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Estimating Drying Curves and Diffusion Coefficients in Coffee Drying (Castilla Variety) through Global Optimization Strategies

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Abstract

Background/Objectives: We present an alternative for estimating drying curves and diffusion coefficients of coffee beans (Castilla variety), based on global optimization strategies. **Methods:** Four optimization algorithms were tested for adjusting drying curves. Based on the parameters that were found, we determined the diffusion coefficient. Algorithms were tuned up on 11 non-linear systems, prior to using them for adjusting the curves. Their performance were assessed through error dispersion analysis, as well as through the number of evaluations of the objective function and run time. **Findings:** On non-linear systems, Particle Swarm Optimization (PSO) and Drone Squadron Optimization (DSO) exhibited the best performance in terms of error. When used for estimating drying curves, PSO, DSO and Genetic Algorithms (GA) achieved determination coefficients beyond 0.99. Even so, GA had the lowest run time. **Applications:** Our experiments offer an alternative with excellent precision for estimating parameters of the drying function and of its diffusion coefficients for different coffee beans.

Keywords: Coffee drying curve, Diffusion coefficient, Metaheuristic

1. Introduction

Determining the mathematical structure of the drying curve and estimating from it the diffusion coefficient of coffee beans while drying them, is a fundamental step for modelling dryers that guarantee an ideal control of such process[1-4]. Coffee has a high humidity removal requirement, so this step becomes vital. In a general sense, the estimation is made by adjusting experimental data to empirically pre-established models[5-7]. An alternative estimation procedure focuses on using global optimization strategies for calculating the parameters governing the solution of the humidity diffusion equation, based on Fick's second law. Metaheuristics have been used to tackle non-linear systems for several years now[8-10] but in this study, the third version of generalized differential evolution (GDE. Their stochastic nature allows them to escape local optima and to find the global solution within a defined search space[11]. A Scopus search shows that there has been quite a lot of work on developing and using metaheuristics through the last decades (Figure 1).

Some metaheuristics are inspired in natural systems (such as ant colonies or evolutionary mechanisms). Others are founded in the behavior of a base population (such as Particle Swarm Optimization). Metaheuristics inspired in artificial systems, such as drone squadrons, have also recently appeared[12].

Presents the results of adjusting drying curves and of calculating the corresponding diffusion coefficients, through global optimization strategies. To do, we begin at Fick's second law applied to Castilla variety coffee beans that have been dried by thermal radiation within an electric oven controlled at 50°C +/- 2°C. As a preliminary step, we tune the optimization algorithms on diverse

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non-linear systems, based on the real roots theorem[13, 14] for creating the objective function and for laying out the minimization problem.

2. Materials and Methods

We divided our experiments into two parts. The first one deals with the selected metaheuristics operating over non-linear systems. The second one focuses on using the metaheuristics for estimating the parameters of the non-linear drying equation, which was derived from applying Fick's second law to the drying of coffee beans.

2.1 Experiments Related to the Metaheuristics Over Non-Linear Systems

We evaluated 11 systems through 4 different algorithms: Drone Squadron Optimization (DSO), Trust Region with Dogleg (TRD), Genetic Algorithms (GA), and Particle Swarm Optimization (PSO). All tests were run in Matlab R2018b, in a computer with processor Intel Core i5-7200U, with 12GB DDR4 memory. In the first case (i.e. DSO), we used the functions provided by the creators of the method[12].

In the second case, we used the Matlab function *fsolve*. For the remaining two, we used the already implemented models within a Matlab toolbox. In all cases, the objective function was built up following Equations 1 and 2, where represents the number of variables in each function, and is the total number of functions.

$$f_1\left(x_1, x_2, \ldots, x_n\right) = 0$$

$$f_2\left(x_1, x_2, \ldots, x_n\right) = 0 \tag{1}$$

$$f_n\left(x_1, x_2, \ldots, x_n\right) = 0$$

$$f_{obj}\left(x_1, x_2, \ldots, x_n\right) = \sum_{i=1}^{k} (\mathrm{f_i}\left(x_1, x_2, \ldots x_n\right))^2 \tag{2}$$

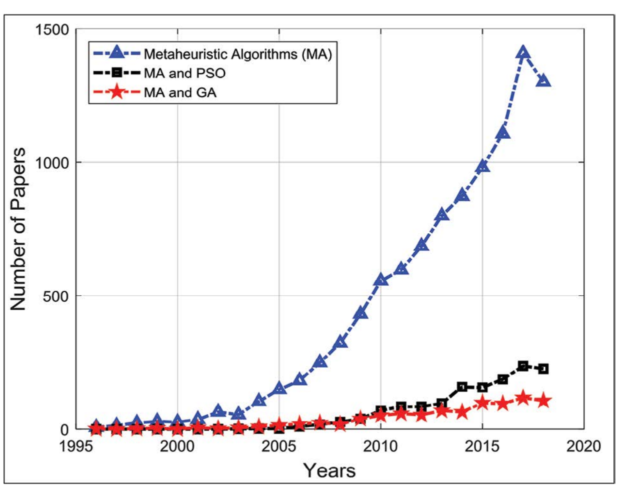

Figure 1. Number of SCOPUS records regarding metaheuristics.

