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Sigmoid Neutralization Response of Acidic Soapstock Waste by Mineralized Phosphorite Residues: A 4-Parameter Logistic Approach

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ABSTRACT
This study investigates the neutralization behavior of an acidic wastewater (AWW)–mineralized mass (MM) system at mass ratios ranging from 100:10 to 100:40, processed at 333 K for 30 min. The evolution of pH as a function of MM dosage and the corresponding CaO content (%) in the solid phase were quantitatively evaluated. The solution pH increased sigmoidally from 4.10 to 7.30, while the CaO content rose from 23.92% to 36.96%, approaching a saturation plateau at higher MM dosages. The pH–dose relationship was described using four-parameter logistic (4PL), Gompertz, and Weibull models, all showing a high goodness of fit ($R^2 \geq 0.97$). Model comparison based on AICc and BIC criteria indicated that the Gompertz model provided the best statistical performance, whereas the 4PL model ensured clearer physicochemical interpretability. A strong positive correlation between pH and CaO content was established (Pearson $r = 0.9649$, $n = 7$, $p < 0.001$), enabling estimation of CaO content from pH values. Numerical inversion of the 4PL model combined with a multi-model ensemble approach was used to determine optimal MM dosages for target pH levels. The recommended operating conditions were identified as 100:32 for pH 6.5, 100:36 for pH 6.8, and 100:38 for pH 7.0, with a stabilization zone observed at 100:37–100:40.

Keywords: neutralization, dose–response, 4-parameter logistic (4PL), pH–CaO correlation, operational optimization.

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Introduction

Acidic wastewater generated during the processing of soapstock in the fat-and-oil industry represents a significant environmental challenge due to its low pH, high salt content, and elevated concentrations of organic and inorganic contaminants [[1], [2], [3]]. Improper handling or disposal of such effluents may lead to soil acidification, groundwater contamination, and adverse effects on aquatic ecosystems. Therefore, the development of effective and resource-efficient neutralization strategies remains an important task for both environmental protection and industrial sustainability [[4], [5], [6], [7]].

In parallel, large volumes of mineralized phosphorite residues are accumulated during phosphate mining and beneficiation, particularly in the Central Kyzylkum region [[8], [9], [10]]. These low-grade materials are typically characterized by high CaO content and limited direct industrial use, resulting in long-term storage and associated environmental risks. Recent studies have highlighted the potential of such calcium-rich mineral residues to serve as neutralizing agents for acidic waste streams, thereby enabling simultaneous wastewater treatment and waste valorization [[11], [12], [13], [14]].

Neutralization processes involving heterogeneous mineral systems often exhibit non-linear behavior due to buffering effects, phase transformations, and saturation phenomena [[15], [16], [17]]. However, many previous studies have relied on linear or simplified empirical approaches, which do not adequately describe the full pH response over a wide range of reagent dosages. In particular, the sigmoidal nature of pH variation during neutralization and its quantitative relationship with solid-phase CaO enrichment have received limited attention in the context of waste-derived mineral reagents [[18], [19]].

The objective of this study is to investigate the neutralization of acidic wastewater using mineralized phosphorite mass from the Central Kyzylkum region, with a focus on the sigmoidal pH–dose response and its mathematical description. By applying four-parameter logistic (4PL), Gompertz, and Weibull models, the work aims to identify optimal operating mass ratios and to establish a quantitative relationship between solution pH and CaO content in the solid phase. This approach provides a predictive basis for process optimization under experimentally defined conditions.

