SUPPLEMENTARY INFORMATION

Recovery of Scandium and Neodymium from Blast Furnace Slag using Acid Baking – Water Leaching

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Experimental design

Extraction efficiency of target element *i* (y_i) was calculated as outlined in Eq. (1).

$$y_i = \frac{C_i V_i}{m_o} \times 100 \qquad \text{[Eq. 1]}$$

where C_i is the concentration of the analyte in the leachate, V_i is the volume of the leachate, and m_o is the weight of each element in the utilized feed slag sample.

To estimate the extraction efficiency of target elements ($\hat{y}_i$) and predict the optimum conditions, the empirical model shown in Eq. (2) was fit to the experimental data using multiple Linear Least Squares Regression (mLLSR) presented in Eq. (3).

$$\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 X_1 + \hat{\beta}_2 X_2 + \hat{\beta}_3 X_3 + \hat{\beta}_4 X_4 + \hat{\beta}_5 X_5 + \hat{\beta}_6 X_6 \qquad \text{[Eq. 2]}$$

where $\hat{\beta}$ is the vector containing each of the model parameters, $\hat{\beta}_0$ corresponds to the baseline bias for the analyte, $\hat{\beta}_1$ corresponds to the baking temperature, $\hat{\beta}_2$ corresponds to the acid to slag mass ratio, $\hat{\beta}_3$ corresponds to the baking time, $\hat{\beta}_4$ corresponds to the water to acid-baked slag ratio, $\hat{\beta}_5$ corresponds to the agitation rate, and $\hat{\beta}_6$ corresponds to the water to slag mass ratio (before baking).

$$\hat{\beta} = (\mathrm{X}^T\mathrm{X})^{-1}(\mathrm{X}^T\mathrm{Y}_i) \qquad \text{[Eq. 3]}$$

where X is the experimental design matrix (Table S2), and $\mathrm{Y_i}$ is the response matrix including the actual extraction efficiencies for analyte *i*.

The significance of the model parameters was determined using 95% confidence intervals ($CI_{95\%}$), based on a two-tailed t-distribution presented in Eq. (4). The variance of each parameter ($s^2_{\hat{\beta}}$) was estimated by the square of the pooled standard deviation of the pairs of replicate runs. To simplify the empirical model and leave only the parameters which have a significant effect, any parameters for which the confidence interval includes zero were removed from the model.

$$CI_{95\%} = \hat{\beta}_j \pm t_{m,\,0.05/2} \times \sqrt{\frac{s^2_{\hat{\beta}}}{n_j}} \qquad \text{[Eq. 4]}$$

Analysis of variance (ANOVA) was conducted for the simplified models to assess the goodness of model fit. The coefficient of determination (R^2), a measure of the correlation between the measured extraction efficiencies (y_i) and the predicted values ($\hat{y}_i$), was determined on the basis of Eq. (5). The significance of the models was evaluated by an *F* test (Eq. (6) and (7)), and the adequacy of the models was assessed by an *R* test (Eq. (8) and (9)).

$$R^2 = 1 - \frac{ResSS}{TSS_{cfm}} = \frac{RSS_{cfm}}{TSS_{cfm}} = \frac{\sum_{k=1}^{p} \left(\hat{y}_{i,k} - \bar{y}_i\right)^2}{\sum_{k=1}^{p} \left(y_{i,k} - \bar{y}_i\right)^2}$$

[Eq. 5]

$$ResSS = \sum_{k=1}^{p} \left(\hat{y}_{i,k} - y_{i,k}\right)^2 = TSS_{cfm} - RSS_{cfm}$$

[Eq. 6]

$$Reject\ H_o\ if: F = \frac{RSS_{cfm}}{ResSS} \times \frac{dof_{ResSS}}{dof_{RSS_{cfm}}} > F_{dof_{RSS_{cfm}}, dof_{ResSS}, 0.05}$$

[Eq. 7]

$$SSLF = ResSS - SSPE = ResSS - s_{\hat{\beta}}^{\ 2} \times m$$

[Eq. 8]

$$Reject\ H_o\ if: R = \frac{SSLF}{SSPE} \times \frac{dof_{SSPE}}{dof_{SSLF}} > F_{dof_{SSLF}, dof_{SSPE}, 0.05}$$

[Eq. 9]

Table S1. Summary of -1, 0, and +1 factor levels for operating parameters.