Table 1. Parameters used in the algorithm

Algorithm	Parameter
DSO	Number of teams: 20 Number of drones per team: 50 Maximum evaluations: 500000 Tolerance: 1e-20
TRD	Maximum evaluations: 500000 Tolerance: 1e-20
GA	Population: 1000 Maximum evaluations: 500000 Tolerance: 1e-20
PSO	Number of particles: 1000 Maximum evaluations: 500000 Tolerance: 1e-20

Table 2. Experimented non-linear systems

System	Interval	Equations
S_1	[-5,5]	$f_1 = x_2{}^2 - 1$ (3) $f_2 = \sin(x_1 - x_2)$ (4)
S_2 Effati-Grosan1	[-2,2]	$f_1 = \cos(2x_1) - \cos(2x_2) - 0.4$ (5) $f_2 = 2(x_2 - x_1) + sin\,(2x_2) - \sin(2x_1) - 1.2$ (6)
S_3 Effati-Grosan2	[-2,2]	$f_1 = \exp(x_1) + x_1 * x_2 - 1$ (7) $f_2 = sin(x_1 * x_2) + (x_1 + x_2) - 1$ (8)
S_4 Reactor	[0,1]	$\gamma = 1000; D = 22; \beta_{1=}2; \beta_{2=}2; R = 0.935$ $f_1 = (1-R) * \left(\frac{D}{10(1+\beta_1)} - x_1\right) * \exp\left(\frac{10x_1}{1+\frac{10x_1}{\gamma}}\right) - x_1$ (9) $f_2 = x_1 - (1+\beta_2)x_2 + (1-R)\left(\frac{D}{10} - \beta_1 x_1 - (1+\beta_2)x_2\right) * \exp\left(\frac{10x_2}{1+\frac{10x_2}{\gamma}}\right)$ (10)
S_5 Steering Problem	[0.06,1] y [-2,2]	ψ_0 =1.3954170041747090114; ϕ_0 =1.7461756494150842271; ψ_1 =1.7444828545735749268; ϕ_1 =2.0364691127919609051; ψ_2 =2.0656234369405315689; ϕ_2 =2.2390977868265978920; ψ_3 =2.4600678478912500533; ϕ_3 =2.4600678409809344550; $E_i = x_2(\cos(\phi_i) - \cos(\phi_0)) - x_2x_3(\sin(\phi_i) - \sin(\phi_0)) - (x_2\sin(\phi_i) - x_3)x_1$ (11) $F_i = -x_2\cos(\psi_i) - x_2x_3\sin(\psi_i) + x_2\cos(\psi_0) + x_3x_1 + (x_3 - x_1)x_2\sin(\psi_0)$ (12) $y_i = \left(E_i(x_2\sin(\psi_i)) - F_i(x_2\sin(\phi_i) - x_3)\right)^2 + (F_i(1 + x_2\cos(\phi_i)) - E_i(x_2\cos(\psi_i) - 1))^2 - ((1 + x_2\cos(\phi_i))(x_2\sin(\psi_i) - x_3)x_1 - (x_2\sin(\phi_i) -$

(*continued*)

		$x_3)(x_2\cos(\psi_i) - x_3)x_1)^2$ Para i = 1,2,3	(13)
S_6	[-1,1]	$f_1 = 3x_1 - \cos(x_2x_3) - 0.5$ $f_2 = {x_1}^2 - 81(x_2 + 0.1)^2 + \sin(x_3) + 1.6$ $f_3 = \exp(-x_1x_2) + 20x_3 + \frac{10\pi-3}{3}$	(14) (15) (16)
S_7 Non-smooth nonlinear system	[-1,1]	$f_1 = {x_1}^2 - {x_2}^2$ $f_2 = 1 - abs(x_1 - x_2)$	(17) (18)
S_8 Merlet Problem	[0,2π]	$f_1 = -\sin(x_1)\cos(x_2) - 2\cos(x_1)\sin(x_2)$ $f_2 = -\cos(x_1)\sin(x_2) - 2\sin(x_1)\cos(x_2)$	(19) (20)
S_9 Floudas Problem	[0.25,1] [1.5,2π]	$f_1 = 0.5\sin(x_1x_2) - 0.25\frac{x_2}{\pi} - 0.5x_1$ $f_2 = \left(1 - \frac{0.25}{\pi}\right)(\exp(2x_1) - e) + e\frac{x_2}{\pi} - 2ex_1$	(21) (22)
S_{10}	[0,1] *n=10*	$f_i = x_i - \frac{1}{2n}(\sum_{j=1}^{n} x_j^3 + i) \quad i = 1,2,3,\ldots\ldots\ldots.n$	(23)
S_{11}	[0,1] *n=10*	$f_i = x_i - exp(\cos(i\sum_{j=1}^{n} x_i) \quad i = 1,2,3,\ldots\ldots\ldots.n$	(24)

The parameters of each algorithm were adjusted in such a way that they all performed under equal conditions, as indicated in Table 1.

