Comparison of five commonly used thin-layer moisture transfer models in fitting the re-wetting data of barley

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Abstract: Five commonly cited thin-layer rewetting models, including Page, Diffusion, Approximate form of diffusion, Exponential, and Polynomial were compared for their abilities to the fit the experimental re-wetting data of barley based on the root mean square error (*RMSE*) and mean relative error (MRE) of estimate of the measured and simulated moisture contents. The comparison shows the Page model is the most suitable model (average, *RMSE* = 0.176% d.b. and *MRE* = 0.713% d.b.) followed by the Diffusion model (average *RMSE* = 0.199% d.b. and *MRE* = 0.862% d.b) to fit the re-wetting experimental data of barley. The Approximate form of diffusion, the Exponential and the Polynomial models have less fitting ability then the Page and Diffusion models for the entire period (> 4 days) of re-wetting of 33 tests at different combinations of temperatures (5.7- 46.3°C) and relative humidity (48.2%-88.6%). The Page and Diffusion models were found to be the most suitable equations, to describe the thin-layer re-wetting characteristics of barley over a typically five day re-wetting. These two models can be used for the simulation of deep-bed re-wetting of barley occurring during ventilated storage.

Keywords: Thin-layer, barley, re-wetting parameters, temperature, relative humidity

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1 Introduction

Moisture adsorption and desorption are important concern when developing simulation models for deep bed drying and aeration of grain. In the early stage of deep bed drying, the lower layer of grain desorbs moisture while the upper layer of grain adsorbs it. Thin-layer moisture transfer equations are used in deep bed grain drying and re-wetting simulation models. Therefore the validity of the deep bed drying or re-wetting model mostly depends on how accurately the thin-layer drying and re-wetting equations used in the model represent the thin-layer moisture transfer characteristics. Moreover, the grain is exposed to fluctuating air temperatures and relative humidity caused by drying and re-wetting cycles in low temperature drying. Grain prepared by desorption has a higher moisture content at a given relative humidity than grain prepared by adsorption. The difference between the adsorption and desorption relationship is important when assessing the thin-layer drying or re-wetting equations (Digvir et al. 1988). Moisture adsorption occurs when the vapor pressure within kernels is lower than that of the surrounding air. The moisture adsorbing environments can exist in the field before harvesting and subsequently during harvesting, holding, transportation, drying and storage of crops (Kunze and Prasad, 1978).

Friesen and Huminiki (1986) stated that for both the near-ambient and natural drying process, it is common to run the fan continuously even if it involves running the fan during periods of high ambient relative humidity which can cause re-wetting of grain. It is desirable to know how fast a grain bed would re-wet in a high humidity environment.

Most of the earlier studies on thin-layer moisture

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transfer relationships were concerned with thin-layer drying of cereal grains and oilseeds (Basunia and Abe, 2003, 2005a, 2005b; Digvir and Sokhansanj, 1986, 1988; Misra and Brooker, 1980) or a short duration and yet very little work was done on thin-layer re-wetting barley. Sokhansanj et al. (1984) stated that the drying rate of wheat, barley and canola changes as a result of re-wetting. Limited work has been done in developing thin-layer re-wetting equations for barley to develop thin-layer adsorption equations.

Basunia and Abe (2003) conducted a study on thin-layer re-wetting and moisture adsorption isotherms characteristics of barley over a wide range of temperature and relative humidity. They fitted only a single thin-layer drying equation to describe the moisture re-wetting characteristics of barley. So there is need to find out the best fitted equation to describe the rewetting characteristics of barley from low to high temperature which is commonly used in barley drying and re-wetting. Similar studies were conducted by Basunia and Rabbani (2011) to select the best fitted equation in rewetting rough rice.

The object of this work is to determine the rate of moisture transfer in re-wetting barley over a range of temperatures and relative humidity, and to find the most suitable thin-layer re-wetting model for barley which can be used in simulating moisture transfer during ventilated storage.

2 Mathematical equations to predict thin-layer rewetting

The drying characteristics of grains have been examined by many researchers and various models for the prediction of the drying rate have been performed with more or less success. Mathematical modeling of drying or re-wetting is crucial for optimizing operating parameters and performance improving the performance of drying systems. The most commonly used thin-layer rewetting or drying models of grain are Diffusion (Newman, 1931), Approximate form of diffusion (Boyce, 1965), Page (Page, 1949), Exponential (Digvir et al, 1991) and Polynomial (Wang, 1978).