Experimental part

Materials. As feedstocks, the present study used AWW produced during the acid treatment of cottonseed soapstock at “Urganch Yog‘-Moy” JSC and MM stored in the Central Kyzylkum region. According to the results of laboratory analyses, the AWW had pH 2.0 (strongly acidic), COD of 947.2 mg $O_2 \cdot L^{-1}$, BOD_5 of 380.2 mg $O_2 \cdot L^{-1}$, and total hardness of 140.5 mg-eq$\cdot L^{-1}$. Major cations were Na^+ (43,158 mg$\cdot L^{-1}$), Mg^{2+} (1,824 mg$\cdot L^{-1}$), Ca^{2+} (300 mg$\cdot L^{-1}$), and NH_4^+ (100 mg$\cdot L^{-1}$), while major anions were SO_4^{2-} (48,145 mg$\cdot L^{-1}$), Cl^- (38,116 mg$\cdot L^{-1}$), and HCO_3^- (3,446 mg$\cdot L^{-1}$). Besides, AWW contained 2.1 wt% total organics and 1.64 wt% total SO_3. The phosphorite residues of the Central Kyzylkum region represented low-grade mineralized mass of the following composition, wt%: P_2O_5 15.09, CaO 43.17, Al_2O_3 1.22, Fe_2O_3 1.34, MgO 1.21, F 1.7, CO_2 14.01, SO_3 2.17, and moisture 9.11. Due to the high CaO content, these residues can be used as the basic neutralizing agent for AWW treatment. The combined use of AWW and MM not only reduces ecological hazards but also opens up new sources of secondary raw materials for fertilizers and other products [[20], [21], [22], [23]].

In order to investigate neutralization, AWW and MM were mixed at different mass ratios from 100:10 to 100:40, enabling quantitative assessment of pH changes upon increasing phosphorite addition. Mixing was performed at 333 K (≈60 °C) to accelerate acid-base reactions and ensure a homogeneous medium. Each experiment was carried out under intense agitation for 30 min, during which the liquid phase reached quasi-equilibrium. Afterwards, the mixtures were dried at 353 K (≈80 °C) to eliminate moisture and accurately determine CaO in the final solid phase; such drying conditions also contribute to residual acid reactions being completed [[22], [23]]. In systematic variation through the mass ratios, the pH increased from 4.10 to 7.30, while the content of CaO in the solid phase increased from 23.92 wt% to 36.96 wt% (Table 1).

Methods. All experimental procedures reported in this study were carried out by the authors under laboratory conditions. Standard analytical methods cited from the literature were used solely as reference protocols for measurements, whereas sample preparation, neutralization experiments, data acquisition, and data processing were performed independently within the framework of this work.

This methodological approach offered the possibility to obtain a complete picture of the neutralization process, find the optimum mass ratio, and obtain reliable data for mathematical modeling. Moreover, experimental conditions were chosen considering realistic technological parameters in accordance with industrial reprocessing practice. pH and CaO content were selected as main performance indicators of the neutralization efficiency. pH was measured using a laboratory pH meter with an ion-selective electrode; the instrument was calibrated before each run with standard buffer solutions (pH 4.00, 7.00, and 9.18).

In order to avoid the effects of temperature, the measurements were performed after attaining equilibrium at 333 K for every mixture.

Table 1 - Composition of neutralization products derived from acidic wastewater (AWW) and the Central Kyzylkum mineralized phosphorite mass

Mass ratio (AWW:MM)	pH	CaO, %
100:10	4.1	23.92
100:15	4.81	27.95
100:20	5.62	28.66
100:25	5.9	32.68
100:30	6.33	35.48
100:35	6.74	36.74
100:40	7.3	36.96

The measurement of the content of CaO was done using the traditional method of complexometric titration using an EDTA solution to titrate calcium ions (Ca^{2+}), and murexide indicator. To maintain analytical accuracy, each assay was carried out in triplicate and mean values were provided as a result. Additionally, some of the samples were confirmed through the gravimetric method, where calcium was precipitated from solution as $CaCO_3$, and the mass correlation between that precipitation and the amount of CaO was determined mathematically via stoichiometry. The estimated overall analytical uncertainty was controlled to ±0.02 for pH and ±0.3% for CaO. The use of both complexometric and gravimetric methods enabled the researcher to collect a reliable dataset that is suitable for the mathematical modeling of neutralization reactions. For a mechanistic yet parsimonious description of the process, the four-parameter logistic (4PL) model was adopted, as it captures the sigmoidal pH–dose dependence effectively. The general form of the 4PL used in this work is:

$$\boldsymbol{y(x) = A1 + \frac{A2 - A1}{1 + (\frac{x}{x_0})^{-n}}}$$

Here, *A1* denotes the initial lower asymptote (acid-region pH), *A2* the upper asymptote (neutral/alkaline region), *x* the half-response mass (dose at which *pH≈(A1+A2)/2*), and *n* the transition steepness, which reflects buffer capacity and the sharpness of the reaction front [24].