We ran 50 repetitions of each algorithm and for each non-linear system. Using that information, we calculated the following indices: minimum error, average error, maximum error, Standard Deviation (SD), SR factor (i.e. the number of times that the algorithm achieved an error at least as good as the tolerance), average run time (seconds), average number of function evaluations, and number of different found solutions. The non-linear systems we used are shown in Table 2.

2.2 Application of Fick's Second Law and the Drying Equation

Based on Fick's second law[14, 15], humidity loss within the bean is given by Equation (25),

$$\frac{dM}{dt} = \nabla \cdot \left(\mathrm{D}\nabla \mathrm{M}\right) \tag{25}$$

Where M is the bean humidity in dry basis (d.b) assuming a cylindric geometry for coffee beans, the solution of the aforementioned equation follows a summation of decreasing exponentials, Equation (26), where Mo and Me represent the initial and equilibrium humidity, respectively, measured in dry basis, r is the average grain radius, and D is the effective diffusion coefficient.

$$\frac{M - M_e}{M_o - M_e} = \frac{6}{\pi^2}\sum_{n=1}^{\infty}\frac{1}{n^2}\exp(-D\frac{n^2\pi^2 t}{r^2}) \tag{26}$$

A more general solution[16] is shown in Equation (27):

$$\frac{M - M_e}{M_o - M_e} = \sum_{i=1}^{\infty} A_i \exp(-k_i * t) \tag{27}$$

From (27), the effective diffusion coefficient can be calculated by dividing the first factor $k_{i=1}$ into π^2 and multiplying the result by the squared value of the average grain radius. Using real data from drying tests, we can use the algorithms for finding parameters A_i and k_i from Equation (27), as well as for estimating M_e. The objective function for this case is shown in Equation (28), where M^* follows Equation (27), and where M represents a vector with 22 elements corresponding to real data from the drying process of coffee beans. Data estimated by the model are then compared against real data through the root mean squared error (RMSE), shown in Equation (29), and through the determination coefficient shown in equation (30) (γ^2), where N is the number of data samples, M is the experimental value of humidity, and M^* is the humidity estimated through the model.

$$\mathrm{f_{obj}} = \sum\left(\mathrm{M} - \mathrm{M}^*\right)^2 = 0 \tag{28}$$

$$RMSE = \sqrt{\frac{\sum_1^N\left(M - M^*\right)^2}{N}} \tag{29}$$

$$\gamma^2 = 1 - \frac{\sum_1^N\left(M - M^*\right)^2}{\sum_1^N\left(M - \bar{M}\right)^2} \tag{30}$$

3. Results and Discussion

3.1 Experiments Related To the Metaheuristics Over Non-Linear Systems

We present the performance metrics of each nonlinear system mentioned in Table 2. We also provide a box plot of the errors calculated throughout 50 repetitions of each algorithm. For 9 out of the 11 experiments, PSO yielded the lowest error, followed by DSO. TRD always found the solution with the lowest number of function evaluations, thus requiring the least computation time. However, because of its nature, TRD can only find one solution in problems with multiple ones. GA was the approach with the second-best run time. The algorithms that find the highest number of solutions are: GA, DSO and PSO. Furthermore, and disregarding TRD, DSO is the approach with the lowest dispersion, followed by GA and PSO, respectively. Tables 3 to 13 and Figures 2 to 12 corroborate the previously described analysis.

Table 3. Performance parameters of system S_1

Alg.	Min. Error	Med. Error	Max Error	Mean Error	SD	SR	Mean Time	Eval.	No. Sol.
PSO	1,8339E-22	7,093E-21	2,9945E-19	4,1467 E-20	7,0669E-20	0,58	9,035	256940	4
TRD	1	1	1	1	0	0	0,01	23	1
GA	1,2053E-14	2,2596E-11	7,7093E-09	4,3288 E-10	1,3903E-09	0	0,744	58020	1
PSO	0	1,1464E-28	2,6734E-22	5,4083 E-24	3,7801E-23	1	2,05	61160	4

Table 4. Performance parameters of system S_2

Alg.	Min. Error	Med. Error	Max Error	Mean Error	SD	SR	Mean Time	Eval.	No. Sol.
PSO	1,0275E-20	7,6982 E-19	4,5731E-18	1,2173E-18	1,2204E-18	0	11,35	257860	1
TRD	2,7988E-14	2,7988 E-14	2,7988E-14	2,7988E-14	6,375E-30	0	0,07	1024	1
GA	3,1484E-12	1,5381E-10	2,8663E-09	3,9356E-10	5,8028E-10	0	0,84	65540	1
PSO	0	3,1122E-27	5,5694E-24	3,7204E-25	1,0417E-24	1	2,5	76380	1