The following models were therefore chosen for this

study to fit the observed rewetting data.

(1) The most commonly used empirical equation to describe the thin-layer drying and re-wetting of cereals is that of Page (Page, 1949):

$$M_R = \frac{M_t - M_e}{M_e - M_i} = \exp\left(-K \times t^N\right) \tag{1}$$

where, M_R is the moisture ratio; M_t is the measured moisture content at any time in dry-basis,%; M_e is the equilibrium moisture content in dry-basis, %, M_i is the initial moisture content in dry-basis,%, t is the re-wetting time, min; and K, N are the re-wetting parameters.

(2) Simplifications of the well-known diffusion model for large drying or r-wetting times that is frequently used to predict the drying and re-wetting of grain are given as:

$$M_{R} = C \times \exp\left(-\frac{\pi^{2} D t}{R^{2}}\right)$$
(2)

where, $C = 6/\pi^2$, *t* is the drying time in hour, h; *D* is the diffusion coefficient, m²/h; *R* is the sphere radius, m.

(3) Approximate form of diffusion equation (Boyace, 1965) for thin layer-drying or rewetting can be written as

$$M_R = a \exp\left(-K \times t\right) \tag{3}$$

where, a is product dependent constant; t is the re-wetting time, min; and K is the re-wetting parameter.

(4) Exponential model (Lewis, 1921) can be written as

$$M_R = \exp\left(-K \times t\right) \tag{4}$$

where, t is the re-wetting time; min, K is the re-wetting parameters.

(5) Second order polynomial equation (Thompson et al., 1968; Wang and Singh, 1978) is of the from

$$M_R = a + bt + ct^2 \tag{5}$$

where, t is the re-wetting time, min; a is the product dependent constant and b, c are the re-wetting parameters.

3 Materials and methods

The range of re-wetting conditions for the experiment is presented in Table 1. The procedure to determine weight data of the sample in thin-layer rewetting, and adsorption equilibrium moisture content of barley were described elsewhere (Basunia and Abe, 2003, 2005a). Thin-layer re-wetting characteristics of barley were determined at temperature ranging from 5.7 to 46.3°C and for relative humidity ranging from 48.2% to 88.6%, with initial moisture contents in the range of 10.26% to 11.54% (d.b.). The data of sample weight, and dry and wet bulb temperatures of the re-wetting air were recorded continuously throughout the re-wetting period for each test. The re-wetting process was terminated when the change of moisture content in 24 h was less than 0.1% (d.b.) (weight change was less than 0.05 g). Normally such an experiment lasts for 4-6 days. The final points were recorded as the dynamic equilibrium moisture contents. Each data file consisted of more than 300 measured points.

Re-wetting parameters of these models were found for each linear regression test. The coefficients of determination R^2 were all above 0.90. The 33 sets of values for different parameters were used in a multiple regression procedure to find expressions for each parameter of the model equations.

The measured and simulated moisture contents were compared and statically analyzed for determining the best fit equation. The root mean square error (*RMSE*) and mean relative error (*MRE*) indicate the fitting ability of a model to a data set. The smaller the *RMSE* and *MRE* values, the better the fitting ability of an equation. For the same data set, the equation giving the smallest *RMSE* and *MRE* values, respectively, represents the best fitting ability (Iglesias and Chirife, 1976, Chen and Morey, 1989).

The *RMSE* is expressed as

$$RMSE = \sqrt{\frac{\sum_{i=1}^{m} \left(M_i - M_s\right)^2}{df}}$$
(6)

where, M_s is the simulated moisture content in dry-basis and *df* is the degree of freedom. For large data set, as in this experiment, it is defined as

$$RMSE = \sqrt{\frac{\sum_{i=1}^{m} \left(M_{i} - M_{s}\right)^{2}}{m}}$$
(7)

where, m is the number of data points.

