

Lixa v0.1.2: an open-source, image-informed framework for closed-loop design of leaching processes for domestic critical-mineral recovery, from the pore to the plant scale

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Code and data: the Lixa v0.1.2 source code, the ore and reagent databases, the figure scripts, the data series behind every figure and the complete output of the worked example are available from the author on request by email (shahram.asgari@uga.edu).

Lixa v0.1.2: an open-source, image-informed framework for closed-loop design of leaching processes for domestic critical-mineral recovery, from the pore to the plant scale

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Abstract.

Leaching takes a metal out of a rock and into a solution. In the United States, rare earth elements, lithium and scandium occur mostly in rocks where the metal is thinly spread through a porous matrix: weathered clays, coal ash, lithium claystones and bauxite residue. For such rocks the leaching recipe (reagent, concentration, temperature, particle size, liquid-to-solid ratio and contact time) decides whether a deposit can be worked, and the pore structure of the rock sets how fast the solution reaches the metal. The recipe is still found by months of bench tests, without the pore structure. Lixa is a Python framework that joins the two. From an image of the rock it reads porosity, connected porosity, specific surface, tortuosity and permeability. These numbers tune a multi-host kinetic model built from shrinking-core dissolution, Langmuir ion exchange and a reagent balance that includes carbonate and silicate gangue. A differential-evolution search then finds the recipe with the highest net value per tonne within reagent and effluent limits, and the same kinetics project it to a heap or to a well field, where the image permeability sets the injection pressure. Each numerical part was checked against an exact solution: lattice Boltzmann flow to 0.12 percent, column transport to 0.004 in relative concentration, kinetics to better than one part in a thousand. The shipped presets for clay-hosted rare earths and coal fly ash are consistent with published recovery ranges. For a weathered-clay ore the search returns ammonium sulfate near 0.3 mol L^{-1} at room temperature, the concentration used in practice, in 6 s. Lixa is a screening tool that gives the first design point for bench work; it does not replace a feasibility study.

1 Introduction

Leaching moves a metal from an ore, a rock that holds enough of the metal to be worth processing, into a solution. A reagent is brought into contact with the crushed or buried rock, the metal dissolves or is displaced from the mineral surfaces, and the metal-bearing solution is drawn off for recovery in later steps. The contact can take place in a stirred tank at the bench; in a heap, a pile of crushed ore several metres high on a liner that is irrigated from the top and drained at the base over weeks or months; or in situ, where the solution is injected through one well, travels through the undisturbed rock and is pumped back from a neighbouring well. In every setting the operator chooses a recipe: the reagent, its concentration, the temperature, the particle size, the volume of solution per kilogram of ore and the contact time. For a dilute ore the recipe decides almost everything. Reagent is usually the largest operating cost. The recovery, the fraction of the metal that reaches the solution, sets the revenue. Both depend on the recipe, and the right recipe depends on the ore. It is still found by trial, from bottle tests through columns to a pilot heap, over months.

The ores that matter most for rare earth elements (REE), lithium and scandium in the United States are of this dilute kind. In the weathered granites of the southeastern states the rare earths are not bound inside a mineral; they are adsorbed on the surfaces of kaolinite and halloysite, held by electrostatic charge, and can be displaced by a salt solution. In coal fly ash they sit in glassy and calcium-rich grains at a few hundred parts per million (Taggart et al., 2016; King et al., 2018). Lithium occurs in illite and smectite claystones of the Great Basin (Benson et al., 2023), and scandium is dispersed through the iron oxides of bauxite residue (Borra et al., 2015). All three metals are on the critical minerals list of the U.S. Geological Survey (2022), and the United States imports most of its rare earth compounds and metals (U.S. Geological Survey, 2025). These feedstocks share one property that makes them hard. The metal is spread through a porous matrix at low concentration, so the solution has to travel through that matrix to reach it, and the rate at which it does so depends on the pore structure: the volume of open space, whether that space connects, the mineral surface the solution touches and the length of the paths through it. Measuring these properties from images is routine in the geosciences (Blunt et al., 2013; Gostick et al., 2016; Jung et al., 2023). For leaching design the pore structure is rarely measured, and it is not used in the search for the recipe.

The models that support that search are mature, but each covers one piece. Speciation codes such as PHREEQC resolve which dissolved species a solution contains, but not how the solution moves through an ore (Parkhurst and Appelo, 2013). Shrinking-core and multi-reactant particle models describe how one mineral grain reacts from the outside in (Levenspiel, 1999; Dixon and Hendrix, 1993). Heap models treat the flow of solution through a whole pad (Bartlett, 1998; Bouffard and Dixon, 2001), and in-situ recovery is modelled with reservoir-scale flow codes (Seredkin et al., 2016). Pore-scale simulators compute the properties that govern how a reagent reaches a grain (Blunt et al., 2013; Jung et al., 2023). No open tool links these pieces. An image of the ore cannot inform the kinetics, the kinetics cannot drive an automated search for the recipe, and the result cannot be carried to a heap or a well field with the same model. Closing that gap is also the kind of problem that current federal research programmes on critical minerals ask for, for example the critical-materials challenge named in the Department of Energy's Genesis Mission (Executive Office of the President, 2025b) and the production measures of Executive Order 14241 (Executive Office of the President, 2025a).

This paper presents Lixa, a framework that makes that chain. It answers, in order, how solution moves through a given ore, how fast the metal comes out and what the reagent is spent on, how that changes between a beaker, a column, a heap and a well field, which recipe gives the highest net value within reagent and effluent limits, and whether that recipe can be run at full scale. The central design choice is one kinetics engine for every scale. A beaker, a laboratory column, a lift of a heap and a flow path between two wells differ in only two things: the mass of ore that each litre of solution contacts, and how the solution moves from one control volume to the next. A recipe tuned in a beaker can therefore be projected to the field without re-fitting, and properties read from an image carry through the whole chain. One example runs through the paper, a weathered granite clay of the kind found in the southeastern United States, holding 800 g of rare earth oxide per tonne. Section 2 describes the model and Sect. 3 the software. Section 4 checks each numerical component against an exact solution. Section 5 compares the shipped ore presets with published leaching data. Section 6 runs the chain on the example from an image to a plan. Section 7 reports the computing cost, and Sect. 8 states the limits of the approach. Appendix A follows one complete run from the command line to the plan.