Table 5. Performance parameters of system S_3

Alg.	Min. Error	Med. Error	Max Error	Mean Error	SD	SR	Mean Time	Eval.	No. Sol.
PSO	0	8,9584E-20	3,6093E-18	5,3938E-19	8,8476E-19	0,3	9,4	215420	1
TRD	3,8153E-16	3,8153E-16	3,8153E-16	3,8153E-16	0	0	0,0357	371	1
GA	5,0763E-13	2,4242E-11	2,6606E-09	1,6026E-10	4,3463E-10	0	0,786	62060	1
PSO	1,2326E-32	2,9091E-27	1,409E-24	6,314E-26	2,2251E-25	1	2,3317	71320	1

Table 6. Performance parameters of system S_4

Alg.	Min. Error	Med. Error	Max Error	Mean Error	SD	SR	Mean Time	Eval.	No. Sol.
PSO	1,0373E-18	0,00013344	0,00021157	8,8752E-05	6,8347E-05	0	10,6	248760	6
TRD	0,00658607	0,00658607	0,00658607	0,00658607	4,3808E-18	0	0,118	1838	1
GA	4,0146E-10	0,00342213	0,00342213	0,00197748	0,00159535	0	0,832	62400	7
PSO	0,00013344	0,00342213	0,00342213	0,00197523	0,0016489	0	9,91	287060	3

Table 7. Performance parameters of system S_5

Alg.	Min. Error	Med. Error	Max Error	Mean Error	SD	SR	Mean Time	Eval.	No. Sol.
PSO	0	2,3743E-23	9,9434E-21	1,6135E-21	2,9529E-21	1	0,61	15520	10
TRD	6,3055E-05	6,3055E-05	6,3055E-05	6,3055E-05	0	0	0,121	2320	1
GA	7,5294E-31	1,6309E-21	2,9894E-14	1,3332E-15	5,4604E-15	0,56	0,71	52000	13
PSO	4,9698E-45	7,9425E-35	1,4391E-28	3,1266E-30	2,0363E-29	1	1,35	40880	4

Table 8. Performance parameters of system S_6

Alg.	Min. Error	Med. Error	Max Error	Mean Error	SD	SR	Mean Time	Eval.	No. Sol.
PSO	3,6968E-19	1,9676E-17	2,3582E-16	2,4689E-17	3,4329E-17	0	13,72	271340	2
TRD	1,3913E-13	1,3913E-13	1,3913E-13	1,3913E-13	1,02 E-28	0	0,128	922	1
GA	1,7831E-11	2,3324E-09	1,4885E-07	1,0683E-08	2,4049E-08	0	1,166	80540	2
PSO	5,668 E-28	6,7856E-26	1,2286E-22	3,9806E-24	1,859 E-23	1	3,782	92220	2

Table 9. Performance parameters of system S_7

Alg.	Min. Error	Med. Error	Max Error	Mean Error	SD	SR	Mean Time	Eval.	No. Sol.
PSO	0	1,9391E-19	9,0159E-18	7,3066E-19	1,4323E-18	0,24	9,112	250540	2
TRD	1,9586E-16	1,9586E-16	1,9586E-16	1,9586E-16	4,9804E-32	0	0,016	99	1
GA	5,2018E-15	3,1169E-12	3,5762E-10	2,3253E-11	5,9341E-11	0	0,72	56060	2
PSO	0	5,7816E-28	1,8956E-25	1,0547E-26	3,4236E-26	1	2,238	67260	2

Table 10. Performance parameters of system S_8

Alg.	Min. Error	Med. Error	Max Error	Mean Error	SD	SR	Mean Time	Eval.	No. Sol.
PSO	0	5,9904E-20	1,1227E-17	1,1758E-18	2,3313E-18	0,4	7,473	233840	13
TRD	3,3732E-19	3,3732E-19	3,3732E-19	3,3732E-19	9,7274E-35	0	0,1436	1506	1
GA	1,7621E-13	6,7734E-11	7,2592E-08	1,7153E-09	1,0245E-08	0	0,7823	61440	13
PSO	3,7058E-32	4,5792E-27	1,8525E-22	5,4656E-24	2,7311E-23	1	2,385	73580	13

Table 11. Performance parameters of system S_9

Alg.	Min. Error	Med. Error	Max Error	Mean Error	SD	SR	Mean Time	Eval.	No. Sol.
PSO	0	1,1007E-18	3,6223E-18	1,3002E-18	9,8647E-19	0,04	9,25	268220	2
TRD	3,525 E-06	3,5248E-06	3,5248E-06	3,5248E-06	1,2834E-21	0	0,122	1809	1
GA	1,3791E-13	1,1343E-11	9,8939E-08	2,1308E-09	1,399 E-08	0	0,69	53780	2
PSO	2,4652E-31	4,8317E-27	2,6892E-24	1,4256E-25	4,4408E-25	1	2,28	70500	2

Table 12. Performance parameters of system S_{10}

Alg.	Min. Error	Med. Error	Max Error	Mean Error	SD	SR	Mean Time	Eval.	No. Sol.
PSO	2,9816E-16	8,0839E-16	4,4508E-15	9,7024E-16	7,064 E-16	0	20,377	247160	2
TRD	5,0506E-17	5,0506E-17	5,0506E-17	5,0506E-17	6,2255E-33	0	0,0385	409	1
GA	1,2451E-07	9,0443E-07	6,2273E-06	1,6489E-06	1,6644E-06	0	4,1905	134060	2
PSO	7,2985E-25	1,5173E-23	4,9538E-22	3,9933E-23	7,9738E-23	1	8,57	172680	2