The MRE is defined as

$$MRE = \frac{100}{m} \sum_{i=1}^{m} \frac{(M_{t} - M_{s})}{M_{t}}$$
(8)

4 Results and discussions

4.1 Expressions for the parameters of Model Equation (1) (Page model)

The multiple regression analysis for *K* as a function of temperature *T* in $^{\circ}$ C and relative humidity *R*_{*H*} in decimal, yielded:

 $K = -0.00108 + 0.0000105 T + 0.00158 R_H$ (9) with a coefficient of determination R^2 of 0.896.

It was observed that *N* varies between 0.882 - 0.978 with in the temperatures and relative humidity studied. Hence for analysis and interpretations of the results, an overall average value of *N* from all tests was used. The mean value of *N* for 33 tests was 0.952. This effectively assumes *N* to be a product-dependent constant. Tables 1 and 2 show the values of root mean square error (*RMSE*) and mean relative error (*MRE*) of estimate, respectively, of moisture content of all tests when the parameter *N* was fixed at this overall average of 0.952. The average *RMSE* and *MRE* values of 33 tests were only 0.176% (d.b.) and 0.713% (d.b.) for a fixed value of *N* as a product-dependent constant seems valid for representing the re-wetting rate data of barley.

 Table 1
 Values of the root mean square errors (RMSE) of each test (number of observations in each test is more than 300)

 for the five model equations

Temperature / ⁰ C	Relative Humidity/%	Page equation /% (d.b.)	Diffusion equation /% (d.b.)	Approximate form of Diffusion equation/% (d.b.)	Exponential equation /% (d.b.)	Polynomial Equation /% (d.b.)
5.7	69.8	0.213	0.324	1.068	0.874	0.889
5.7	80.1	0.199	0.110	0.796	1.771	0.495
6.2	88.2	0.213	0.417	0.723	2.785	1.669
7.9	65.9	0.088	0.218	1.652	0.196	0.495
9.4	75.8	0.087	0.100	0.340	1.253	0.959
9.4	87.0	0.117	0.473	1.349	1.349	3.374
13.4	63.7	0.145	0.094	0.671	0.200	0.465
13.4	76.4	0.284	0.094	0.575	0.575	1.735

Temperature / ⁰ C	Relative Humidity/%	Page equation /% (d.b.)	Diffusion equation /% (d.b.)	Approximate form of Diffusion equation/% (d.b.)	Exponential equation /% (d.b.)	Polynomial Equation /% (d.b.)
13.4	87.0	0.298	0.474	1.253	1.253	1.581
18.7	55.6	0.107	0.148	0.905	0.780	0.194
18.7	77.1	0.220	0.168	0.339	0.379	1.578
19.4	64.2	0.223	0.136	1.014	0.816	0.407
19.4	71.3	0.265	0.034	0.282	0.753	0.697
19.4	86.2	0.201	0.426	0.827	0.774	2.283
23.3	71.6	0.100	0.142	0.138	0.518	0.625
24.3	59.2	0.207	0.158	0.107	0.112	0.203
24.3	84.6	0.137	0.350	0.579	1.113	1.312
29.8	48.2	0.127	0.135	0.497	0.439	0.249
29.8	88.6	0.122	0.394	0.610	1.216	1.774
31.2	57.5	0.149	0.142	0.088	0.050	0.196
31.2	66.8	0.058	0.104	0.146	0.108	0.263
35.0	60.7	0.234	0.256	0.181	0.225	0.264
35.0	73.1	0.069	0.058	0.129	0.405	0.536
35.0	80.9	0.116	0.077	0.345	0.797	0.969
39.7	64.3	0.031	0.109	0.085	0.083	0.242
39.7	81.5	0.381	0.288	0.119	0.343	0.677
41.2	50.3	0.084	0.146	0.094	0.118	0.277
41.2	69.5	0.095	0.107	0.128	0.241	0.295
41.2	82.2	0.262	0.181	0.107	0.361	1.113
44.6	58.0	0.149	0.225	0.128	0.142	0.227
44.6	64.6	0.152	0.158	0.246	0.132	0.412
44.6	76.5	0.360	0.133	0.289	0.088	0.340
46.3	81.1	0.275	0.172	0.094	0.404	0.502
	Average	0.176	0.199	0.482	0.626	0.827

Note: **RMSE of estimate of predicted moisture content with more than 300 observations for each test.

