uncertainties associated with the estimates, it can be said that in all the estimates there was a low degree of uncertainty when comparing the range of the 99% credibility interval with the average of the estimates.

Table 2. Comparison and parameter estimates for the Yoon-Nelson model.

z (cm)	Parameter	Ang et al. (2019)	Present work	Rel. Dev. (%)
5	k_{YN} (min^{-1})	1.68	0.75 (0.60 ; 0.95)	55.35
	τ (min^{-1})	2.87	3.21 (2.96 ; 3.45)	11.84
10	k_{YN} (min^{-1})	1.18	0.48 (0.42 ; 0.58)	59.32
	τ (min^{-1})	6.85	7.63 (7.33 ; 7.95)	11.39
15	k_{YN} (min^{-1})	0.93	0.48 (0.43 ; 0.55)	48.38
	τ (min^{-1})	10.53	11.23 (10.93 ; 11.52)	6.65

Table 3. Comparison and parameter estimates for the Thomas model.

z (cm)	Parameter	Ang et al. (2019)	Estimate	Rel. Dev. (%)
5	k_{TH} (mL mg^{-1}·min^{-1})	2.47	1.43 (1.19; 1.73)	42.10
	q_{TH} (mg g^{-1})	482.29	509.73 (469.35; 549.62)	5.69
10	k_{TH} (mL mg^{-1}·min)	1.68	0.91 (0.78 ; 1.06)	45.83
	q_{TH} (mg g^{-1})	582.28	607.76 (583.28; 632.96)	4.37
15	k_{TH} (mL mg^{-1}·min)	1.87	0.91 (0.80; 1.10)	51.33
	q_{TH} (mg g^{-1})	563.83	596.68 (581.17; 613.66)	5.82

Table 4. Comparison and parameter estimates for the Clark model.

z (cm)	Parameter	Estimate
5	r (min^{-1})	1.061 (0.942; 1.202)
	n	2.368 (2.081; 2.658)
10	r (min^{-1})	0.703 (0.657; 0.755)
	n	2.660 (2.362; 2.956)
15	r (min^{-1})	0.921 (0.878; 0.964)
	n	3.674 (3.283; 4.085)

Table 5. Comparison and parameter estimates for the Yan model.

z (cm)	Parameter	Present study
5	q_y (mg g^{-1})	465.32 (437.21; 494.33)
	a_y	2.34 (2.09; 2.65)
10	q_y (mg g^{-1})	583.95 (559.91; 607.59)
	a_y	3.51 (3.06; 3.99)
15	q_y (mg g^{-1})	583.84 (568.00; 599.11)
	a_y	5.13 (4.44; 5.86)

The estimated and experimental breakthrough curves are shown in Figure 4. From the result, a good agreement was observed between the experimental and estimated data for the Yan model, which is mostly contained within the credibility interval in. $z = 5$ cm .