Table 13. Performance parameters of system S_{11}

Alg.	Min. Error	Med. Error	Max Error	Mean Error	SD	SR	Mean Time	Eval.	No. Sol.
PSO	4,7024E-16	1,3411E-14	0,16103138	0,01034948	0,035	0	10,021	404820	12
TRD	1,18567336	1,18567336	1,18567336	1,18567336	1,346E-15	0	0,211	5822	1
GA	2,265E-07	0,00776249	0,72393666	0,06910478	0,119	0	12,151	796000	15
PSO	2,3979E-22	1,7261E-19	0,40680825	0,03206816	0,073	0,26	193,74	5758800	12

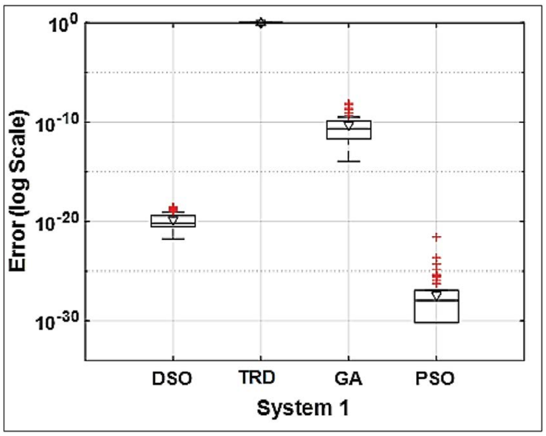

Figure 2. Box plot – Errors of system S_1.

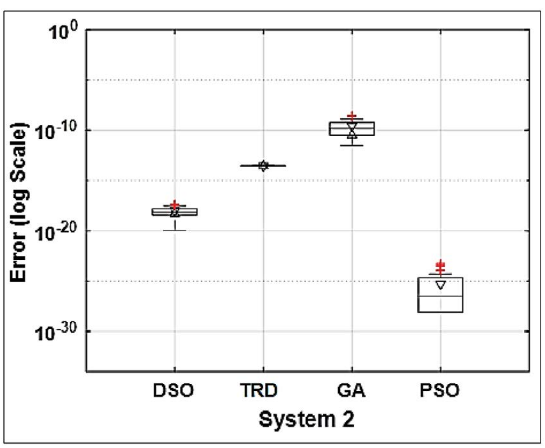

Figure 3. Box plot – Errors of system S_2.

3.2 Application of Fick's Second Law and the Drying Equation

For the drying curves and for the calculation of the diffusion coefficients, we considered that in 10 out of the 11 previous experiments, the standard deviation of error was below 1%. Since each repetition can take several minutes, we decided to run a single repetition of each algorithm for this section. But, we considered drying curves with two, three and four components. In the first case, we ran tests with DSO, GA, and PSO using 1000 and 100 search agents. Based on the resulting data, we selected a population of 100 search agents for the drying curves with 3 and 4 components. The average coffee bean radius used in the estimation of the diffusion coefficient was 5.5 mm. Units of the coefficient are, thus, given in mm^2/min. Tables 14 to 17 and Figures 13 to 16 shows the details of the fitting, as well as the models found for the diffusion coefficients.

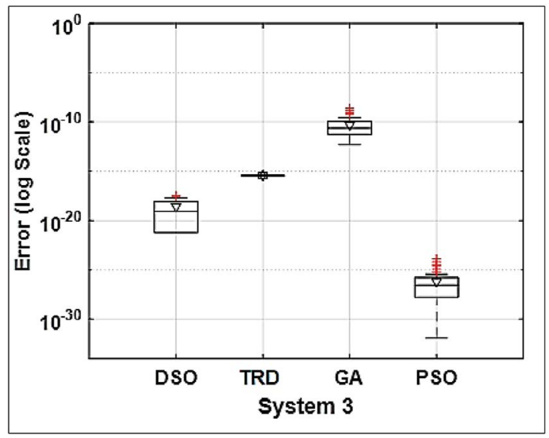

Figure 4. Box plot – Errors of system S_3.

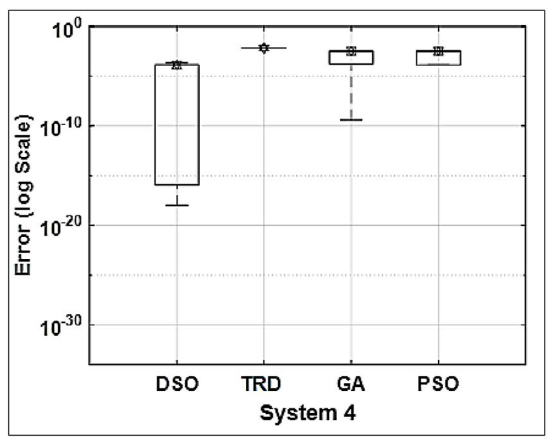

Figure 5. Box plot – Errors of system S_4.