Parameter estimation was performed by nonlinear least squares; starting values were anchored to the observed minimum and maximum pH, and 95% confidence intervals were obtained by bootstrap resampling (≥1000 replicates) [25]. Model selection relied on AICc [26] and BIC [27], with the lowest scores indicating the preferred specification. As alternatives to 4PL, Weibull and Gompertz functions were also evaluated. Weibull model (four-parameter, CDF form):

$$y\,(x) = A2 - (A2 - A1)e^{-(\frac{x}{\lambda})^{\beta}}$$

Here, *λ* is the scale parameter, and *β* is the shape parameter; in practice, the Weibull specification captures the gradual, decelerating approach to the plateau as the dose increases.

Gompertz model.

$$y\,(r) = A1 + (A2 - A1)\; e^{-exp[-k(x - x_0)]}$$

This model describes an initial lag phase, a period of accelerating growth, and a final brief saturation stage; it is thus better suited to asymmetric response curves [28]. All models were validated by residual diagnostics (residuals vs. fitted values, Q–Q plots, and Cook's distance) and weighted regression was applied when heteroscedasticity was detected. The key benefit of the 4PL formulation derives from the physicochemical interpretability of the parameters: A1 corresponds to the starting acidic baseline, A2 to the final neutral/alkaline plateau, x0 to the half-response dose (i.e., operational mass ratio at the midpoint of the process), and n describes the transition steepness (i.e., process sensitivity), thereby elevating the analysis of neutralization from simple empirical observation to a predictive, parametric basis. In this regard, numerical inversion of the 4PL model was also implemented to calculate the required mass ratio for a given target pH, which allows for actionable decisions in industrial practice. In all, the 4PL constitutes a rigorous mathematical representation of full sigmoidal neutralization behavior and returns results that are at once reliable and practically useful, while Weibull and Gompertz provide supporting checks and further insight when asymmetry in the process response is present.

Although standard analytical approaches reported in the literature were used as methodological references, all experimental work and data presented in this article were generated by the authors.

Results and Discussion

The results presented below were obtained exclusively from experiments conducted in this study. All data points correspond to independently performed neutralization tests at defined AWW:MM mass ratios, and no secondary or literature-derived datasets were used in the analysis.

The AWW:MM ratios tested in this research ranged from 100:10 to 100:40, all trials carried out on day 333 K; all agitation times lasted 30 minutes and were performed according to protocols described in the 'Materials and Methods' section. The solution's pH was monitored after each experiment, and the mass fraction of CaO contained within the solid portion of the solution was computed and expressed as a percentage of that solution mass. Solutions were two-point calibrated with buffers, one at pH 4.00 and the other at pH 7.00, before obtaining the pH measurements of each solution; all solutions were corrected for temperature variations by using ATC. The electrodes utilized for pH measurements were cleaned before each use, and electrode drift was accounted for. The results of CaO determinations were obtained through STN methods; sample treatments and measurements of ions using the ion-selective electrode were consistently performed in the same manner from run to run. The major contributors to uncertainty associated with analysing the data were identified as, but are not limited to, electrode drift, the effects of ionic strength, and the potential for heterogeneity in the samples being analysed; therefore, the responses obtained from calibrating and controlling test solutions were completed before each measurement series began. The resulting raw dataset covered AWW:MM points 100:10, 100:15, 100:20, 100:25, 100:30, 100:35, and 100:40. The corresponding pH values were 4.10, 4.81, 5.62, 5.90, 6.33, 6.74, and 7.30, and CaO contents were 23.92%, 27.95%, 28.66%, 32.68%, 35.48%, 36.74%, and 36.96%, respectively (Table 1). Descriptive statistics confirmed data stability and controlled dispersion. For pH, N = 7, min = 4.10, max = 7.30, mean = 5.829, SD = 1.105, and CV = 18.95% (Table 2).