2 Model description

2.1 Overview

Figure 1 shows the workflow. The pore stage turns a greyscale image of the ore into five numbers: porosity ϕ , connected porosity ϕ_{eff} , specific surface per bulk volume S_V , tortuosity τ and permeability k . The first four describe how much open space the ore has, how well it connects, how much mineral surface the solution can reach and how far the solution has to detour; the fifth says how easily the solution flows under pressure. Three of them (ϕ_{eff} , τ and S_V) adjust the kinetic parameters of the ore. The permeability bypasses the laboratory stage and sets the hydraulics of the in-situ model. The kinetics turn the ore description, the pore numbers and a recipe into the metal released and the reagent consumed over time. The reactors place that chemistry in a batch vessel, a column, a heap lift or a streamtube between wells. The search runs on the batch reactor, which is cheap enough to test hundreds of recipes in seconds, and returns the recipe with the highest net value per tonne. The plant stage then runs the column reactor once at full scale with that recipe, and the economics turn recovery and reagent use into revenue, cost and net present value. The pore stage computes geometry and flow only; solute transport and reaction are solved at the reactor scale, with the pore numbers as parameters. Every input is a validated data model with units and bounds, so an impossible value fails at the door instead of producing a quiet wrong result three stages later.

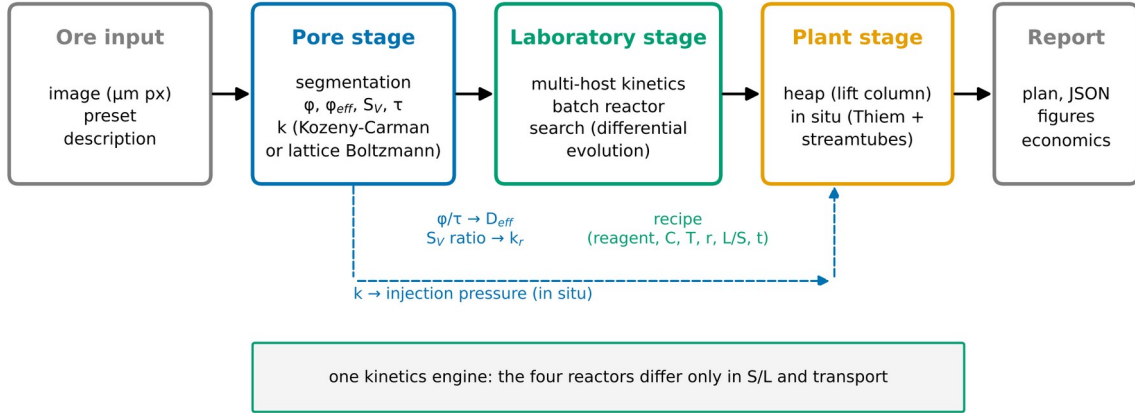


Figure 1. Workflow of Lixa. Boxes are the stages; arrows are the quantities that pass between them. The pore-scale permeability bypasses the laboratory stage and sets the injection pressure of the in-situ model. One kinetics engine serves all four reactor types; S/L is the solid-to-liquid ratio.

2.2 Pore-scale characterisation

The input is a greyscale image, for example one slice of an X-ray micro-tomography scan, in which the open pores are dark and the minerals are light. Pixels are classed as pore or solid with Otsu's method (Otsu, 1979), which tries every grey-level cut and keeps the one that separates the two classes most cleanly. When the classes are far apart a range of cuts works equally well, and Lixa takes the middle of that range. A three-phase option separates grey gangue from a bright ore mineral with a second cut. Porosity is the

fraction of pore pixels. Connected porosity is the fraction of pore pixels in 4-connected clusters that reach from the inlet side to the outlet side; an isolated pocket counts toward the porosity but carries no flow.

The specific surface is the pore-solid boundary per unit volume, where the chemistry happens. It is measured by counting the pore-solid transitions along every row and every column of the image, which are intercept counts on two orthogonal families of test lines. For an isotropic boundary the intercepts per unit line length, P_L , give the surface per unit volume by the stereological relation

$$S_V = 2 P_L, \quad (1)$$

where S_V is the pore-solid interface area per bulk volume (m^{-1}) and P_L is the number of intercepts per unit length of test line (m^{-1}), averaged over both families. The boundary length per image area is $L_A = (\pi/2) P_L$, so $S_V = (4/\pi) L_A$; the count itself already equals $2 P_L$ and carries no further factor. Versions before 0.1.2 applied $4/\pi$ a second time and overestimated S_V by 27 percent; the error was found in review and is corrected here.

Tortuosity is geodesic. A breadth-first search from the inlet face gives every connected pore pixel its shortest 4-connected path length through the pore space; the mean of those lengths at the outlet face divided by the straight-line length of the sample is τ . Straight channels give $\tau = 1$. Because the path is 4-connected, a channel at 45° reports $\sqrt{2}$ times its true tortuosity; the measure is adequate for isotropic pore space and is stated here so that it is not mistaken for a Euclidean one. Permeability is estimated by default from the porosity and the surface with the Kozeny-Carman relation (Carman, 1937), which treats the pore space as a bundle of channels whose conductance rises steeply with porosity and falls with the surface per unit of solid,

$$k = \frac{\phi_{\text{eff}}^3}{c S_s^2 (1 - \phi_{\text{eff}})^2}, \quad S_s = \frac{S_V}{1 - \phi_{\text{eff}}}, \quad c = 5, \quad (2)$$

where k is the permeability (m^2), ϕ_{eff} is the connected porosity, S_s is the surface per solid volume (m^{-1}) and c is the Kozeny constant. An image that does not percolate returns $k = 0$ and is flagged.

Permeability can also be computed directly by simulating the flow through the image with a lattice Boltzmann method (LBM). The solver uses the D2Q9 velocity set, in which fluid populations move between neighbouring pixels in nine directions, and BGK collision, which relaxes them toward local equilibrium with relaxation time $\tau_{\text{LB}} = 1$ and hence a kinematic viscosity $\nu = (\tau_{\text{LB}} - 1/2)/3$ in lattice units. A constant body force g along the flow direction drives the flow. The force enters through the scheme of Guo et al. (2002), in which half of it is added to the velocity,

$$\rho u_x = \sum_i c_{ix} f_i + \frac{1}{2} \rho g, \quad (3)$$

where ρ is the fluid density, u_x the velocity along the flow, c_{ix} the x component of lattice velocity i and f_i the population moving in that direction. Solid pixels use half-way bounce-back, which places the no-slip wall half-way between the last fluid pixel and the first solid pixel (Krüger et al., 2017). The image is padded with copies of its edge columns, so the periodic seam in the flow direction joins two faces of the same geometry. The run stops when the mean velocity over the whole image changes by less than one part in 10^7 between

checks 50 steps apart, or at a step cap of 20 000, in which case the result is flagged as not converged. Darcy's law then converts that velocity into a permeability in physical units,

$$k = \frac{u_s \nu}{g} \Delta x^2, \quad (4)$$

where u_s is the mean velocity over the whole image including the solids, Δx is the pixel size (m), and u_s , ν and g are in lattice units.