Table 2 Values of the mean relative error (*MRE*) of each test (number of observations in each test is more than 300) for the five model equations

Temperature / ⁰ C	Relative Humidity/%	Page equation /% (d.b.)	Diffusion equation /% (d.b.)	Approximate form of Diffusion equation/% (d.b.)	Exponential equation /% (d.b.)	Polynomial Equation /% (d.b.)
5.7	69.8	0.766	1.581	6.745	4.650	5.870
5.7	80.1	0.063	0.265	3.756	8.000	2.707
6.2	88.2	1.314	1.760	2.831	10.954	4.150
7.9	65.9	0.336	0.517	10.145	0.921	13.339
9.4	75.8	0.631	0.641	1.657	5.920	8.774
9.4	87.0	0.647	1.940	5.053	8.060	6.564
13.4	63.7	0.541	0.118	4.452	0.690	1.152
13.4	76.4	1.537	0.261	2.628	5.460	5.345
13.4	87.0	0.199	3.087	4.398	6.960	12.010
18.7	55.6	0.864	0.500	5.756	4.828	0.340
18.7	77.1	0.700	0.709	1.333	3.290	6.525
19.4	64.2	0.925	2.192	3.362	0.753	2.909
19.4	71.3	1.054	0.038	0.865	3.330	5.627
19.4	86.2	1.148	1.597	2.947	4.260	5.145
23.3	71.6	0.214	0.488	0.606	2.192	5.067
24.3	59.2	0.498	0.822	0.422	0.406	1.449
24.3	84.6	0.338	1.118	1.959	0.668	2.522

(10)

Temperature / ⁰ C	Relative Humidity/%	Page equation /% (d.b.)	Diffusion equation /% (d.b.)	Approximate form of Diffusion equation/% (d.b.)	Exponential equation /% (d.b.)	Polynomial Equation /% (d.b.)
29.8	48.2	0.162	0.701	2.176	2.936	1.007
29.8	88.6	0.576	1.245	1.684	3.339	12.855
31.2	57.5	0.067	0.720	0.245	0.119	0.794
31.2	66.8	0.006	0.511	0.627	0.368	1.169
35.0	60.7	0.617	1.425	0.795	1.082	1.803
35.0	73.1	0.174	0.258	0.474	1.540	4.155
35.0	80.9	0.219	0.001	1.128	2.608	7.948
39.7	64.3	0.680	1.832	0.222	0.337	0.514
39.7	81.5	1.244	0.749	0.326	1.124	5.156
41.2	50.3	0.562	1.007	0.413	0.591	1.007
41.2	69.5	1.390	0.343	0.517	1.117	0.990
41.2	82.2	0.663	0.087	0.110	1.124	8.734
44.6	58.0	0.177	1.053	0.528	0.705	0.918
44.6	64.6	1.829	0.017	1.127	0.520	1.377
44.6	76.5	1.839	0.177	0.922	0.281	0.384
46.3	81.1	1.544	0.686	0.320	1.529	3.441
	Average	0.713	0.862	2.137	2.747	4.295

Note: *MRE of estimate of predicted moisture content with more than 300 observations for each test

The highest *RMSE* was 0.381%, (d.b.) and the lowest was 0.031%, (d.b.) only. Similarly, the highest *MRE* was 1.839%, (d.b.) and the lowest was only 0.006%, (d.b.). The average *RMSE* and *MRE* of estimate between the measured and predicted values of moisture contents for the full data set were 0.176%, (d.b.) (Table 1), and 0.713%, (d.b.) (Table 2) only, respectively. These very low *RMSE* (0.00176 d.b.) and *MRE* (0.00713 d.b.) show the accuracy of the model to predict the moisture content at any time during the re-wetting period. The *RMSE* and *MRE* of individual test are shown in Table 1 and Table 2, respectively.

4.2 Expressions for the parameter of Model Equation (2) (Diffusion model)

It was observed that C varies between 0.888 - 0.994 within the ranges of temperatures and relative humidity studied. Hence for analysis and interpretations of the results, an overall average value of C from all tests was used. The average value of C for 33 tests was 0.957. This effectively assumes C to be a product-dependent constant instead of 0.608 for a perfectly spherical grain kernel as in Equation (2). Tables 1 and 2, respectively, show the values of root mean square error of estimate (*RMSE*) and mean relative error (*MRE*) of moisture content of all tests when the parameter C was fixed at this overall average of 0.957. The average *RMSE* value of

33 tests was only 0.199%, (d.b.) and *MRE* was 0.862%, (d.b.) for a fixed value of C = 0.957. The expression relating diffusivity, D in m² h⁻¹, and re-wetting air temperature, T in ⁰C, was found as

$$D = 2.2554 \times 10^{-3} \exp\left(-\frac{4724.32}{T+273.15}\right)$$

with a coefficient of determination 0.953.