Table 2 - Descriptive statistics for pH and CaO (%): N, Min, Max, Mean, SD, CV (%)

Metric	N	Min	Max	Mean	SD*	CV, %
pH	7	4.10	7.30	5.829	1.105	18.95
CaO, %	7	23.92	36.96	31.770	5.035	15.85

*SD — sample standard deviation**;** CV (%) = SD / Mean × 100**.**

For CaO, N=7, a minimum of 23.92% to a maximum of 36.96%. The mean CaO content was 31.770% with SD=5.035 and CV=15.85%. This data preliminarily indicates that there is a sigmoidal increase with respect to the pH levels and near-saturation of CaO. The dataset is sufficiently informative for future stages of modelling. The increase of the AWW:MM ratio caused an increase in the pH of the solutions. An initial monotonic increase and a distinct sigmoidal response was seen as the AWW:MM ratio was increased from 100:10 to 100:40. The growth rate of the pH-response increased between the AWW:MM ratios of 100:20 - 100:30, followed by a plateau from 100:35 - 100:40. This response demonstrated that the Neutralisation process occurred stepwise during Buffering and Carbonation. Four-parameter Logistic, Gompertz, and Weibull Models were fitted to the pH-dose data according to the procedures and constraints set forth in Materials and Methods; these three models all fitted the data adequately with minor differences in goodness of fit. The Gompertz model yielded the lowest AICc and BIC and thus emerged as the preferred specification; its $R^2 = 0.989$ indicates a high explanatory power. The Weibull model achieved $R^2 = 0.987$ with competitive AICc/BIC values. Although the 4PL model also produced $R^2 \approx 0.989$, it was penalized more strongly by AICc and therefore ranked slightly lower. Figure 1 presents the observed points and the three fitted curves on a single plot, clearly illustrating the sigmoidal trajectory.

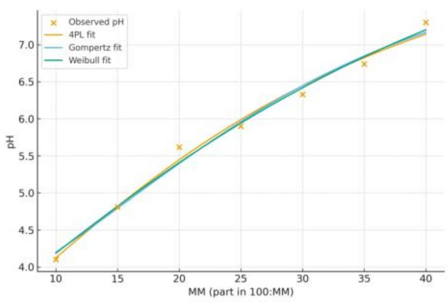

Figure 1 - pH vs. MM: observed data points with fitted 4PL, Gompertz, and Weibull curves

Figure 2 residual distribution for the best-fitting model, confirming the absence of systematic patterns.

Random dispersion of the residuals around zero indicates that the model is correctly specified. The physical interpretation of the 4PL parameters is convenient: the lower asymptote is $A_1 \approx 3.03$ and the upper asymptote is $A_2 \approx 9.50$. For 4PL, the half-response dose EC_{50} (x_0) ≈ 27.93, meaning that the response reaches its midpoint at this dose, and the slope parameter $n \approx 1.55$ reflects a moderately sharp transition. In the Gompertz model, the upper asymptote is $a \approx 8.82$, while the shape parameter $c \approx 0.043$ indicates a gradually advancing neutralization front; the half-response occurs at $x_{50} \approx 11.87$, i.e., at a lower dose. For the Weibull model,

the upper asymptote is $a \approx 9.50$ and the shape parameter $c \approx 0.659$, capturing dynamics that accelerate initially and then decelerate; the corresponding half-response is $x_{50} \approx 14.18$, which marks the dose yielding the median response. Table 3 reports the goodness-of-fit indicators—R^2, AICc, and BIC—enabling direct comparison among the models.

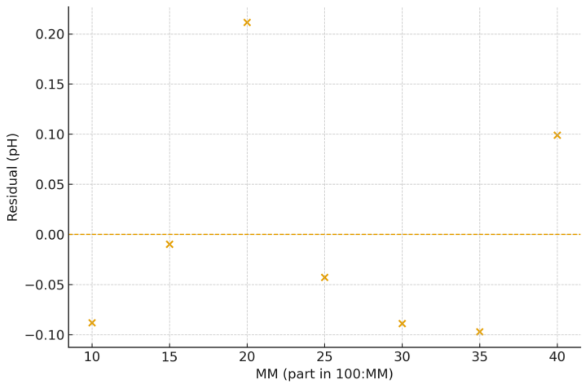

Figure 2 - Residuals for the best-fitting model (Weibull).

