of drying power and moisture content on Midilli et al. models' constants and coefficients by multiple regression, It can be seen that, this model was in good agreement with the experimental results. Model 9 gave a highest EF value and lowest chi-square and thus, were selected to represent the microwave drying of POP. To validate the suitability of the models, the experimental and predicted drying characteristics were compared (fig 5). The experimental data are closely correlated with the computed data for the Midilli et al. Based on the results, it is concluded that the microwave drying of POP for all power ranges shows acceptable agreement with the experimental results.

Effective moisture diffusivity :

The effective moisture diffusivity of a material characterizes its intrinsic mass transfer property of moisture in the sample. The mechanism of movement/removal of moisture from interior to the surface of POP during the microwave operation was only due to diffusivity as explained by Fick's second law. The effective moisture diffusivity (which is affected by composition, moisture content, temperature, and porosity of the material) was used to explain the mechanism of moisture movement during drying process. The following assumptions were made: The molded and tempered rectangular POP cuboids were assumed as a slab (since, the height is small when compared with length and breath); Moisture is initially uniformly distributed throughout the mass of a sample; Mass transfer is symmetric with respect to the center, Surface moisture content of the sample instantaneously reaches equilibrium with the condition of surrounding air, Resistance to mass transfer at the surface is negligible, when compared to internal resistance of the sample, Mass transfer follows diffusion mechanism, and shrinkage is negligible.

$$MR = \frac{8}{\pi^2} \exp\left[-\frac{\left(D_{eff} .\pi^2\right)}{T^2} t \right]$$

This, could be further simplified to a straight-line relation. The effective moisture diffusivities are determined by typically plotting the linear relationship between ln(MR) and drying time for various microwave output powers and initial moisture content. The method of slopes was used in which the slopes of the graph (Fig. 6 and Fig.7) for different microwave output powers (540, 360 and 180W), initial moisture content of sample (70, 75 and 80 %) and sample thicknesses (11,12,13 and 14mm), were used to calculate the effective moisture diffusivity. The details of effective moisture diffusivity values (D_{eff}) and the corresponding values of coefficients of determination R^2 are presented in Table 3 and Table 4. The presence of maximum moisture content in samples responded quantitatively faster to microwaves resulting in immediate and complete drying of POP.

Conclusion :

The drying characteristics of POP were made under microwave conditions using three different power supplies, initial moisture contents, and sample geometries. The measured moisture ratio was analyzed for its dependency on the above-mentioned variables. The suggested models for the microwave drying of ceramic materials were analyzed and the results of the statistical data were reported. An empirical model was developed based on Midilli et al.'s equation to represent the present experimental results. This present proposed model should be useful for the design and scale up of the microwave drying process for ceramic industries.

Nomenclature :

X_o	initial moisture content (gm.gm^{-1} solid)
X_c	equilibrium moisture content (gm.gm^{-1} solid)
X	moisture content at time t (gm.gm^{-1} solid)
r_{avg}	Average regression coefficient
$MR_{exp,i}$	'ith' experimental moisture ratio
$MR_{pred, i}$	'ith' predicted moisture ratio
$MR_{exp\ avg}$	average value of experimental moisture ratio
a,b, c, k	Empirical coefficients in models
M	moisture content (g water/g dry solids)

Me	equilibrium moisture content (g water/g drysolids)
M_0	initial moisture content (g water/g dry solids)

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Table (1) : Mathematical models tested for the moisture ratio values of POP.

No	Model Name	Equation	References
1	Newton	MR = exp(-kt)	Ayensu [9].
2	Page	MR = exp($-kt^n$)	Agarwal and singh [10].
3	Henderson	MR = a exp(-kt)	Pal and Chakraverthy [12].
4	Logarithmic	MR = a exp(-kt) +c	Yagcioglu et al [13],
5	Wang and Singh	MR = $1+at+bt^2$	Wang and Singh [14].
6	Diffusion	MR = a exp(-kt)+ (1-a)exp(-kbt)	Akpinar et al, [15].
7	Verma	MR = a exp(-kt)+(1-a)exp(-gt)	Verma et al [16].
8	Two term exponential	MR = a exp(-kt)+(1-a)exp(-kat)	Sharaf-Elden et al [17].
9	Midilli	MR = a exp(-k(t^n))+ b t)	Midilli et al [18].

Table 2 : Result of statistical analyses on the modeling of moisture content and drying time.

