Supplementary Information

Determination of Thermal Process Kinetics by Artificial Neural Networks: A Review Considering Isothermal and Non-Isothermal TG And DSC Data

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Table S1. Comparative analysis between the characteristics of neural networks, studied systems and results obtained in the literature works

Reference	Neural Network Type	Material used	Input	Output	Number of hidden layers	Treatment/kinetic model	Accuracy/results
Isothermal							
Sebastião *et al.*[1]	Multilayer Perceptron (MLP)	rhodium(II) acetate	time in isothermal TG data	conversion degree curve $\alpha(t)$ and E_a	1	adjustment of $\alpha(t)$ curves using sigmoide activation function in the intermediate layer; determination of Ea through the optimized weight	MSE = 0.04
Sebastião *et al.*[2]	MLP	rhodium(II) acetate	time in isothermal TG data	contribution of the kinetic models	1	the authors determined the kinetic model contribution to adjust the isothermal experimental data	MSE = 0.03
Ferreira *et al.*[3]	MLP	efavirenz and lamivudine	time in isothermal TG data	contribution of the kinetic models and rate constant	1	the authors determined the kinetic model contribution to adjust the isothermal experimental data and the rate constant of the process	MSE = 0.02
Ferreira *et al.*[4]	MLP	thalidomide	time in isothermal TG data	conversion degree curve $\alpha(t)$ and E_a	1	the authors compared the thermal decomposition process under isothermal and nonisothermal conditions (by MLP and isoconversional model)	MSE = 10e-7
Ferreira *et al.*[5]	MLP	automotive polyurethane	time in isothermal TG data	conversion degree curve $\alpha(t)$ and E_a	1	the authors compared the thermal decomposition process under isothermal and nonisothermal conditions (by MLP and isoconversional model)	MSE = 10e-7 (average)
Non isothermal							
Conesa *et al.*[6]	MLP	simulated data, cellulose, polyethylene and lignin	non-isothermal TG data	rate constant, k_{ref}, activation energy, E_a, and reaction order, n	1	the authors assumed a one process described be a n-th order reaction	only mentions it is in the same order of magnitude as previous data
Burgaz *et al.*[7]	MLP	polymer poly(ethylene oxide)/n% clay, with n = 0, 5, 10, 15, 20, and 100	temperature and clay wt.%	mass loss	2	normalized data/kinetic parameters non determined	$R^2 > 0.999$

Table S1. Comparative analysis between the characteristics of neural networks, studied systems and results obtained in the literature works (cont.)

Reference	Neural Network Type	Material used	Input	Output	Number of hidden layers	Treatment/kinetic model	Accuracy/results
Rojek *et al.*[8]	self-organization map (SOM)	caffeine and excipients	temperature associated with 16 percent mass loss	map of similarity between different samples	2D grid with 5 × 5 neurons	compatibility study between caffeine and excipients based on thermal analysis	the outcomes of SOM studies were confirmed by complementary techniques - DSC and FTIR
Çepelioğullar *et al.*[9]	MLP	refuse-derived fuel	temperature and heating rate	mass loss	2	normalized data/kinetic parameters non determined	MSE = 0.04
Monticeli *et al.*[10]	MLP	curaua, jute, kenaf, and ramie fibers	time, temperature and heating rate	mass loss	1	normalized data/kinetic parameters non determined	$R^2 > 0.99$
Araujo *et al.*[11]	MLP	chitosan raw material	temperature and heating rate	mass loss, contribution kinetic model	1	activation energy by Vyazovkin methodology, contribution model	MSE = 2.3e10-5
Araújo *et al.*[12]	Hopfield	Brazilian petroleum coke	temperature	distribution of activation energy model (DAEM) and parameters q, m, n for Cai-Liu model	–	DAEM, Miura and Maki method, Cai-Liu model	MSE 8.2e10-5
Wakimoto *et al.*[13]	MLP	simulated data	temperature and heating rate	E_a, A and mass loss	1	DAEM, Miura and Maki method	$R^2 > 0.999$
				DSC			
Sbirrazzuoli and Brunel[14]	MLP	simulated data	320 thermograms with n = 2, E_a and ln(A)	$\Delta H, E_a, \ln(A)$	1	feedforward neural networks have been used for kinetic parameters determination in differential scanning calorimetry	MSE = 1e-7
Sbirrazzuoli and Brunel[15]	MLP	simulated data	320 thermograms with n = 2, E_a and ln(A)	$\Delta H, E_a, \ln(A)$	1	the difference between the 2 works is the algorithm used to optimize the ANN	MSE = 1e-8
Araujo *et al.*[16]	Hopfield	losartan potassium	temperature in the DSC data at 3 heating rates	$Ea, \ln(A)$ and n order of reaction	3 neurons	the authors determined the kinetic parameters for polymorphic conversion using DSC data and HNN	MSE = 1e-8 (average)