The pore numbers enter the kinetics as ratios to the values of the preset at which the rate constants were fitted. Porosity and tortuosity scale the effective diffusivity of the layer that builds up on a reacting grain, $D_{\text{eff}} \propto \phi_{\text{eff}}/\tau$, so a more open and less tortuous pore space admits the reagent faster. The specific surface, converted to a mass basis with a grain density of 2.65 t m^{-3} , scales the rate constant of the surface reaction. The surface ratio is clamped to the range 0.2 to 5, because an image at micrometre resolution sees only a small part of the true reactive surface, which includes roughness far below the pixel size.

2.3 Leaching kinetics

An ore holds its target metal in one or more host phases, each with a share of the target and its own release mechanism. A host that an acid or an organic ligand dissolves, such as the calcium-rich glass in fly ash, is treated by dissolution. A metal that is adsorbed on a surface and displaced by another ion, as the rare earths on clay are, is treated by ion exchange. The recovery of the ore is the share-weighted sum of the host conversions, where the conversion X of a host is the fraction of it that has reacted or released its metal. Stoichiometry is counted per metal atom: an oxide grade such as total rare earth oxide (TREO) is converted with the molar mass per rare earth atom (RE_2O_3 counted as $\text{REO}_{1.5}$, 165 g mol^{-1}), so that one mole of target consumes the ions of one trivalent ion.

For dissolution the shrinking-core model is used (Levenspiel, 1999), in which a spherical grain reacts from the outside in, the unreacted core shrinks and a leached layer builds up around it. While that layer is thin the surface reaction sets the rate (reaction control); as it thickens, diffusion of the reagent through it to the core sets the rate (diffusion control). Under reaction control the integrated law is $1 - (1 - X)^{1/3} = k_r t$, whose rate form is

$$\frac{dX}{dt} = 3 k_r (1 - X)^{2/3}, \quad (5)$$

where X is the conversion of the host (0 to 1), t is time (h) and k_r is the reaction-control rate constant (h^{-1}). Under diffusion control the integrated law is $1 - 3(1 - X)^{2/3} + 2(1 - X) = k_d t$, whose rate form is

$$\frac{dX}{dt} = \frac{k_d}{2[(1 - X)^{-1/3} - 1]}, \quad (6)$$

where k_d is the diffusion-control rate constant (h^{-1}). The two mechanisms act as resistances in series: the combined rate is the harmonic combination of the two rate expressions, $dX/dt = (1/\rho_{\text{react}} + 1/\rho_{\text{diff}})^{-1}$, where ρ_{react} and ρ_{diff} are the right-hand sides of Eqs. (5) and (6), so that the slower step controls at each moment. The two rate constants depend on the driving-ion concentration, the particle radius, the surface ratio from the image, the pore geometry and the temperature,

$$k_r = k_{\text{ref}} \frac{1 \text{ mm}}{r} s a^n \exp \left[-\frac{E_a}{R_g} \left(\frac{1}{T} - \frac{1}{T_{\text{ref}}} \right) \right], \quad (7a)$$

$$k_d = \frac{3600 D_{\text{eff}}}{r^2} \frac{\phi_{\text{eff}}/\tau}{(\phi_{\text{eff}}/\tau)_{\text{ref}}} a \exp \left[-\frac{E_a}{2R_g} \left(\frac{1}{T} - \frac{1}{T_{\text{ref}}} \right) \right], \quad (7b)$$

where k_{ref} is the rate constant at 25 °C, unit concentration and 1 mm radius (h^{-1}), r is the particle radius (m), s is the surface ratio from the image, a is the concentration of the driving ion (the proton for acids, mol L^{-1}), n is the reaction order, E_a is the activation energy (J mol^{-1}), R_g is the gas constant, T is the temperature (K), $T_{\text{ref}} = 298.15$ K, and D_{eff} is the diffusivity through the leached layer at the reference geometry ($\text{m}^2 \text{s}^{-1}$). The exponentials are the Arrhenius temperature dependence; the diffusion term uses half of the activation energy.

Rare earths in weathered clays are held on the clay surfaces by electrostatic charge, and a salt solution releases them by placing a competing cation on the same sites (Moldoveanu and Papangelakis, 2012). The fraction released at equilibrium rises with the cation concentration along a Langmuir curve, steep at low concentration and flat at high concentration, so beyond a certain concentration more salt frees little more metal. The approach to that equilibrium is first order in time,

$$X_{\text{eq}} = X_{\text{max}} \frac{K_{\text{ex}} C}{1 + K_{\text{ex}} C}, \quad \frac{dX}{dt} = k_{\text{ex}} (X_{\text{eq}} - X), \quad (8)$$

where X_{eq} is the released fraction at equilibrium, X_{max} is the largest fraction that can be released at all, C is the concentration of the displacing cation (mol L^{-1} ; for ammonium sulfate twice the salt molarity, and the proton concentration when an acid acts on an exchange host, with the same K_{ex}), K_{ex} is the exchange affinity (L mol^{-1}) and k_{ex} is the rate of approach (h^{-1}). K_{ex} does not depend on temperature in this version, so the exchange equilibrium is temperature independent; k_{ex} scales with $r^{-1/2}$ and with an Arrhenius factor of 15 kJ mol^{-1} . The exchange is reversible, so metal re-adsorbs where the solution is depleted in cation, and the re-adsorbed amount is limited to the metal present in the solution of that control volume. Charge balance sets the cation demand at $3/z$ moles per mole of trivalent rare earth, for a cation of charge z .

