Supplementary Materials

Process Design Aspects for Scandium-Selective Leaching of Bauxite Residue with Mineral Acids

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Table S1. Examples of Sc Concentration (g/t) in global Resources being (or, to be) Industrially Exploited for Scandia (Sc oxide)/Sc Production.

Location (Resource Owner)	Resource	Sc Concentration (typical values)
China, Bayan Obo (Baotou Steel Group's)	REE-Fe-Nb-Sc Ore or, Tailings [18]	100–500 ([19], § Sc mineral.)
Russia, Kola Peninsula, Kovdor (Kovdorskiy GOK, Eurochem)	Baddeleyite (ZrO_2) (with Apatite & Iron Ore)	500 (avg.) ([20], Table 1)
Australia, NSW (Scandium International Mining Corp.)	Ni-Co Laterite	100–235 [21]
Australia, QLD (Australian Mines Ltd.)	Ni-Co Laterite	110 (avg.) [22]
Russia, Ural Aluminium Plant (UC RUSAL)	BR	90 (avg.) ([23], Table 7)

Table S2. Recovery (% w/w) of Sc and other REEs by mild leaching with different acids (ambient conditions, mechanical stirring, optimized acid feed concentration for max. total REEs recovery, Liquid to Solids ratio 50:1 (L/kg dry BR), 1h mixing time [Slide14 of 30].

Acid	La	Yb	Y	Sc	Fe
H_2SO_4	32	52	77	52	4
HNO_3	35	70	96	78	3
HCl	37	57	80	68	12
Aqua Regia	68	74	68	83	16

Text S1. Mathematical Method for the Interpretation of the Kinetic Experimental Data

By using multiple least squares regression, the correlation parameters *m* and *k* of Equation (1) are converted to concentration dependent functions. The mathematical terms for the kinetic data processing are described in Table S3(a), while the visualization of this method with a short description is presented in Table S3(b), and a characteristic example has been included in Table S3(c).

The advantage of this data interpretation method is that Sc leaching yield is expressed as an explicit function of feed acid concentration and mixing residence time, without the need for iterative calculations. The polynomials fitting is a simple and explicit interpolation method, while the 4th order offers for the specific data series the best combination of low prediction error and few curve fluctuations. However, the probable fluctuations in these predictions regard to only intermediate values of this method that are finally, in the most

cases, symmetrically absorbed and generally attenuated, by the following LSRL fitting of the linearized 1st order kinetics (Table S3(b)).

Table S3. (a) Description of kinetic data processing in mathematical terms. (b) Scheme for a comprehensible visual presentation of kinetic data processing. (c) An example of calculations.

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(a)	From the 5 experimentally tested mixing residence times (τ_i, $i=1…5$), i.e., $\tau_1=5min$, $\tau_2=15min$, $\tau_3=30min$, $\tau_4=45min$, $\tau_5=60min$, are derived: • $m(C_{Af})$= - Slope of LSRL {pairs (τ_i, $ln[1- \eta pol_i(C_{Af})/$ $/ \eta_{L/Sc-max.}(C_{Af})])$}, • $k(C_{Af})$ = Interception Point of LSRL { pairs (τ_i, $ln[1-\eta pol_i(C_{Af})//\eta_{L/Sc-max.}(C_{Af})])$}, where: $\eta pol_i(C_{Af})$ = 4th ord. Polynomial LSR {pairs (C_{Afj}, $\eta exp.\mid C_{Afj}$, τ_i)}, j=1..13 (or C_{Afj} = 0.0 M, 0.23M, 0.30M, … ,3.60M), i=1…5, where: $\eta exp.$ is the experimentally measured Sc yield for concentration C_{Afj} after τ_i mixing residence time, • $\eta_{L/Sc-max.}(C_{Af})$ = 1.01 · MAX [$\eta pol_i(C_{Af})$] , for i=1...5. *Note: $\eta_{L/Sc-max.}$ is taken as 1.01 times (or, 1% more than) the maximum appearing yield in the [0,60] min time interval, as far as any derived logarithmic values from 1st order kinetics linearization to be valid.*