Random dispersion of the residuals around zero indicates that the model is correctly specified. The physical interpretation of the 4PL parameters is convenient: the lower asymptote is $A_1 \approx 3.03$, and the upper asymptote is $A_2 \approx 9.50$. For 4PL, the half-response dose EC_{50} (x_0) ≈ 27.93, meaning that the response reaches its midpoint at this dose, and the slope parameter $n \approx 1.55$ reflects a moderately sharp transition. In the Gompertz model, the upper asymptote is $a \approx 8.82$, while the shape parameter $c \approx 0.043$ indicates a gradually advancing neutralization front; the half-response occurs at $x_{50} \approx 11.87$, i.e., at a lower dose. For the Weibull model, the upper asymptote is $a \approx 9.50$ and the shape parameter $c \approx 0.659$, capturing dynamics that accelerate initially and then decelerate; the corresponding half-response is $x_{50} \approx 14.18$, which marks the dose yielding the median response. Table 3 reports the goodness-of-fit indicators—R^2, AICc, and BIC—enabling direct comparison among the models.

The table also includes an interpretation of the EC_{50} (x_0) and n parameters to guide practical dose selection. While the Gompertz model attains the lowest AICc/BIC, indicating the statistically preferred specification, the 4PL parameters remain the most operationally intuitive.

Table 3 - Parameter estimates and goodness-of-fit statistics for pH models (4PL, Gompertz, Weibull)

Model	4PL	Gompertz	Weibull
Lower asymptote (y↓)	3.03	~0.00	~0.00
Upper asymptote (y↑)	9.50	8.82	9.50
EC50, x_{50}	27.93	11.87	14.18
n (slope/shape)	1.55	0.043	0.659
R^2	0.989	0.989	0.987
AICc	−2.998	−17.255	−15.903
BIC	−23.214	−25.417	−24.066

Accordingly, we recommend balancing statistical optimality with physicochemical interpretability. For example, in production terms, the 4PL x_0 points to the transition region around pH = 6.2–6.3. By contrast, Gompertz and Weibull emphasize the early-transition segment more strongly and are useful for assessing reagent economy. Residual diagnostics confirmed adequacy across the main domain, with minor edge deviations that may arise from buffer phases and solid-phase formation. Overall, the pH–dose response corroborates the multistage nature of neutralization. In the next step, the CaO–dose results are integrated to recommend a clear optimal dose window. In the AWW–MM system, the association between pH and CaO (%) is strongly positive: Pearson r = 0.96490, n = 7, p = 0.000435 (Table 4).

Table 4 - Pearson correlation (pH vs. CaO), significance, sample size, 95% confidence interval for r, and linear regression summary (slope, intercept, R^2).

Metric	Value
Pearson r	0.96490
p-value	0.000435
n (observations)	7
95% CI (r, lower)	0.77494
95% CI (r, upper)	0.99498
Linear slope, dCaO/dpH	4.39823
Slope 95% CI (lower)	3.02215
Slope 95% CI (upper)	5.77431
Intercept (CaO % at pH = 0)	6.13460
R^2	0.93104

This implies that as pH increases, the CaO fraction in the solid phase also increases monotonically; the 95% confidence interval for the Pearson correlation is [0.77494, 0.99498]. A simple linear regression (CaO = 6.13460 + 4.39823·pH) yielded R^2 = 0.93104, indicating that ≈93% of the variance in CaO is explained by pH (Figure 3). In the scatter plot of Figure 3 (markers = observations), the least-squares regression line shows that a one-unit increase in pH raises CaO by ~4.40% (95% CI for the slope: [3.02215, 5.77431]).

These quantitative results are mechanistically consistent with: (a) consumption of free acidity during neutralization, leading to a pH rise; (b) increasing buffering strength (phosphate–calcium and carbonate buffers) as pH grows; (c) formation of carbonate and Ca–phosphate phases (e.g., brushite/apatite), which transfers Ca species to the solid phase and increases CaO (%); and (d) emergence of a plateau at high pH due to solubility constraints and slower phase-growth kinetics.

As a result, CaO can be practically predicted from on-line pH control; for example, at pH ≈ 6.8, CaO≈6.13460+4.39823×6.8≈36.0%. The strong, monotonic pH–CaO association, together with the plateau observed in the upper segment of the pH–dose curve (zone of sharply diminishing marginal gains) forming around 100:37–100:40, informed the dose selection for target pH. Accordingly, the required doses were obtained by numerical inversion of the 4-parameter logistic (4PL) model (the primary specification described in Materials and Methods) and stabilized via triangulation with Gompertz, Weibull, and local linear interpolation (see Table 5).