Model Name	Constants	R^2
Newton	k = 0.0023	0.99843
Page	k = 0.0060, n = 0.8258	0.99845
Henderson	a = 0.9694, k = 0.0022	0.99750
Logarithmic	a = 0.6376, k = 0.0056, c = 0.3990	0.99264
Wang and Singh	a = -0.0025, b = 0.000003	0.99587
Diffusion	a = 1.0000, k = 0.0023, b = 1.0000	0.99831
Verma	a = 0.9694, k = 0.0022, g = 1.0000	0.99750
Two term exponential	a = 0.9944, k = 0.0023	0.99831
Midilli	a = 3.3357, k = 0.9366, n = 0.0884, b = -0.0006	0.99999

Table (3) :The estimated effective moisture diffusivity values and statistical analysis of linear model at various microwave output powers for sample thicknesses of 0.013m.

Sl no	Moisture content	Power output	Slope $x10^3$	D_{eff} x 10^8 ($m^2 s^{-1}$)	R^2
1	80	180	5.187	2.218	0.9929
2	80	360	3.872	1.656	0.9910
3	75	180	3.209	1.372	0.9909
4	70	180	2.727	1.166	0.9902
5	75	360	2.359	1.009	0.9894
6	75	540	2.002	0.856	0.9891
7	80	540	1.665	0.712	0.9877
8	70	360	1.519	0.650	0.9875
9	70	540	1.347	0.576	0.9876

Table (4) :The estimated effective moisture diffusivity values and statistical analysis of linear model at uniform microwave output power of 180W and initial moisture content of 80% for varied sample thicknesses.

Sl no	Sample thickness(m)	Slope $x10^3$	D_{eff} x 10^8 ($m^2 s^{-1}$)	R^2
1	0.011	8.47	2.6927	0.9967
2	0.012	6.84	2.5429	0.9928
3	0.013	5.17	2.1014	0.9919
4	0.014	4.15	1.9187	0.9915

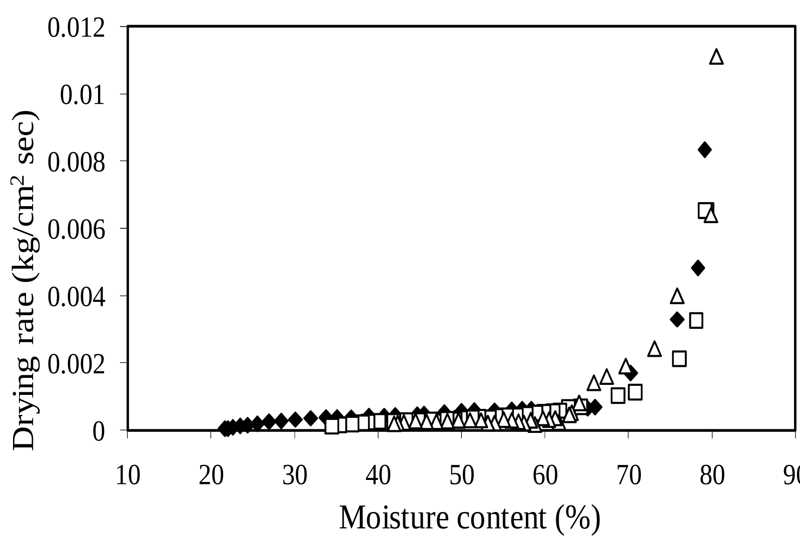

Fig ure (1) : Drying rate versus moisture content of POP at different power ranges (♦,P-180W, □,P- 360W, Δ,P-540W) Conditions: Initial moisture content-70%, Geometry- Cylinder