The driving ion is consumed by three sinks. The first is the stoichiometric demand of the target reaction. The second is carbonate gangue, the part of the rock that is not the target and reacts with acid as fast as the acid arrives; it is treated as an instantaneous titration, so wherever free acid and carbonate coexist in a control volume the smaller of the two is consumed at once. The third is silicate gangue, a slow sink whose rate decays in proportion to the capacity still available, so its total demand is bounded. Metal released and reagent consumed are computed from the realised change in conversion over each time step, not from the instantaneous rate, so the mass balance closes exactly, also when an exchange host re-adsorbs metal. When the demand of a step is larger than the reagent present, the conversion change is scaled back to what the solution can pay for. A weak acid therefore stalls in a carbonate-rich ore, because the acid is spent on the gangue before it reaches the metal.

All control volumes of a reactor advance together in vectorised numpy. Exchange hosts use the exact exponential solution at fixed concentration. Dissolution hosts take a midpoint step. The common sub-step is bounded in three ways: by 0.2 divided by the local slope of the dissolution rate with respect to conversion, $2 k_r a^n (1 - X)^{-1/3} + k_d a$, with finished hosts dropped; by $2/k_{\text{ex}}$ for the exchange coupling; and by a 30 percent drawdown of the reagent per step. A floor of one four-hundredth of the transport step keeps any cell from stalling; it binds only for rate constants above about 10^4 h^{-1} , far above the preset values, and the accuracy figures of Sect. 4 hold below that. A predictor-corrector on the concentration gives second-order coupling between the hosts and the solution.

2.4 Reactors

The reactors differ in the mass of ore that each litre of solution contacts and in how the solution moves. The batch reactor, which represents a bottle-roll test, is one control volume in which the whole mass of ore meets the whole volume of solution at once. Its solid-to-liquid ratio is $S/L = (L/S)^{-1}$ in kg L^{-1} , where L/S is the liquid-to-solid ratio in litres of solution per kilogram of ore. Recovery is the share-weighted conversion over the hosts. Reagent use in $\text{kg per tonne of ore}$ has two parts: the part consumed by the chemistry, from the ions consumed, the ions per mole of reagent and the molar mass, and the share of the free reagent that is not recycled. The recycle fraction is a property of the reagent in the database (0.8 for the two sulfate salts, 0 for the acids), and for the exchange ores the unrecycled free salt is most of the reported reagent per tonne, which is why the liquid-to-solid ratio sets the reagent cost.

The column is a one-dimensional advection-dispersion-reaction problem on N cells of length Δz : the solution is carried along by the flow and spreads by dispersion, the mixing that arises from the range of speeds along different pore paths. The pore velocity is $v = q/\varepsilon_b$, where q is the superficial velocity and ε_b the bed porosity, and the dispersion coefficient is $D = \alpha_L v + D_m$, where α_L is the dispersivity and D_m the molecular diffusivity. Transport is solved explicitly: first-order upwind differences for advection and central differences for dispersion, with the time step set by the stricter of the Courant and diffusion limits. The upwind scheme adds a numerical dispersion of $(v \Delta z/2)(1 - Co)$, where Co is the Courant number, which is subtracted from the physical coefficient down to a floor of 20 percent of the physical value. The inlet is a flux (Danckwerts) condition, advective inflow at the feed concentration and no dispersive flux across the inlet face, and the outlet has zero gradient. Both faces are closed to dispersion, so the scheme conserves dissolved mass; versions before 0.1.2 used a fixed concentration at the inlet ghost cell, which let dissolved metal leave the column backwards by dispersion and lost about six percent of the released metal in the in-situ runs. After every transport step each cell reacts with $S/L = \rho_{\text{bed}}/\varepsilon_b$. Recovery is what has been collected at the outlet. It lags the recovery measured on the solids by the metal still travelling down the column, and both are reported.

A heap is modelled as the column at the lift height, irrigated at the design rate, with a field dispersivity of at least five percent of the height. A real heap has dry zones, preferential channels and compacted patches that the solution never wets, so a solution-ore contact efficiency η caps the recovery, and the stoichiometric reagent demand, at the fraction η of the ore; the unrecycled share of the applied solution is spent regardless.

For in-situ recovery the permeability from the pore stage decides whether the design flow can be injected at all, since the pressure needed to push solution into a tight formation is bounded by fracturing and by the permit. The steady radial pressure rise at an injection well is given by the Thiem relation (Thiem, 1906),

$$\Delta p = \frac{Q \mu}{2\pi k b} \ln \left(\frac{r_e}{r_w} \right), \quad (9)$$

where Δp is the pressure rise (Pa), Q is the injection rate ($\text{m}^3 \text{s}^{-1}$), μ the fluid viscosity (Pa s), k the permeability (m^2) from the pore stage, b the thickness of the ore layer (m), r_e the distance between wells (m) and r_w the well radius (m). If Δp exceeds the allowed pressure, the flow is cut to the largest feasible value and the result is flagged. Between the wells the formation is a bundle of streamtubes, each a flow path from the injection well to the recovery well with its own travel time, modelled as a column of length r_e . The travel times are the quantiles of a log-normal distribution whose median is the pore volume of the

well pattern divided by the flow and whose log standard deviation $\sigma_{\ln}$ stands for the permeability heterogeneity of the formation; the tube flows are normalised so that they sum to Q . Each tube runs the column model with the velocity that gives its travel time and a dispersivity of ten percent of the spacing. The recoveries are averaged and multiplied by a sweep efficiency, the share of the ore that the solution ever contacts. Reagent per tonne is the stoichiometric part, scaled by the sweep efficiency, plus the unrecycled share of all the salt injected over the leach.

2.5 Objective and search

The search maximises the net value per tonne of ore, the metal recovered times its price less the costs the recipe incurs,

$$J = 1000 w R P - m_{\text{reagent}} c_{\text{reagent}} - \frac{c_{\text{crush}}}{r} - c_t t - c_{\text{opex}}, \quad (10)$$

where J is the net value (USD per tonne of ore), w is the grade as a mass fraction, R the recovery, P the metal price (USD kg⁻¹), m_{reagent} the reagent use (kg t⁻¹), c_{reagent} its price (USD kg⁻¹), c_{crush}/r the crushing cost for a particle radius r in mm, $c_t = 0.02$ USD t⁻¹ h⁻¹ a time cost for tied-up capital and tank occupancy, and c_{opex} a fixed operating cost. The crushing term is zero for the in-situ route, in the search as well as in the plant economics; in versions before 0.1.2 the search charged it for every route. A recipe that needs more reagent than a cap, or that sends out effluent below a pH limit, is penalised rather than forbidden, so the search can cross infeasible regions, but only a recipe that satisfies the limits can be selected.