Factor	Factor Description	Units	-1 Level	0 Level	+1 Level
X_1	Baking temperature	ºC	200	300	400
X_2	Acid to slag mass ratio	g/g_{DBFS}	0.50	1.25	2.00
X_3	Baking time	min	30	60	90
X_4	Water to acid-baked slag ratio	mL/g_{ABBFS}	4	10	16
X_5	Agitation rate	rpm	200	400	600
X_6	Water to slag mass ratio	g/g_{DBFS}	0	1	2

Table S2. 2^{6-2}_{IV} experimental design matrix for empirical model building.

Run	Baking temperature X_1 (°C)	Acid to slag mass ratio X_2 (g/g_{DBFS})	Baking time X_3 (min)	Water to acid-baked slag ratio X_4 (mL/g_{ABBFS})	Agitation rate X_5 (rpm)	Water to slag mass ratio X_6 (g/g_{DBFS})
1	-1	-1	-1	-1	-1	-1
2	-1	1	-1	-1	1	1
3	-1	-1	1	-1	1	1
4	-1	1	1	-1	-1	-1
5	-1	-1	-1	1	-1	1
6	-1	1	-1	1	1	-1
7	-1	-1	1	1	1	-1
8	-1	1	1	1	-1	1
9	1	-1	-1	-1	1	-1
10	1	1	-1	-1	-1	1
11	1	-1	1	-1	-1	1
12	1	1	1	-1	1	-1
13	1	-1	-1	1	1	1
14	1	1	-1	1	-1	-1
15	1	-1	1	1	-1	-1
16	1	1	1	1	1	1
Center-point tests (3 replicates)	0	0	0	0	0	0
	0	0	0	0	0	0
	0	0	0	0	0	0
-1 level	200	0.50	30	4	200	0
0 level	300	1.25	60	10	400	1
+1 level	400	2.00	90	16	600	2

Table S3. The ANOVA results for the empirical extraction models of the studied elements.

	Sc	**Nd**
$\bar{Y}$	36.361	26.647
TSS	45104	23514
TSS_{cfm}	19984	10023
RSS	42191	19849
RSS_{cfm}	17071	6358.6
ResSS	2912.9	3664.7
R^2	0.85424	0.63438
SSPE	20.990	9.7213
SSLF	2891.9	3654.9
$F_{p,n\text{-}p\text{-}1,\alpha}$	19.437	4.6358
F_{test}	49.814	4.8583
$F_{vLF,vPE,\alpha}$	19.429	19.413
R_{test}	18.370	62.662

Table S4. Summary of factor effect coefficients for the studied elements.

Coefficient	**Factor description**	**Sc**	**Nd**
β_0		36.4	26.6
β_1	Baking temp.	-6.1	-4.9
β_2	Acid : Slag	32.1	17.8
β_3	Baking time	0.0	-2.8
β_4	Water : Acid-baked slag	0.0	3.7
β_5	Agitation rate	0.0	0.0
β_6	Water : Slag	0.0	-5.9

Table S5. Experimental conditions for validation tests.

Run	X_1	X_2	X_3	X_4	X_5	X_6
Validation 1	1	1	-1	1	-1	1
Validation 2	1	1	-1	1	-1	-1

Table S6. Predicted and actual extraction efficiency of scandium and neodymium for validation and optimization tests.

	Val 1	**Model-Val 1**	**Val 2**	**Model-Val 2**	**Opt**	**Model-Opt**
Sc	61.3	62.3 ± 3.2	54.0	62.3 ± 3.2	82.5 ± 0.7	74.6 ± 3.2
Nd	32.9	40.1 ± 2.2	47.1	52.0 ± 2.2	80.6 ± 7.7	61.7 ± 2.2
AARD (%)	9.8		11.4		20.6	

Table S7. Coefficients of determination (R^2) showing the pairwise correlations between the extraction efficiency of scandium and neodymium and that of bulk metals (Al, Mg, Ti, Fe, Ca, and Mn).