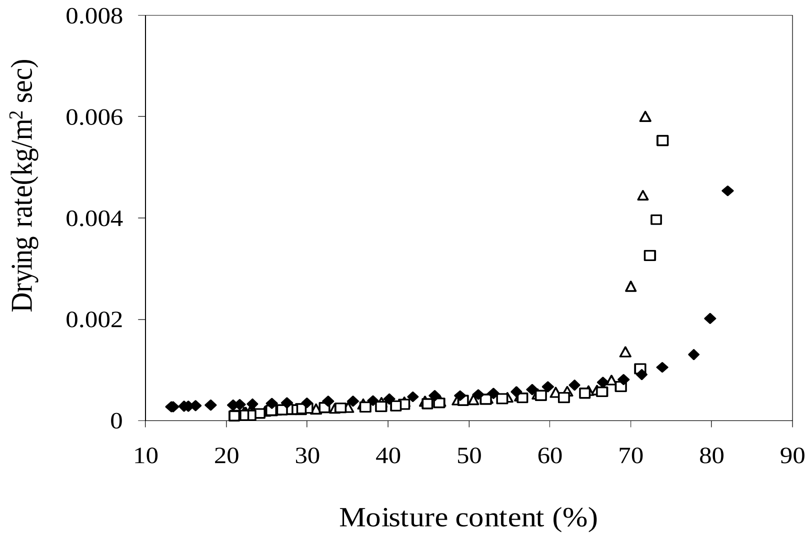

Fig 2: Drying rate versus moisture content of POP at different initial moisture contents (□ Initial moisture content 75%, Δ Initial moisture content 70%, ♦ Initial moisture content 80%) Conditions: Rectangle, Power 180W.

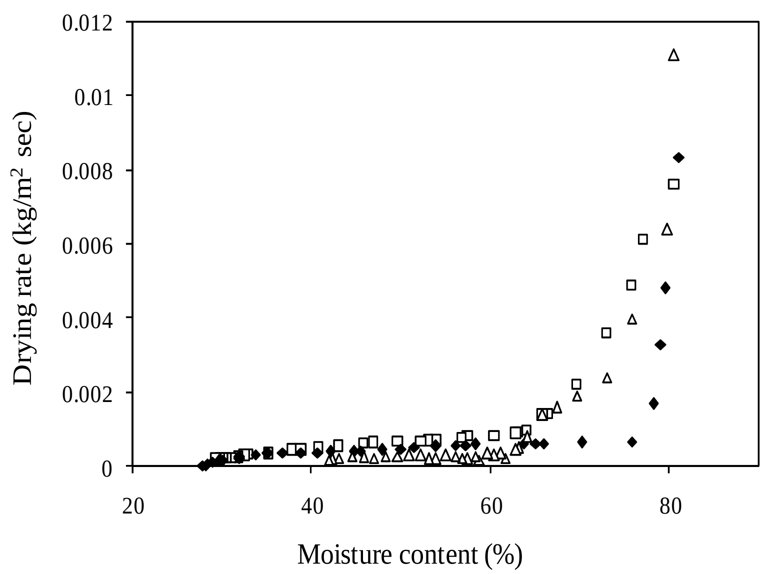

Fig 3: Drying rate versus moisture content of POP at varied geometries. (□ square, Δ cylinder, ♦ rectangle) Conditions : Initial moisture content 70%, Power -360 W

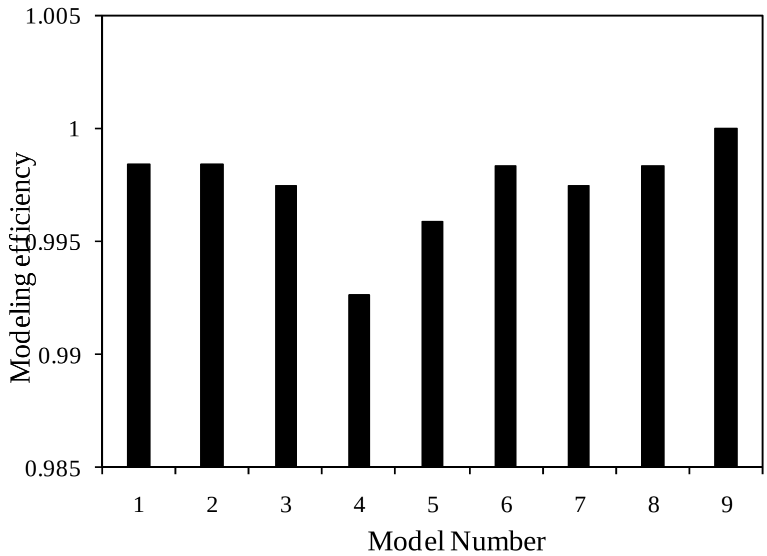

Figure (4) : Modeling efficiency of all basic models in Table (2).