The reagent is a categorical variable and is handled by enumeration. For each compatible reagent, differential evolution (Storn and Price, 1997), a population method that recombines candidate recipes and keeps the better offspring, searches five continuous variables: log concentration, temperature, log particle radius, liquid-to-solid ratio and log time, within bounds set by the user (by default 0.01 to 2 mol L⁻¹, 25 °C, 0.5 to 5 mm, 1 to 5 L kg⁻¹ and 1 to 24 h). The initial population is a Latin hypercube, which spreads the first candidates evenly over the search box, and the budget is honoured in multiples of 40 evaluations per reagent. Differential evolution was chosen over Bayesian optimisation because a batch evaluation costs tens of milliseconds, so hundreds of evaluations are cheap, and because it adds no dependency beyond SciPy. After the search, a one-at-a-time sensitivity changes each variable by 25 percent (5 °C for temperature) in both directions, clipped to the search bounds, and records the change in net value, which identifies the variables a bench programme should pin down first.

2.6 Interpreting an ore description

Ore descriptions in plain language, such as weathered granite clay with adsorbed rare earths, 800 ppm, in-situ wells, no strong acid, are read by a rule-based interpreter. It matches synonyms of each preset, reads the grade as the number with a unit that lies nearest a target-metal keyword, preferring ppm or g t⁻¹ over a percentage because percentages in such sentences usually describe gangue, recognises the process route and exclusions such as no strong acid, and adjusts the carbonate demand on keywords. An optional layer calls a large language model with the same extraction schema. Its output passes through the same validators, so the tool never depends on the model being present or right.

3 Implementation

Lixa is a Python package for Python 3.10 or newer. Its required dependencies are numpy, SciPy, matplotlib, PyYAML, Pillow, pydantic and click; scikit-image, the Anthropic client and phreepy are optional. The package is organised by scale (`lixo.pore`, `lixo.chem`, `lixo.lab`, `lixo.plant`, `lixo.loop`), with a pipeline module and a command-line tool, `lixo`, that exposes each stage (`pore`, `batch`, `column`) and the whole chain (`plan`). Ore presets and reagents are YAML files with literature references (Table 1), and a user file is merged over the built-in set. Each preset also carries the fields that Table 1 omits for space: bulk density, the reference porosity, tortuosity and specific surface at which the rate constants apply, the silicate sink rate and capacity, the protons per metal atom and the metal price. All inputs and results are pydantic models, which gives validation, JSON output and a documented schema. The test suite (46 tests) covers the exact-solution checks of Sect. 4, the mass-balance properties, the input validation, the literature ranges of Sect. 5 and one end-to-end run. A continuous-integration workflow runs it on two Python versions. The module `lixo.chem.phreeqc` writes a PHREEQC input file for the equivalent batch contact (solution, calcite as carbonate gangue, gypsum allowed to precipitate), so any recipe can be checked for free acid, pH and gypsum saturation in a full speciation model. The lattice Boltzmann solver follows the design used in CompLaB (Jung et al., 2023). The code was written with AI-assisted programming tools; the model choices, verifications and interpretations are the author's.

Table 1. Ore presets shipped with Lixa v0.1.2 (diss.: shrinking-core dissolution; exch.: ion exchange; share: fraction of the target metal in that host; TREO: total rare earth oxide). Values are indicative, assembled from Moldoveanu and Papangelakis (2013), Taggart et al. (2016), King et al. (2018), Rioyo et al. (2022), Borra et al. (2015) and Gupta and Krishnamurthy (2005), and are meant to be re-fitted to one bottle-roll test per ore.

Ore preset	Target, grade	CO ₃ demand (mol H ⁺ kg ⁻¹)	Host phase	Mode, share	Kinetic parameters
ion adsorption clay ree	TREO, 800 ppm	0.0	exchangeable REE on kaolinite and halloysite surfaces	exch., 0.90	K_{ex} 40 L mol ⁻¹ , k_{ex} 3 h ⁻¹ , X_{max} 0.97
			residual REE in monazite, zircon and Fe-Mn oxides	diss., 0.10	k_{ref} 2.0×10^{-4} h ⁻¹ , n 0.6, E_a 55 kJ mol ⁻¹ , D_{eff} 2.0×10^{-12} m ² s ⁻¹
coal fly ash ree	REE (metal basis), 500 ppm	2.5	REE in aluminosilicate glass	diss., 0.50	k_{ref} 1.5×10^{-4} h ⁻¹ , n 0.8, E_a 45 kJ mol ⁻¹ , D_{eff} 1.0×10^{-12} m ² s ⁻¹
			REE in Ca phosphate and oxide phases	diss., 0.25	k_{ref} 5.0×10^{-2} h ⁻¹ , n 0.7, E_a 30 kJ mol ⁻¹ , D_{eff} 2.0×10^{-11} m ² s ⁻¹

Ore preset	Target, grade	CO ₃ demand (mol H ⁺ kg ⁻¹)	Host phase	Mode, share	Kinetic parameters
			REE in zircon and monazite (refractory)	diss., 0.25	$k_{\text{ref}} 1.0 \times 10^{-6} \text{ h}^{-1}$, $n 0.5$, $E_a 60 \text{ kJ mol}^{-1}$, $D_{\text{eff}} 1.0 \times 10^{-12} \text{ m}^2 \text{ s}^{-1}$
lithium clay smectite	Li, 3000 ppm	3.0	Li in smectite octahedral sheet	diss., 0.90	$k_{\text{ref}} 1.0 \times 10^{-2} \text{ h}^{-1}$, $n 0.9$, $E_a 50 \text{ kJ mol}^{-1}$, $D_{\text{eff}} 8.0 \times 10^{-12} \text{ m}^2 \text{ s}^{-1}$
			Li in illite and refractory silicates	diss., 0.10	$k_{\text{ref}} 5.0 \times 10^{-4} \text{ h}^{-1}$, $n 0.8$, $E_a 60 \text{ kJ mol}^{-1}$, $D_{\text{eff}} 1.0 \times 10^{-12} \text{ m}^2 \text{ s}^{-1}$
bauxite residue scandium	Sc, 100 ppm	3.5	Sc in goethite and hematite	diss., 0.70	$k_{\text{ref}} 8.0 \times 10^{-3} \text{ h}^{-1}$, $n 1.0$, $E_a 40 \text{ kJ mol}^{-1}$, $D_{\text{eff}} 4.0 \times 10^{-12} \text{ m}^2 \text{ s}^{-1}$
			Sc in Ti and Zr phases (refractory)	diss., 0.30	$k_{\text{ref}} 3.0 \times 10^{-4} \text{ h}^{-1}$, $n 0.7$, $E_a 60 \text{ kJ mol}^{-1}$, $D_{\text{eff}} 1.0 \times 10^{-12} \text{ m}^2 \text{ s}^{-1}$
carbonatite bastnaesite	TREO, 70000 ppm	9.0	bastnaesite (REE fluorocarbonate)	diss., 0.90	$k_{\text{ref}} 2.0 \times 10^{-2} \text{ h}^{-1}$, $n 1.0$, $E_a 35 \text{ kJ mol}^{-1}$, $D_{\text{eff}} 1.0 \times 10^{-11} \text{ m}^2 \text{ s}^{-1}$
			monazite (REE phosphate)	diss., 0.10	$k_{\text{ref}} 3.0 \times 10^{-4} \text{ h}^{-1}$, $n 0.8$, $E_a 65 \text{ kJ mol}^{-1}$, $D_{\text{eff}} 1.0 \times 10^{-12} \text{ m}^2 \text{ s}^{-1}$