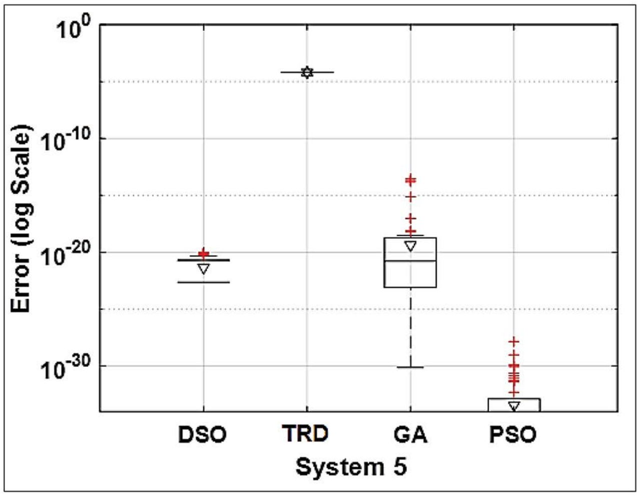

Figure 6. Box plot – Errors of system S_5.

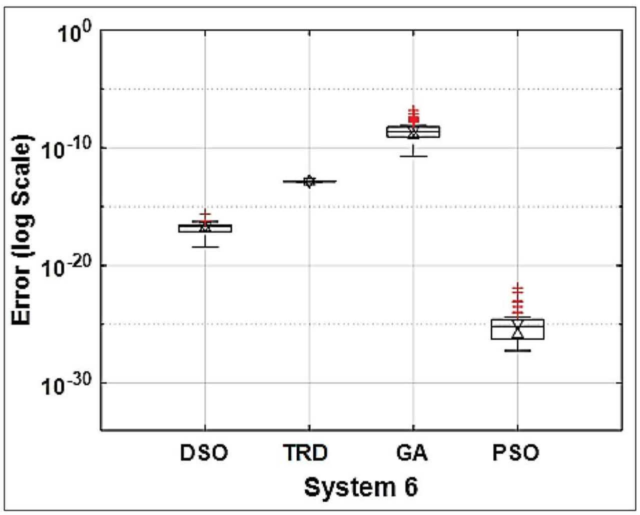

Figure 7. Box plot – Errors of system S_6.

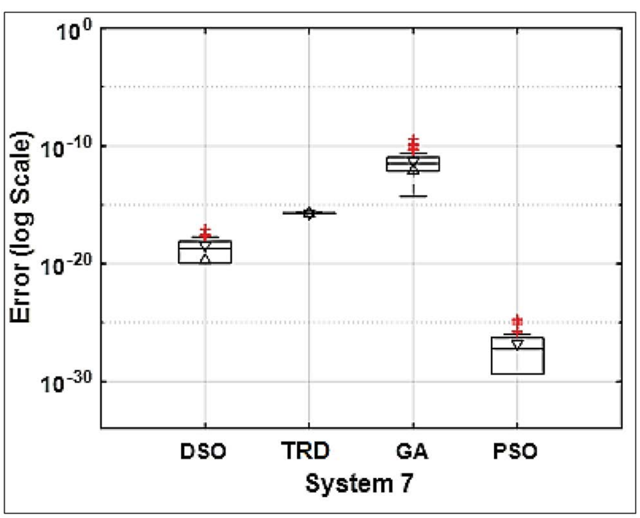

Figure 8. Box plot – Errors of system S_7.

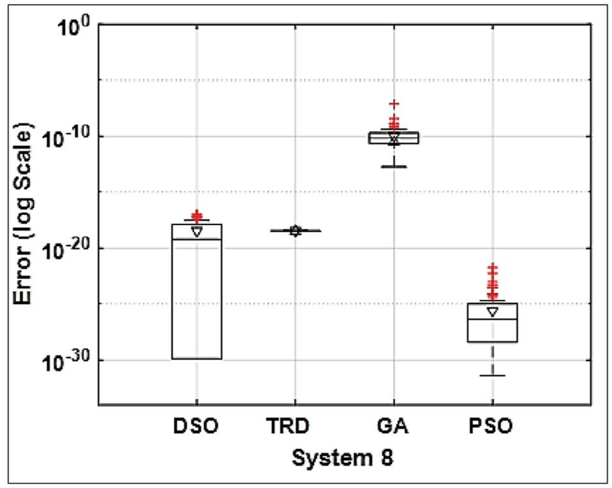

Figure 9. Box plot – Errors of system S_8.