The very low *RMSE* (0.199%, d.b.) and *MRE* (0.862%, d.b.) suggest the accuracy of the model to predict the moisture content at any time during the re-wetting period. The *RMSE* and *MRE* of individual tests are shown in Table 1 and 2, respectively. The highest *RMSE* was 0.473%, (d.b.) and the lowest was 0.034%, (d.b.) is only. Similarly the highest *MRE* was 2.192%, (d.b.) and the lowest was 0.001%, (d.b.) only.

4.3 Expression for the parameter of Model Equation(3) (Approximate form of Diffusion)

The multiple regression analysis for *K* as a function of temperature *T* in $^{\circ}$ C and relative humidity *R*_{*H*} in decimal, yielded:

$$K = -0.00397 + 0.00007 \times T + 0.00539 \times R_H$$
$$(R^2 = 0.95)$$
(11)

The average *RMSE* and *MRE* of estimate between the measured and predicted values of moisture contents for the full data set was 0.482% and 2.137%, (d.b.),

respectively, which are higher than both the Page and Diffusion models. The *RMSE* and *MRE* of individual tests are shown in Table 1and 2, respectively. The highest *RMSE* was 1.652%, (d.b.) and the lowest was only 0.085%, (d.b.). The highest *MRE* was 10.145%, (d.b.) and the lowest was 0.110%, (d.b.).

4.4 Expression for the parameter of Model Equation(4) (Exponential)

The multiple regression analysis for *K* as a function of temperature *T* in ${}^{\circ}$ C and relative humidity *R*_{*H*} in decimal, yielded:

 $K = -0.00634 - 0.0000728T + 0.00965R_H$ (12) with a coefficient of determination R^2 of 0.89.

It was observed that the value of a varies between 0.832-0.931 with in the temperatures and relative humidity studied. Hence for analysis and interpretations of the results, an overall average value of a from all tests was used. The average value of a for 33 tests was 0.89. The highest *RMSE* was 2.785%, (d.b.) is and the lowest was only 0.050%, (d.b.) (Table 1). The highest *MRE* was 10.954%, (d.b.) and the lowest was 0.119%, (d.b.) (Table 2). The average *RMSE* and *MRE* of estimate between the measured and predicted values of moisture contents for the full data set were 0.626% and 2.747%, (d.b.) which are much higher than the Page and the Diffusion models.

4.5 Expressions for the parameters of Model Equation (5) (2nd order polynomial)

The multiple regression analysis for *b* as a function of temperature *T* in $^{\circ}$ C and relative humidity *R*_H in decimal, yielded:

 $b = 0.00383 - 0.0000001 \times T - 0.00765 \times R_H$ (13) with a coefficient of determination R^2 of 0.90.

The regression analysis for *c* as a function of function of temperature *T* in ${}^{\circ}C$ and relative humidity R_{H} in decimal, yielded:

$$c = -0.00000282 - 0.0000001 \times T + 0.0000082 \times R_H$$
(14)

with a coefficient of determination R^2 of 0.81.

It was observed that a varies between 0.826-0.942 with in the temperatures and relative humidity studied. Hence for analysis and interpretations of the results, an overall average value of a from all tests was used. The average value of *a* for 33 tests was 0.892.

The highest *RMSE* was 3.374%, (d.b.) and the lowest was 0.194%, (d.b.) (Table 1). Similarly, the highest *MRE* was 13.339%, (d.b.) and the lowest was 0.340%, (d.b.) (Table 2). The average *RMSE* and *MRE* of estimate between the measured and predicted values of moisture contents for the full data set was 0.827% and 4.295% (d.b.), respectively, which are higher than both the Page and Diffusion models. The *RMSE* and *MRE* of individual test are shown in Table 1 and 2. It is worth mentioning that the Polynomial model did fit well approximately for the first half hour and then there was a large variation between the measured and predicted moisture content for long duration. So this model is not suitable for predicting long term moisture adsorption and desorption process of grains.

