XIV ENCAT
Encontro de Catálise do Norte, Nordeste e Centro-Oeste
Catálise: Impulsionando a transição energética para um futuro mais sustentável
17-19 novembro 2024 • Fortaleza
SBCAT SOCIEDADE BRASILEIRA DE CATÁLISE

ÁREA: Métodos computacionais e novos temas para transformações catalíticas

Nonlinear Regression in Adsorption Studies: Which software to use?

Joacy B. Lima[1,*], Cicero W. B. Bezerra[1], Francisco A. Silva[2] , Leonardo B. Cantanhede[2]

[1]Laboratório de Interfaces e de Materiais, Universidade Federal do Maranhão (UFMA), São Luís - MA, 65085-580, Brasil
[2] Programa de Pós-Graduação em Química, Instituto Federal de Educação, Ciência, Tecnológica do Maranhão (IFMA), São Luís - MA, 65030-005, Brasil

**E-mail: joacy.lima@ufma.br*

Abstract

This study compares the performance of Excel 365, RStudio, Jupyter Notebook, Origin, and Matlab for nonlinear regression in adsorption studies. Nonlinear regression is vital for modeling adsorption processes or any other process involving adsorption, such as the removal of methylene blue by activated carbon from monkfish seeds (CAFT). The experimental setup involved kinetic and isotherm models, specifically pseudo-second-order kinetics and the Langmuir isotherm, using a Gauss-Newton algorithm based on the least squares method applied to experimental data from methylene blue adsorption (pH 5.5) on CAFT, an activated carbon from monkfish seeds. Data input varied in complexity and time from one program to another. Excel 365, for example, was easy to use and required minimal programming knowledge. Nonlinear regressions were performed using the Solver add-in or Gauss-Newton algorithm. RStudio offered advanced statistical tools for nonlinear regression via the nls function but required knowledge of R programming. Jupyter Notebook, similar to RStudio, allowed for multiple programming languages like Python, nonlinear regressions were performed using the curve_fit function. Origin is specially designed for scientific data analysis and offered intuitive tools for nonlinear regression without programming knowledge but lacks a free version. Finally, Matlab provided extensive mathematical modeling capabilities, with nonlinear regression available through the Curve Fitter tool. It requires programming knowledge and is not free, though a mobile version is available. The results of the kinetic and isotherm modeling are presented in Tables 1 and 2. As expected, all software produced comparable statistical results with minimal differences but differed greatly in ease of use, availability, and graphical illustration capabilities. [1,2]

Table 1 – Kinetic parameters and statistical analysis.

Parameters	Excel	RStudio	Jupyter Notebook	Origin	Matlab
q_{eq}	3.78E+02	3.78E+02	3.78E+02	3.78E+02	3.78E+02
k_2	4.04E-04	4.04E-04	4.04E-04	4.04E-04	4.04E-04
R^2	0.9818	0.9818	0.9818	0.9818	0.9818
SSR	1.61E+03	1.61E+03	1.61E+03	1.61E+03	1.61E+03
SST	8.85E+04	8.85E+04	8.85E+04	—	—
MSR	1.46E+02	1.46E+02	1.46E+02	1.46E+02	—
SE	1.21E+01	1.21E+01	1.21E+01	—	1.21E+01
SE(q_{eq})	4.70E+00	4.70E+00	4.70E+00	4.70E+00	—
SE(k_2)	3.53E-05	3.53E-05	3.53E-05	3.53E-05	—
Stat t(q_e)	8.04E+01	8.04E+01	8.04E+01	—	—
Stat t(k_2)	1.15E+01	1.15E+01	1.15E+01	—	—
p-value(q_e)	0	0	0	—	—
p-value(k_2)	1.85E-07	1.85E-07	1.85E-07	—	—

Table 2 – Adsorption isotherm parameters and statistical analysis.

Parameters	Excel	RStudio	Jupyter Notebook	Origin	Matlab
q_{max}	5.16E+02	5.16E+02	5.16E+02	5.16E+02	5.16E+02
K_L	4.33E-03	4.33E-03	4.33E-03	4.33E-03	4.3E-03
R^2	0.9869	0.9869	0.9869	0.9869	0.9869
SSR	3.31E+02	3.31E+02	3.31E+02	3.31E+02	3.31E+02
SST	2.52E+04	2.52E+04	2.52E+04	—	—
MSR	6.62E+01	6.62E+01	6.62E+01	6.62E+01	—
SE	8.14E+00	8.14E+00	8.14E+00	—	8.14E+00
SE(q_{max})	7.42E+00	7.42E+00	7.42E+00	7.42E+00	—
SE(K_L)	3.28E-04	3.28E-04	3.28E-04	3.28E-04	—
Stat t(q_{max})	6.96E+01	6.96E+01	6.96E+01	—	—
Stat t(K_L)	1.32E+01	1.32E+01	1.32E+01	—	—
p-value(q_{max})	1.16E-08	1.16E-08	1.16E-08	—	—
p-value(K_L)	4.49E-05	4.49E-05	4.49E-05	—	—

Keywords: computational tools, mathematical modeling, data analysis

References

[1] Bates, D. M.; Watts, D. G. Nonlinear regression analysis and its applications. John Wiley & Sons, 1988.

[2] Tran, H. N. et al. Mistakes and inconsistencies regarding adsorption of contaminants from aqueous solutions: A critical review, Water Research 120 (2017) 88-116.

Acknowledgment

JBL thanks the IFMA Postgraduate Program in Chemistry for supporting his postdoctoral internship.