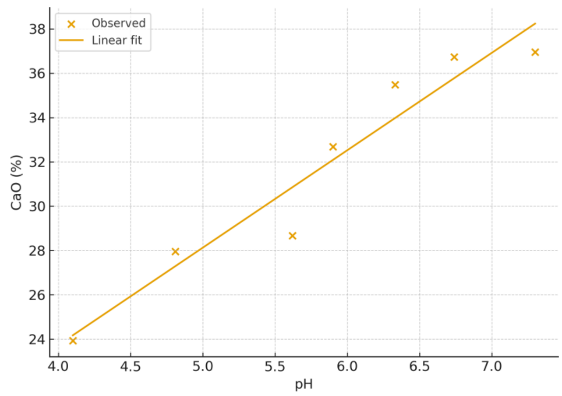

Figure 3 - Relationship between pH and CaO (%) in the AWW–MM system (n = 7).
Markers indicate observations; line shows the least-squares linear fit (CaO = 6.13460 + 4.39823·pH; R^2 = 0.93104; p < 0.001).

All computations were interpreted strictly within the observed range (MM = 10–40). For each target pH, the ensemble median across the four approaches was adopted as the recommended dose, whereas the model min–max defined the operational control window.

Table 5 - Target pH → recommended dose (100:MM), based on 4PL inversion with multi-model triangulation (Gompertz, Weibull, and local linear interpolation)

Target pH	**6,5**	**6,8**	**7.0**
4PL (MM)	30.67	34.63	37.63
Gompertz (MM)	32.55	36.38	38.74
Weibull (MM)	32.00	35.52	37.57
Linear interp. (MM)	32.07	35.54	37.32
Ensemble median (MM)	32.07	35.98	37.60
Recommended (100:MM)	100:32	100:36	100:38*
Operational window	100:31–100:33	100:35–100:37	100:37–100:40

Accordingly, the most suitable settings are pH 6.5 → ~100:32, pH 6.8 → ~100:36, and pH 7.0 → ~100:38. Because the last setting lies very close to the onset of the plateau, a cost-aware operating policy is to start at 100:37 and, under on-line pH control, adjust 37 → 38 only if required.

Conclusions

The neutralization of acidic wastewater by the Central Kyzylkum mineralized mass exhibited a clear sigmoidal pH response within the investigated mass ratio range of 100:10–100:40. Under the applied conditions (333 K, 30 min), the solution pH increased from 4.10 to 7.30, while the CaO content in the solid phase rose from 23.92% to 36.96%, indicating progressive incorporation of calcium-bearing components during neutralization.

Mathematical description of the pH–dose relationship using four-parameter logistic (4PL), Gompertz, and Weibull models demonstrated a high goodness of fit ($R^2 \geq 0.97$). Although the Gompertz model showed the most favorable statistical criteria (AICc/BIC), the 4PL model provided parameters with clearer physicochemical interpretation, enabling identification of the transition region and the onset of saturation. Based on model inversion and multi-model comparison, the optimal operating mass ratios were determined as 100:32 for pH 6.5, 100:36 for pH 6.8, and 100:38 for pH 7.0, with a stabilization (plateau) zone observed at 100:37–100:40.

A strong positive correlation between pH and CaO content was established (Pearson r = 0.9649, $p < 0.001$), demonstrating that pH can serve as a reliable operational indicator for estimating CaO enrichment in the solid phase under the investigated conditions. This relationship provides a quantitative basis for process control and dose selection during neutralization.

The conclusions of this study are limited to experimentally measured pH and CaO parameters and their mathematical interpretation. Potential effects related to corrosion behavior, environmental impact, carbonation processes, and the agronomic suitability of the solid product were not evaluated and therefore remain outside the scope of the present work. These aspects should be addressed in future investigations.

Conflicts of interest. On behalf of all authors, the corresponding author states that there is no conflict of interest.

CRediT author statement: **S. Shamuratov**: Conceptualization, Methodology, Software, Data curation, Writing draft preparation, Supervision, Software, Validation, Reviewing and Editing; **U. Baltaev, U. Alimov, M. Jabbarov, A. Madaminov**: Visualization, Investigation.