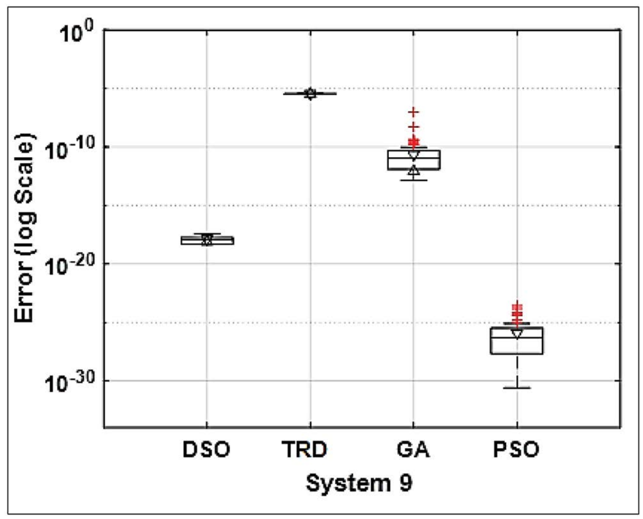

Figure 10. Box plot – Errors of system S_9.

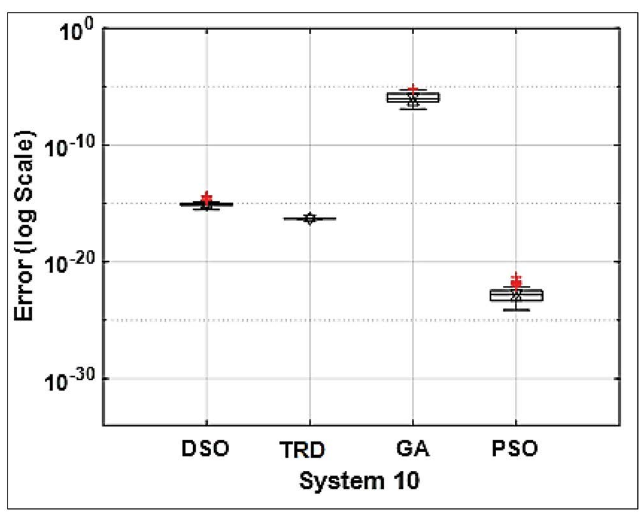

Figure 11. Box plot – Errors of system S_{10}.

Note that the best fitting models are achieved by GA, PSO, and DSO, in that order. Moreover, GA was more computationally efficient. These algorithms also allowed, because of their formulation, to limit the search domain to logical operating ranges. Our data is comparable to previously published results[16].

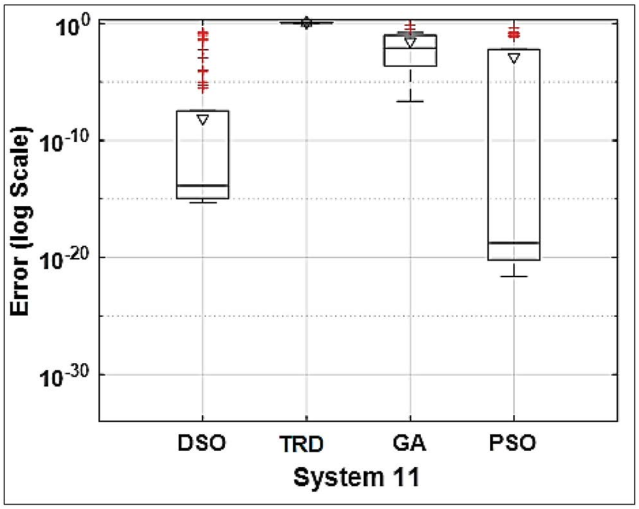

Figure 12. Box plot – Errors of system S_{11}.

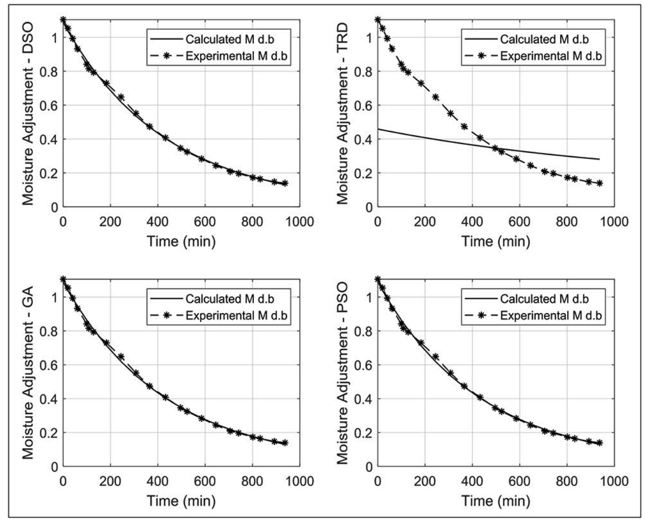

Figure 13. Drying curves fitted with different optimization algorithms, for a summation of two exponentials – Algorithms: DSO, GA, and PSO with initial population of 1000.