TG: thermogravimetry; DSC: differential scanning calorimetry; MSE: mean squared error; E_a: activation energy; HNN: Hopfield Neural networks; A: pre-exponential fator; FTIR: Fourier transform infrared spectroscopy.

References

1. Sebastião, R. C. O.; Braga, J. P.; Yoshida, M. I.; *J. Therm. Anal. Calorim.* **2003**, *74*, 811. [Crossref]
2. Sebastião, R. C. O.; Braga, J. P.; Yoshida, M. I.; *Thermochim. Acta* **2004**, *412*, 107. [Crossref]
3. Ferreira, B. D. L.; Araujo, B. C. R.; Sebastião, R. C. O.; Yoshida, M. I.; Mussel, W. N.; Fialho, S. L.; Barbosa, J.; *J. Therm. Anal. Calorim.* **2017**, *127*, 577. [Crossref]
4. Ferreira, B. D. L.; Araújo, N. R. S.; Ligório, R. F.; Pujatti, F. J. P.; Mussel, W. N.; Yoshida, M. I.; Sebastião, R. C. O.; *J. Therm. Anal. Calorim.* **2018**, *134*, 773. [Crossref]
5. Ferreira, B. D. L.; Araújo, N. R. S.; Ligório, R. F.; Pujatti, F. J. P.; Yoshida, M. I.; Sebastião, R. C. O.; *Thermochim. Acta* **2018**, *666*, 116. [Crossref]
6. Conesa, J. A.; Caballero, J. A.; Reyes-Labarta, J. A.; *J. Anal. Appl. Pyrolysis* **2004**, *71*, 343. [Crossref]
7. Burgaz, E.; Yazici, M.; Kapusuz, M.; Alisir, S. H.; Ozcan, H.; *Thermochim. Acta* **2014**, *575*, 159. [Crossref]
8. Rojek, B.; Suchacz, B.; Wesolowski, M.; *Thermochim. Acta* **2018**, *659*, 222. [Crossref]
9. Çepelioğullar, Ö.; Mutlu, İ.; Yaman, S.; Haykiri-Acma, H.; *J. Anal. Appl. Pyrolysis* **2016**, *122*, 84. [Crossref]
10. Monticeli, F. M.; Neves, R. M.; Ornaghi Jr., H. L.; *Cellulose* **2021**, *28*, 1961. [Crossref]
11. Araujo, N. R. S.; Sebastião, R. C. O.; Freitas-Marques, M. B.; da Nova Mussel, W.; Yoshida, M. I.; Virtuoso, L. S.; *Therm. Sci. Eng. Prog.* **2022**, *36*, 101490. [Crossref]
12. Araújo, N. R. S.; Duarte, Á. C. M.; Pujatti, F. J. P.; Freitas-Marques, M. B.; Sebastião, R. C. O.; *Thermochim. Acta* **2021**, *697*, 178847. [Crossref]
13. Wakimoto, S.; Matsukawa, Y.; Numazawa, Y.; Matsushita, Y.; Aoki, H.; *Fuel* **2023**, *343*, 127836. [Crossref]
14. Sbirrazzuoli, N.; Brunel, D.; *Neural Comput. Applic.* **1997**, *5*, 20. [Crossref]
15. Sbirrazzuoli, N.; Brunel, D.; Elégant, L.; *J. Therm. Anal.* **1997**, *49*, 1553. [Crossref]
16. Araujo, B. C. R.; Carvalho, F. S.; Marques, M. B. F.; Braga, J. P.; Sebastião, R. C. O.; *J. Braz. Chem. Soc.* **2020**, *31*, 1392. [Crossref]