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Қышқыл сабын қалдықтарының сигмоидты бейтараптандыру реакциясында минералданған фосфорит қалдықтарын пайдалану: 4 параметрлі логистикалық тәсіл

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ТҮЙІНДЕМЕ
Бұл зерттеуде 333 К температурада және 30 минут өңдеу уақытында 100:10–100:40 массалық қатынастарда «қышқылды ағынды су (AWW) – минералданған масса (ММ)» жүйесінің бейтараптану процесінің жүрісі зерттелді. ММ дозасына байланысты pH өзгерісі және қатты фазадағы CaO мөлшері (%) сандық түрде бағаланды. Ерітінді pH мәні 4,10-нан 7,30-ға дейін сигмоидалы түрде артты, ал CaO мөлшері 23,92%-дан 36,96%-ға дейін өсіп, ММ-нің жоғары дозаларында қанығу платосына жақындады. «pH–доза» тәуелділігі төртпараметрлі логистикалық (4PL), Гомпертц және Вейбулл модельдері арқылы сипатталды, олардың барлығы жоғары сәйкестік дәрежесін көрсетті ($R^2 \geq 0,97$). AICc және BIC критерийлері негізінде жүргізілген модельдерді салыстыру нәтижесінде Гомпертц моделі ең жақсы статистикалық көрсеткіштерге ие екені анықталды, ал 4PL моделі физика-химиялық тұрғыдан неғұрлым айқын интерпретацияланатын параметрлерді қамтамасыз етті. pH пен

CaO мөлшері арасында күшті оң корреляция орнатылды (Пирсон коэффициенті r = 0,9649, n = 7, p < 0,001), бұл CaO мөлшерін pH мәндері арқылы бағалауға мүмкіндік береді. 4PL моделін сандық кері есептеу мультимодельді ансамбльдік тәсілмен біріктіріліп, берілген pH деңгейлері үшін ММ-нің оңтайлы дозаларын анықтау мақсатында қолданылды. Ұсынылған жұмыс режимдері pH 6,5 үшін 100:32, pH 6,8 үшін 100:36 және pH 7,0 үшін 100:38 болып анықталды, ал тұрақтану аймағы 100:37–100:40 аралығында байқалды.

Түйін сөздер: бейтараптандыру, доза–реакция тәуелділігі, төрт параметрлі логистикалық модель (4PL), pH–CaO корреляциясы, технологиялық процесті оңтайландыру.

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Сигмоидная нейтрализационная реакция кислых отходов соапстока с использованием минерализованных остатков фосфоритов: 4-параметрический логистический подход

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АННОТАЦИЯ

В настоящем исследовании изучается поведение процесса нейтрализации системы «кислотные сточные воды (AWW) – минерализованная масса (ММ)» при массовых соотношениях от 100:10 до 100:40 при температуре 333 K и продолжительности обработки 30 мин. Количественно оценена зависимость изменения pH от дозировки ММ, а также соответствующее содержание CaO (%) в твердой фазе. Значение pH раствора возрастало по сигмоидальной зависимости от 4,10 до 7,30, в то время как содержание CaO увеличивалось с 23,92% до 36,96%, приближаясь к плато насыщения при более высоких дозировках ММ. Зависимость «pH–доза» была описана с использованием четырехпараметрической логистической (4PL), моделей Гомпертца и Вейбулла, которые показали высокую степень аппроксимации ($R^2 \geq 0{,}97$). Сравнение моделей на основе критериев AICc и BIC показало, что модель Гомпертца обеспечивает наилучшие статистические показатели, тогда как модель 4PL обладает более четкой физико-химической интерпретируемостью. Установлена сильная положительная корреляция между pH и содержанием CaO (коэффициент Пирсона r = 0,9649, n = 7, p < 0,001), что позволяет оценивать содержание CaO по значениям pH. Численное обращение модели 4PL в сочетании с мультимодельным ансамблевым подходом было использовано для определения оптимальных доз ММ при заданных значениях pH. Рекомендуемые рабочие условия составили 100:32 для pH 6,5, 100:36 для pH 6,8 и 100:38 для pH 7,0, при этом зона стабилизации наблюдалась в диапазоне 100:37–100:40.

Ключевые слова: нейтрализация, зависимость доза–отклик, четырёхпараметрическая логистическая модель (4PL), корреляция pH–CaO, оптимизация технологического процесса.

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