Table 14. Performance parameters for the two-element drying curves – Algorithms: DSO, GA, and PSO with initial population of 1000

Alg.	Error	RMSE	r^2	Time (s)	Evaluation	D (mm^2/min)
DSO	0,00412938	0,01370033	0,99819993	614,4976	500000	0.0064
TRD	2,07362989	0,30701124	0,09606608	4,506210	3329	0.0027
GA	0,00415354	0,01374035	0,9981894	96,52852	79000	0.0072
PSO	0,00410392	0,01365804	0,99821102	3022,018	2426000	0.0067

Table 15. Performance parameters for the two-element drying curves – Algorithms: DSO, GA, and PSO with initial population of 100

Alg.	Error	RMSE	r^2	Time (s)	Evaluation	D (mm^2/min)
DSO	0,00411122	0,01367017	0,9982	616,076	439600	0.0066
TRD	0,29389753	0,11558105	0,87188	43,048	33123	0.0083
GA	0,00419068	0,01380165	0,9982	39,65	32500	0.0072
PSO	0,00410392	0,01365804	0,9982	256,102	219100	0.0067

Table 16. Performance parameters for the three-element drying curves – Algorithms: DSO, GA, and PSO with initial population of 100

Alg.	Error	RMSE	r^2	Time (s)	Evaluation	D (mm^2/min)
DSO	0,0041	0,01365	0,998	638,639	186300	0.0067
TRD	0,05	0,04774	0,978	59,5538	43077	0.0085
GA	0,0042	0,01376	0,998	15,6616	12100	0.0066
PSO	0,0041	0,01366	0,998	216,123	187100	0.0067

Table 17. Performance parameters for the four-element drying curves – Algorithms: DSO, GA, and PSO with initial population of 100

Alg.	Error	RMSE	r^2	Time (s)	Evaluation	D (mm^2/min)
DSO	0,0041162	0,01367845	0,9982	632,908	413200	0.0066
TRD	0,0182917	0,02883469	0,9920	68,4508	53094	0.0083
GA	0,0041548	0,0137424	0,9982	16,8025	13200	0.0066
PSO	0,0041499	0,01373433	0,9982	175,326	144000	0.0073

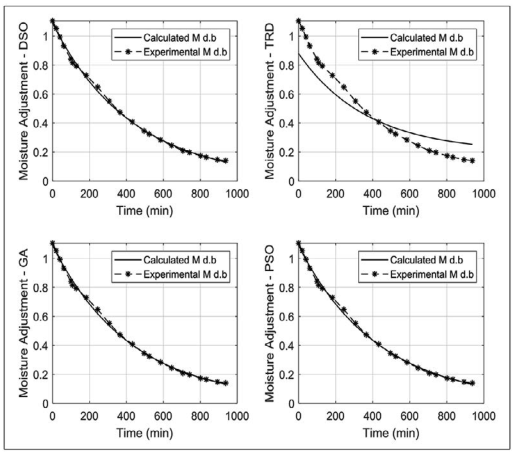

Figure 14. Drying curves fitted with different optimization algorithms, for a summation of two exponentials – Algorithms: DSO, GA, and PSO with initial population of 100.

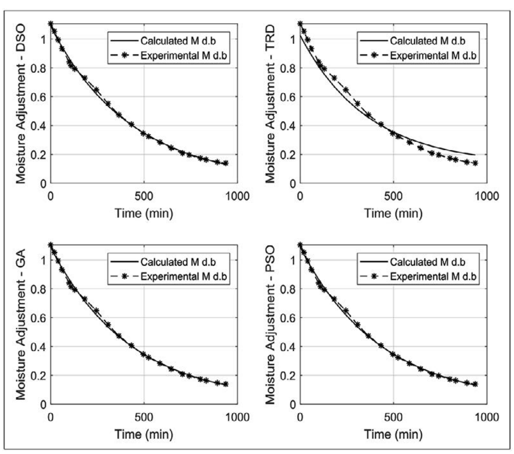

Figure 15. Drying curves fitted with different optimization algorithms, for a summation of three exponentials – algorithms: DSO, GA, and PSO with initial population of 100.

4. Conclusions

Throughout this work we carried out experiments with four metaheuristics for estimating drying curves and diffusion coefficients, based on real data from humidity loss in coffee

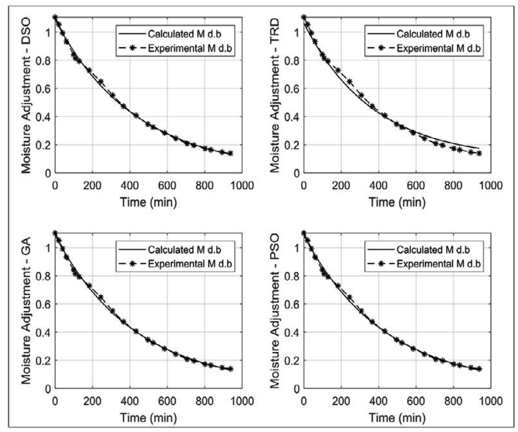

Figure 16. Drying curves fitted with different optimization algorithms, for a summation of four exponentials – algorithms: DSO, GA, and PSO with initial population of 100.

beans from the Castilla variety. Prior to running these tests, we tuned the algorithms on several non-linear systems, finding that PSO, DSO, and GA achieved the lowest error rates. These algorithms were able to achieve correlation coefficients beyond 0.99 when fitting drying curves, with GA representing the alternative with lowest run time. Finding such parameters then allowed estimating the diffusion coefficients, which were located within the expected ranges. Hence, the proposed approach is useful and should be replicated in similar bean drying processes.

5. References

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