4 Model verification

Each numerical component is run on a case with a known exact solution and compared with it (Table 2). These checks establish that the code solves its equations correctly; whether the equations describe real ores is the subject of Sect. 5.

The flow solver (Eqs. 3 and 4) is tested on a straight slot of H fluid pixels between two solid rows. Body-force-driven flow through the slot is Poiseuille flow with a parabolic profile. The reference is the exact average of that parabola over the H fluid rows, with the walls half-way between the last fluid and the first solid row, $g H^2 / (12\nu)(1 + 1/(2H^2))$ in lattice units, scaled by $H/(H + 2)$ because u_s is averaged over all rows including the two solid ones. With $H = 20$ the solver reaches this value to 0.125 percent after 4700

iterations, with a tolerance of 10^{-9} . The profile is parabolic and symmetric to 1×10^{-13} of its maximum (Fig. 2d). The error falls as H^{-2} (1.370 % at $H = 6$, 0.498 % at $H = 10$, 0.125 % at $H = 20$, 0.031 % at $H = 40$), which is the known dependence of the effective wall position of the BGK bounce-back scheme on resolution at $\tau_{LB} = 1$ (Krüger et al., 2017). On the synthetic sample image of Fig. 2a, at a tolerance of 10^{-7} , the solver picks out the preferred flow paths between the grains (Fig. 2c). It gives $k = 7.09 \times 10^{-12} \text{ m}^2$ at $4 \mu\text{m}$ per pixel, against $8.76 \times 10^{-12} \text{ m}^2$ from Kozeny-Carman (Eq. 2) with the same porosity and surface; the two agree within a factor of 1.2, as expected for a channel-bundle relation applied to a grain packing.

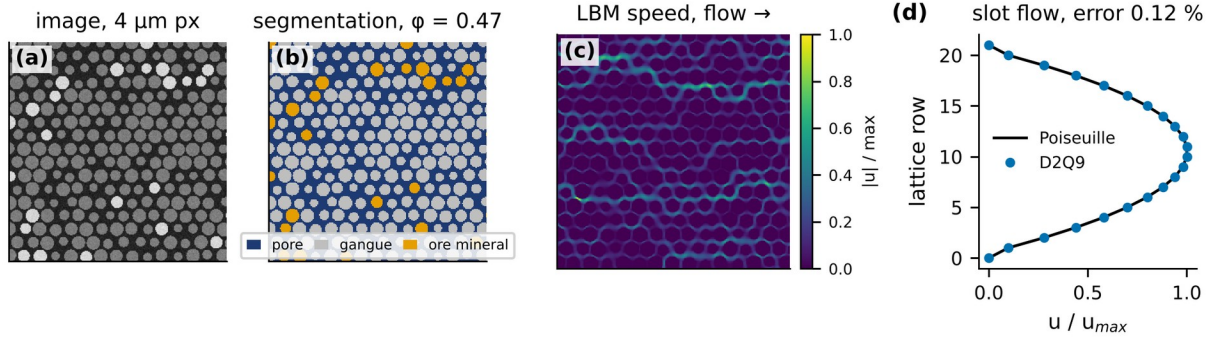


Figure 2. Pore stage. (a) Synthetic sample image at $4 \mu\text{m}$ per pixel: dark pores, grey gangue, bright ore mineral. (b) Three-phase segmentation; porosity 0.47, connected porosity 0.47, tortuosity 1.06. (c) Lattice Boltzmann speed field, flow from left to right. (d) Velocity profile across a slot of 20 fluid pixels against the Poiseuille parabola whose walls sit half-way between fluid and solid pixels.

The kinetics integrator is tested against the integrated shrinking-core laws (Eqs. 5 and 6), which can be written in closed form at constant concentration. For reaction control the largest absolute error in conversion is 1.8×10^{-8} (Fig. 3a). For diffusion control it is 9.3×10^{-4} in the integrated variable (Fig. 3b). An exchange host at fixed concentration (Eq. 8) follows the exponential solution to 3.6×10^{-9} (Fig. 3c). The acid balance of a carbonate-rich fly ash batch closes to $4.4 \times 10^{-16} \text{ mol L}^{-1}$: at every step, free acid plus consumed acid times S/L equals the initial charge (Fig. 3d). The step at $t = 0$ is the instantaneous carbonate titration, which removes half of the charge.