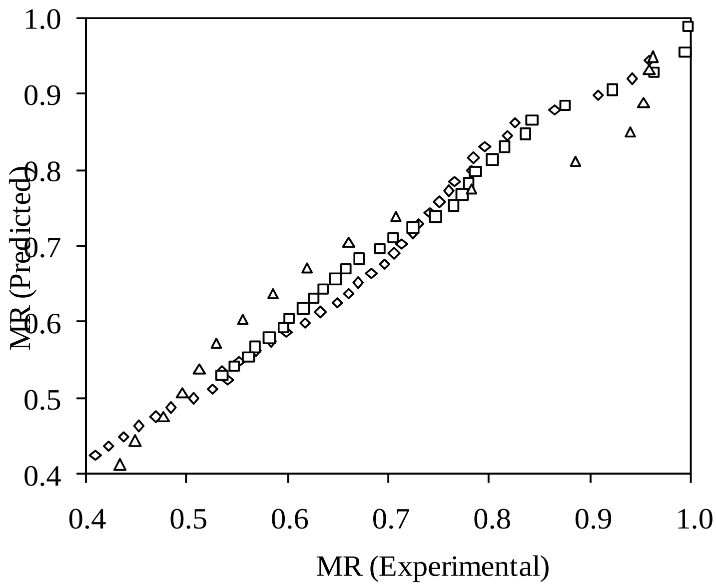

Figure (5) : Predicted and experimental moisture content of POP during microwave drying (◊ Power 180W, □ Power 360 W, Δ Power 540 W).

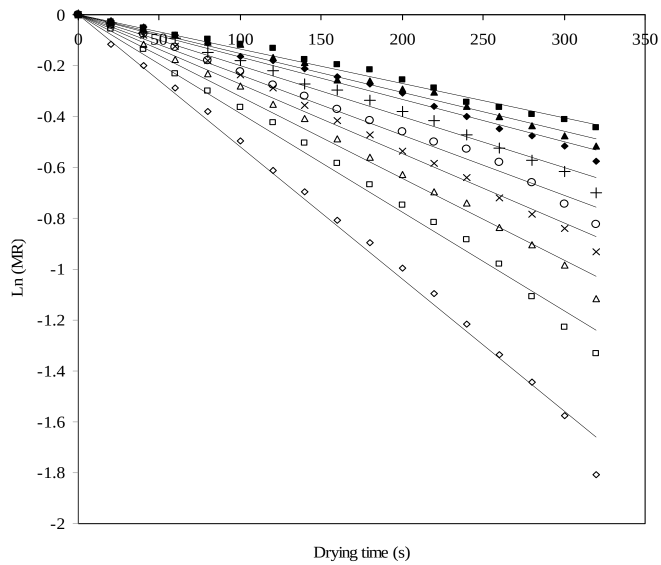

Figure (6) : Drying kinetic relationship of POP at different microwave power ranges for 13 mm sample thickness: ◊ - 180 W, IM 80%; □, 360 W, IM 80%; Δ, 180 W, IM 75%; ×, 180 W, IM 70%; ○, 360 W, IM 75%; +, 540 W, IM 75%; ♦, 540 W, IM 80%; ▲, 360 W, IM 70%; ■, 540 W, IM 70%.

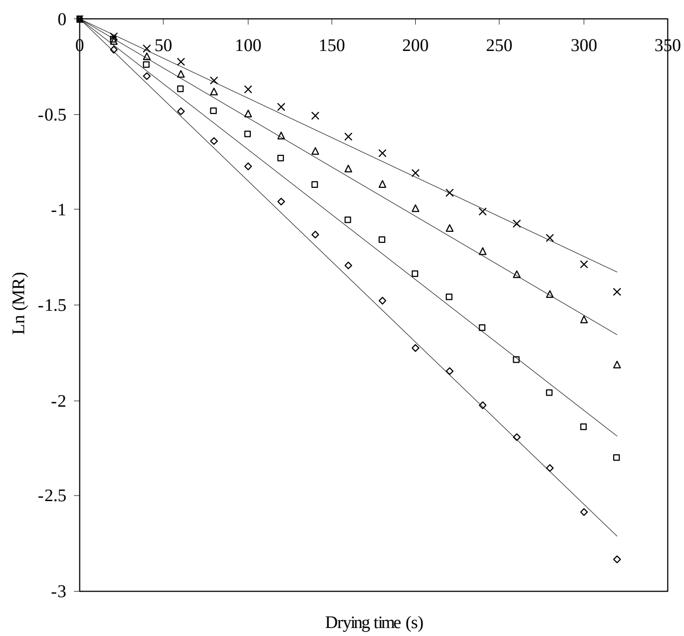

Figure (7) : Drying kinetic relationship of POP at different sample thickness for microwave power 180 W and IM 80. ◊, 14 mm; □, 13mm; Δ, 12mm; ×, 11mm.