From Table 1, it can be observed that for most of the tests RMSE was below 0.20%, (d.b.) both by the Page and Diffusion models. Similarly, from Table 2, it can be observed that for most of the tests MRE was below 0.80%, (d.b.) both by the Page and Diffusion models. It was found the that the numerical difference between the moisture contents predicted by Equation. (1), and with parameter K calculated with Equation. (9) and the observed moisture content did not exceed 0.6%, (d.b.) points in any test conducted at all temperature and relative humidity combination. Similarly, it was found the that the numerical difference between the moisture contents predicted by Equation. (2), with diffusivity calculated with Equation (10) and the observed moisture content did not exceed 0.7%, (d.b.) points in any test conducted at all temperature and relative humidity combination. This amount of error can be accepted for most practical purpose when working with biological products. So the Equations (1) and (9) or the Equations (2) and (10) can be used in a deep bed drying simulation model to predict the re-wetting under high ambient relative humidity conditions.

The moisture simulated by Equation (1) with N = 0.952 and K calculated with Equation. (9), respectively, were compared to observe moisture in Figures 1 and 2. The predicted and observed values were in good agreement. Similar agreements were also observed in

other re-wetting conditions.

The moisture contents simulated by Equation (2) with C = 0.957, and diffusivity D with Equation (10), were compared to observe moisture contents in Figures 3 and 4. The measured and predicted values were in very good agreement. Similar agreements were also observed in other re-wetting conditions.



Figure 1 Comparison between the curves predicted by the Page model with the values of the re-wetting parameter K with Equation (8) and N = 0.952 and experimental points at temperature (T) of 13.4,

23.3, 35.0 and 41.2°C, and various relative humidity (R_H)





31.2 and 35.0°C, and various relative humidity (R_H)



Figure 3 Comparison between the curves predicted by the diffusion model with the values of the diffusivity with equation (9) and the experimental points at temperature (*T*) of 13.4, 23.3, 35.0 and 41.2° C, and various relative humidity (*R_H*)





 35.0° C, and various relative humidity (R_{H})

5 Conclusions

The re-wetting rates of barley from low to high temperatures have been determined. Five models were compared based on root mean square error of estimate (RMSE) and mean relative error (MRE) values. The Page model and the Diffusion model, based on the ratio of the difference between the initial and final moisture content and the equilibrium moisture content, fits the data well with a RMSE error of 0.175%, (d.b.) and 0.199%, (d.b.), respectively, and MRE 0.713%, (d.b.) and 0.862%, (d.b.), respectively. The Page model and the Diffusion model are found to be the most appropriate models for representing the rewetting characteristics of barley. The other three models, the Approximate form of Diffusion, the Exponential and the Polynomial did not fit well compared to the previous two. It was found that the Polynomial model is only valid in shorter term span but not suitable for long time rewetting or drying. The values of RMSE for the approximate form of diffusion, the Exponential and the Polynomial models were 0.482%, 0.626% and 0.827% (d.b.), respectively, and MRE were 2.137%, 2.747% and 4.295%, (d.b.), respectively. The result presented here, over a typical five day re-wetting period, are useful in the longer term moisture transfer process occurring during ventilated storage.

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a product dependent constants in Equations (3) and

Notation

(5), respectively.

- b, c re-wetting parameters in Equation (5).
- C product dependent constant in Equation (2)
- D diffusivity of barley in m²/hr
- K re-wetting parameters in Equations (1), (3) and (4)
- M_e equilibrium moisture content of grain (d.b.)
- M_i initial moisture content of grain (d.b.)
- M_t measured moisture content of grain at any time, dry-basis (d.b.)
- M_s simulated moisture content of grain at any time,

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dry-basis (d.b.)

- M_R moisture ratio
- MRE mean relative error (% dry-basis)
- *m* number of observations in each test
- *N* re-wetting parameters in Equation (1)
- *R* radius of the sphere in m in Equation (1)
- R^2 coefficient of determination
- R_H relative humidity
- *RMSE* root mean square error
- t re-wetting time (min in Equations (1) and (3) to
- (5) and hr in Equation (2)
- T re-wetting temperature (⁰C)