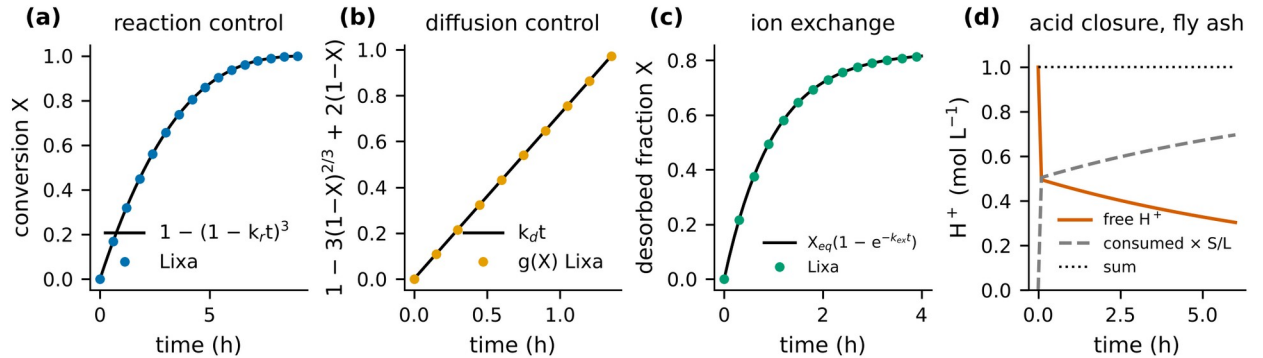


Figure 3. Kinetics verification. (a) Reaction-controlled shrinking core against $1 - (1 - k_r t)^3$. (b) Diffusion-controlled shrinking core: the integrated variable $1 - 3(1 - X)^{2/3} + 2(1 - X)$ against $k_d t$. (c) Ion-exchange host at fixed cation concentration against $X_{eq} [1 - \exp(-k_{ex} t)]$. (d) Acid closure in a batch of coal fly ash with $1 \text{ mol L}^{-1} \text{ HCl}$ at $S/L = 0.2 \text{ kg L}^{-1}$ and 60°C : free acid, consumed acid times S/L, and their sum.

The column scheme is tested with a non-reactive tracer, so that only the transport is checked. The classical Ogata-Banks solution (Ogata and Banks, 1961) applies to a fixed concentration at the inlet; the column uses a flux inlet, for which the semi-infinite solution of van Genuchten and Alves (1982, case A2) is the exact reference. The column Péclet number, the ratio of advection to dispersion, is 25. The concentration is read at mid-column, so the outlet condition does not disturb the comparison. The largest absolute error in relative concentration C/C_0 is 0.0036 with 400 cells. It falls with resolution (0.0316 at 50 cells, 0.0138 at 100 cells, 0.0071 at 200 cells, 0.0036 at 400 cells), at first order as expected for upwind differencing (Fig. 4a). Figure 4b and c show a reacting case: coal fly ash in a 1 m column of 100 cells, 0.5 mm particles, with 1 mol L⁻¹ sulfuric acid at 0.02 m h⁻¹ and 25 °C. The acid front advances only as the carbonate and silicate demand of each cell is paid, so free acid, two protons per mole of the diprotic acid, reaches the outlet after 5.2 d. The dissolved rare earths released by the calcium-rich phase travel ahead of the acid front, because that phase reacts in the near-neutral solution that precedes it, and the band of leached ore moves down the column behind.

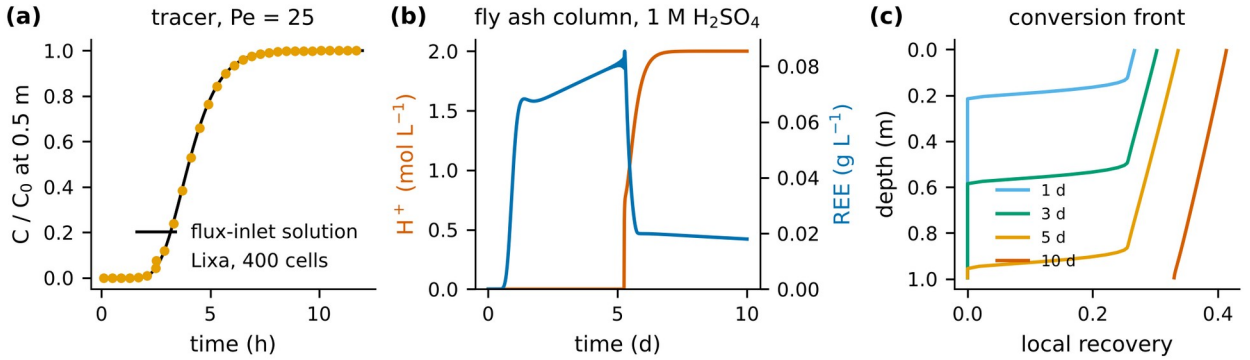


Figure 4. Column reactor. (a) Tracer breakthrough at 0.5 m in a 1 m column, Péclet number 25, against the flux-inlet solution of van Genuchten and Alves (1982). (b) Coal fly ash in a 1 m column of 100 cells, 0.5 mm particles, with 1 mol L⁻¹ H₂SO₄ at a superficial velocity of 0.02 m h⁻¹ and 25 °C: outlet free acid (as H⁺) and outlet rare earth concentration. (c) Local recovery along the column at 1, 3, 5 and 10 d.

Table 2. Verification cases. All of them run in the automated test suite.

Benchmark	Quantity compared	Result
LBM D2Q9, slot flow, $H = 20$	mean velocity vs. exact node average of the Poiseuille parabola	0.125 %, $O(H^{-2})$
LBM profile	asymmetry of the parabola, relative to its maximum	1×10^{-13}
Column tracer, $Pe = 25$, mid-column	C/C_0 vs. flux-inlet solution	0.0036 max. abs., $O(\Delta z)$
Shrinking core, reaction control	$X(t)$ vs. $1 - (1 - k_r t)^3$	1.8×10^{-8} max. abs.
Shrinking core, diffusion control	$g(X)$ vs. $k_d t$	9.3×10^{-4} max. abs.

Benchmark	Quantity compared	Result
Ion exchange, fixed C	X(t) vs. exponential	3.6×10^{-9} max. abs.
Acid balance with carbonate	closure of free + consumed acid	4.4×10^{-16} mol L ⁻¹
Column metal balance	collected + in solution vs. released from solids	2×10^{-3} (unit test)
Economics	hand calculation of Eq. (10) and of the NPV	10^{-6} relative (unit test)