(b)
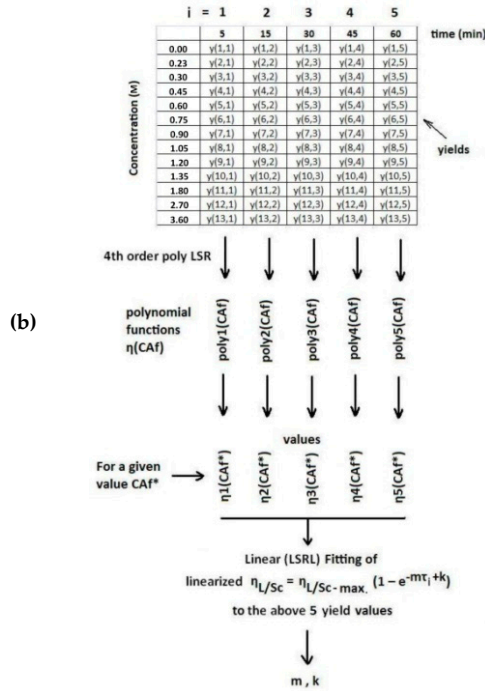
Scheme Description: For each experimental time value there is an experimental series of Sc yields for the different acid feed concentrations (C_{Af}). A different 4th order polynomial function is fitted to each of these 5 series (columns of the above table). Therefore, for any given value of C_{Af} (that is symbolized as $C_{Af}{}^*$) a time-series of leaching yields is predicted. $\eta_{L/Sc-max.}$ is 1% more than the maximum yield of this time-series. The linearized form of eq.(1) is fitted to this time-series to produce values for the *m* and *k* parameters, for the specific feed acid concentration ($C_{Af}{}^*$).

(c)	**Example:** From the experimental data of the Concentration vs. Time table of the above scheme (b), with fitting of 4th order polynomials are produced 5 polynomial functions, one for each experimental mixing residence time value. For example, if $C_{Af}{}^*=0.21M$ (i.e., an intermediate value between experimentally investigated values), these polynomials give: $\eta_{L/Sc}(5min)=13.92\%$, $\eta_{L/Sc}(15min)=19.95\%$, $\eta_{L/Sc}(30min)=24.38\%$, $\eta_{L/Sc}(45min)=22.13\%$, $\eta_{L/Sc}(60min)=30.41\%$. LSRL fitting of linearized eq.(1) onto these 5 values gives: $m=3.5826$ and $k=0.027$, when: $\eta_{L/Sc-max.}=1.01 \cdot MAX[\eta_{L/Sc}(\tau_i)$, $i=1…5] = 1.01 \cdot 30.41\% = 30.71\%$. Therefore: $\eta_{L/Sc}(C_{Af}=0.21M, t) = 30.71\% \cdot (1–e^{-3.5826.t+0.027})$, when $L/S=50$ (L of acid/ kg dry BR).

Text S2. 1st Order Kinetics and Fundamentals of the Thin Film Theory

According to leaching process fundamentals [39], it is referred: "*Mass transfer rates within the porous residue are difficult to assess because it is impossible to define the shape of the channels through which transfer must take place. It is possible, however, to obtain an approximate indication of the rate of transfer from the particles to the bulk of the liquid.*

Using the concept of a thin film as providing the resistance to transfer, the equation for mass transfer may be written as: $dM/dt = k'A(c_s-c)/b''$. The latter equation for constant solvent volume (V) can be transformed [31] to Equation (S1):

$$\frac{dc}{dt} = \frac{K_L A}{V}(c_s - c) \tag{S1}$$

Equation (S1) is a typical 1st order kinetics, when the mass transfer parameters are considered to be constant with time. A visual presentation of this theoretical model, which stands as an equivalent to the experimental behavior of the real leaching process mechanism, is depicted in Figure S1, where at the left is presented an approach of the real diffusion mode and at the right the thin film concept equivalent.

If 1st order kinetics are valid, and given that k' is considered generally as constant for a certain leaching mixture, then the A/b quotient would be considered as constant with time, or otherwise that either the particle size remains approximately intact all over the leaching period, or the thin film layer width (b) varies proportionally with the surface area (A) during particles disintegration [39]. The constant A/b assumption is considered to be valid for a wide variety of leaching cases.
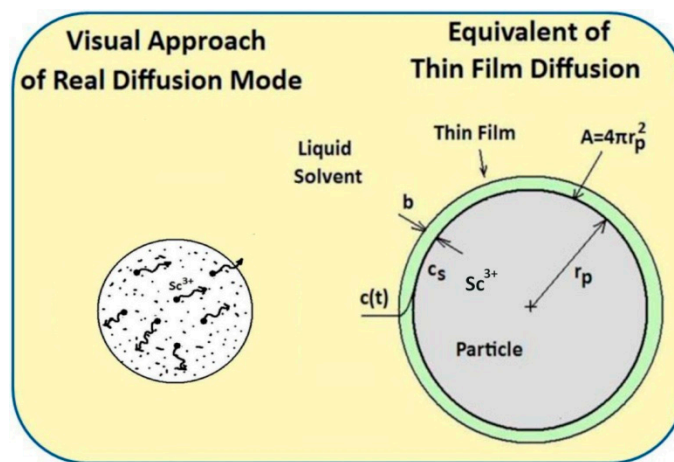

Figure S1. A visual presentation of leaching process mechanism, where at the left appears a visual approach to the real diffusion mode, while at the right appears the equivalent of the thin film diffusion concept [39].