	Al	**Mg**	**Ti**	**Fe**	**Ca**	**Mn**
Sc	0.95	0.85	0.73	0.79	0.39	0.85
Nd	0.85	0.79	0.52	0.75	0.47	0.83

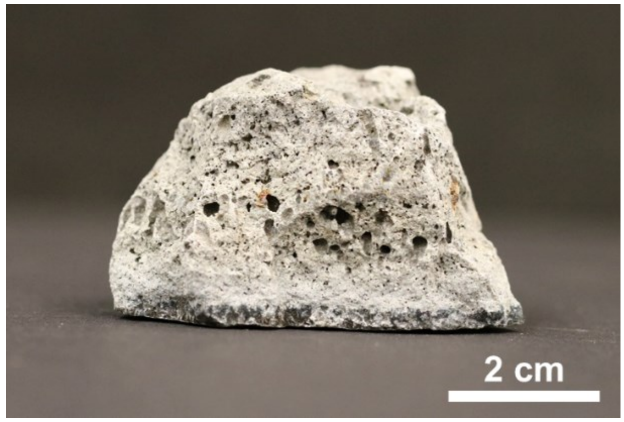

Figure S1. Photo of the blast furnace slag used in this study.

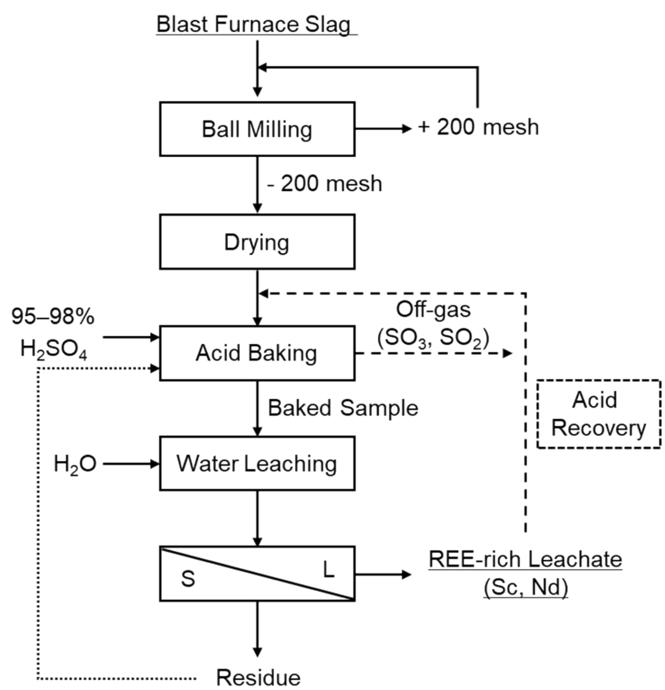

Figure S2. Block flow diagram of the acid baking – water leaching process used in this study.

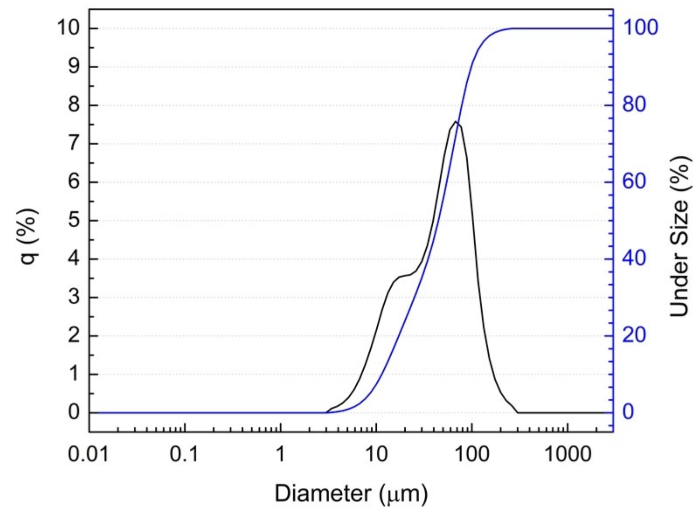

Figure S3. Particle size distribution of ground blast furnace slag sample. The median size is 44.75 µm, mean size is 51.23 µm, D10 is 11.44 µm, and D90 is 98.76 µm.