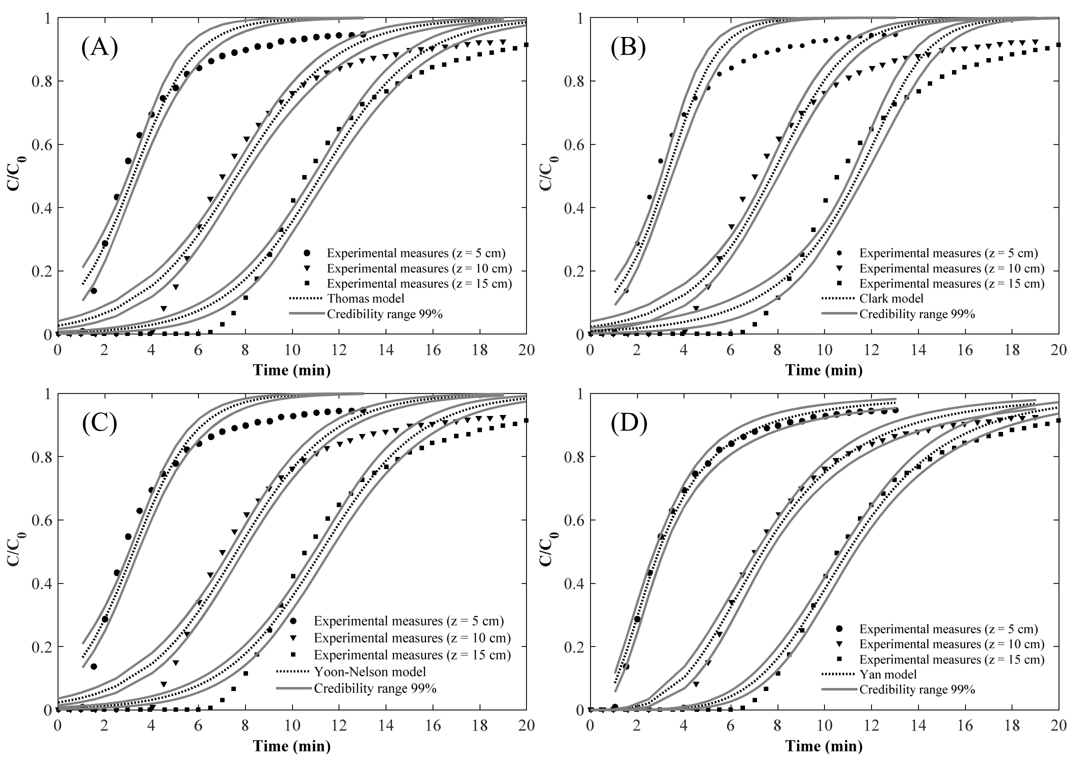

Figure 4. Breaking curve estimates for (A) Thomas, (B) Clark, (C) Yoon-Nelson and (D) Yan models.

In order to quantify the adjustment to the experimental data, the value of the Bayesian criteria for each estimate was calculated as shown in Tables 6 to 8 including the comparison of the results of this study with those of Ang et al. (2019) for Thomas and Yoon-Nelson models.

Table 6: Statistical metrics for model selection at z = 5 cm.

Metric	Model	Present study	Ang et al. (2019)
AIC	Thomas	54.125	95.899
	Yoon-Nelson	54.294	133.422
	Clark	70.119	---
	Yan	10.435	---
AIC_{corr}	Thomas	54.671	96.421
	Yoon-Nelson	54.839	133.944
	Clark	70.664	---
	Yan	10.980	---
BIC	Thomas	28.281	49.208
	Yoon-Nelson	28.366	67.969
	Clark	36.278	---
	Yan	6.436	---

Table 7: Statistical metrics for model selection at z = 10 cm.

Metric	Model	Present study	Ang et al. (2019)
AIC	Thomas	74.288	160.435
	Yoon-Nelson	74.539	256.924
	Clark	105.625	---
	Yan	23.500	---
AICcorr	Thomas	74.651	160.798
	Yoon-Nelson	74.903	257.287
	Clark	105.988	---
	Yan	23.863	---
BIC	Thomas	38.727	81.801
	Yoon-Nelson	38.853	130.045
	Clark	54.396	---
	Yan	13.333	---

According to the model selection criteria, the estimate by the Bayesian technique presented a better result in relation to the study by Ang et al. (2019), because in all the studied cases, lower values for the Bayesian metrics were obtained. This fact corroborates the high value of the relative deviation discussed above.

Table 8: Statistical metrics for model selection at z = 15 cm.

Metric	Model	Present study	Ang et al. (2019)
AIC	Thomas	64.879	208.596
	Yoon-Nelson	64.865	198.020
	Clark	131.191	---
	Yan	25.320	---
AICcorr	Thomas	65.195	208.912
	Yoon-Nelson	65.180	198.336
	Clark	131.507	---
	Yan	25.633	---
BIC	Thomas	34.153	106.012
	Yoon-Nelson	34.146	100.724
	Clark	67.309	---
	Yan	14.373	---

From the results, it was observed that the Yan model presented the best quantitative estimate with the lowest value for the three Bayesian criteria, mainly in. It is worth mentioning that for this bed height, the best estimates were obtained for all models, indicating that they better represent the phenomenon of adsorption in shorter break times.

In addition, it was observed that the Thomas and Yoon-Nelson models presented similar estimates (because they present close values for the metrics AIC, AIC_{corr} and BIC), and, according to the selection criteria, the adjustment to the Yoon model - Nelson overcame the first only when. This is due to the fact that both models are very mathematically similar. However, it is known that the Yoon-Nelson model is the simplest among those analyzed, but the Thomas model loses accuracy for long periods. As reported in the literature, this deficiency is overcome by Yan's model (De Franco et al., 2017).

Among the models studied, the Clark model stands out among the others due to the high values of the Bayesian metrics used (AIC, AIC_{corr}, and BIC), indicating the worst estimate for the rupture curves.

5. CONCLUSION

In this work, the problem of estimating parameters of fixed-bed adsorption was solved, using Bayesian techniques. As a solution methodology, the analytical models of Thomas, Yoon-Nelson, Clark, and Yan were adjusted to experimental data provided in the literature using the Monte Carlo Bayesian technique via Markov Chain implemented with the Metropolis-Hastings acceptance/rejection algorithm. Based on the sensitivity analysis, it was observed that most of the parameters analyzed can be easily estimated, directly implicating the convergence of Markov chains.

Regarding the estimates, the models presented a good fit to the experimental curves, however, the Yan model was more adequate to represent the experimental data and this was the model selected by the Bayesian criteria. Therefore, the Bayesian approach presented itself as an advantageous alternative for the estimation of parameters and selection of models, thus consequently for the prediction of the characteristics of the adsorption system.

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