5 Consistency of the presets with published leaching data

Verification shows that the equations are solved correctly. It says nothing about whether the presets describe real ores. The rate constants of the two presets that can be checked were set from the publications cited below, so Fig. 5 is a consistency check and not an independent validation; the lithium clay, bauxite residue and carbonatite presets have not been compared with data and should be re-fitted before use. Moldoveanu and Papangelakis (2013) report that 0.2 to 0.5 mol L⁻¹ ammonium sulfate releases 80 to 90 percent of the rare earths from Chinese weathered clays within hours, at room temperature and about two litres of solution per kilogram of clay, and that magnesium sulfate is somewhat less effective at the same molarity. The preset gives 84 percent with ammonium sulfate and 81 percent with magnesium sulfate at 0.3 mol L⁻¹ after 2 h (Fig. 5a). The Langmuir form also reproduces the flattening above 0.3 mol L⁻¹, which is why that concentration is used in practice. For coal fly ash the published picture depends on the ash. Taggart et al. (2016) extracted about 70 percent of the rare earths from high-calcium Powder River Basin ashes by heated nitric acid digestion, and King et al. (2018) recovered nearly all of them from such ash with hydrochloric acid, while low-calcium Appalachian and Illinois Basin ashes gave under 40 percent in acid alone and needed an alkaline digestion before the acid to reach 85 percent. The preset is a mixed ash with half of its rare earths in a calcium-rich phase; it gives 68 percent at 85 °C and 28 percent at 25 °C after 4 h in 1 mol L⁻¹ HCl (Fig. 5b), between the two ash classes, and a user should set the share of the calcium-rich phase from the calcium content of the ash in hand. Figure 5c shows the particle-size effect of the shrinking-core model at 60 °C: 9 times more metal in 4 h from 50 µm grains than from 5 mm grains. This is the trade-off that the crushing term of Eq. (10) prices.

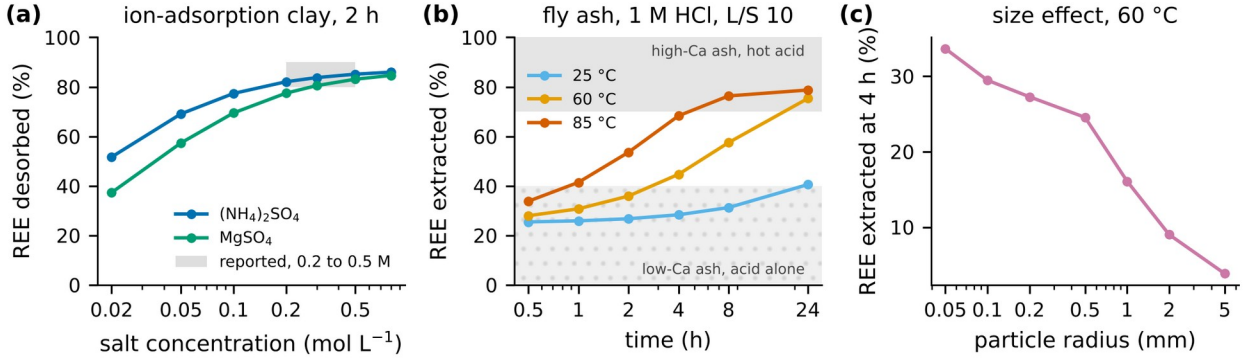


Figure 5. Presets against published behaviour. (a) Rare earths released from weathered clay after 2 h at L/S = 2 and 0.5 mm particles as a function of salt concentration; the band is the range reported by Moldoveanu and Papangelakis (2013) for 0.2 to 0.5 mol L⁻¹. (b) Rare earths extracted from the fly ash preset by 1 mol L⁻¹ HCl at L/S = 10 and 20 µm particles at three temperatures; the upper band is the range reported for high-calcium ash in hot acid and the lower band the range for low-calcium ash in acid alone (Taggart et al., 2016; King et al., 2018). (c) Extraction after 4 h at 60 °C as a function of particle radius.

6 Application: from image to plan

6.1 Searching the recipe

The weathered-clay rare earth preset of the running example (800 ppm TREO, bulk density 1.5 t m⁻³) is searched over all six reagents at room temperature with the default bounds and 480 evaluations, for a heap route (Fig. 6). The search returns ammonium sulfate at 0.31 mol L⁻¹, 1.0 L of solution per kilogram of clay, 1.1 mm particles and 2.5 h. This recipe releases 84 percent of the rare earths, uses 9.0 kg t⁻¹ of salt, of which the unrecycled free salt is the larger part, and leaves a net value of 21.5 USD per tonne (Table 3). The concentration is the one used in industry, and the search found it because the preset's Langmuir curve, fitted to the same literature, flattens near 0.3 mol L⁻¹; the liquid-to-solid ratio sits at the lower bound of the search box, because the unrecycled free salt is proportional to the liquid volume while the recovery is not. Magnesium sulfate is a close second (83 percent, 21.2 USD t⁻¹). That matters, because magnesium sulfate is the reagent preferred for in-situ leaching on groundwater grounds. The dilute acids reach 67 to 79 percent at lower value: a proton enters the exchange with the same affinity as ammonium in this model, but an acid is dearer per mole of displacing ion and is also consumed by the silicate sink. Citric acid cannot compete. The sensitivity (Fig. 6c) names the two variables a bench programme should pin down first: the liquid-to-solid ratio, which sets reagent per tonne, and the concentration, which sets the exchange equilibrium.

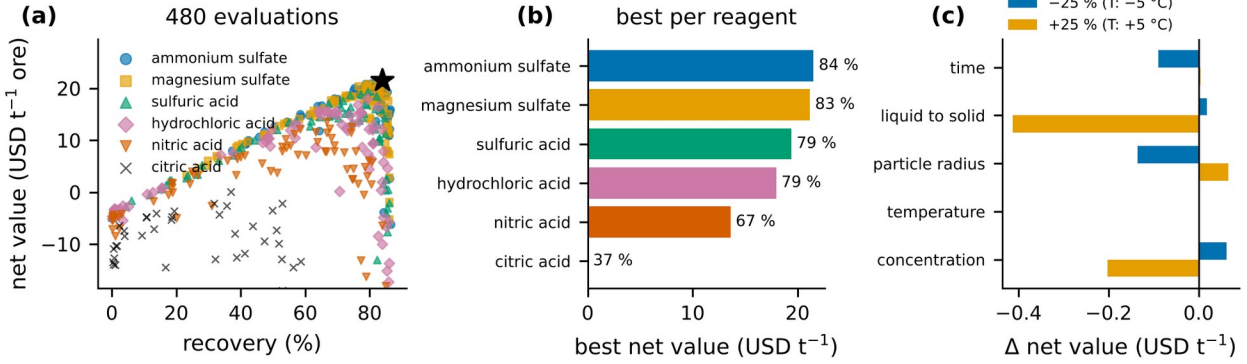


Figure 6. The Lixa search on the weathered-clay rare earth preset. (a) All 480 evaluations, net value against recovery, by reagent; the star is the selected recipe. (b) Best net value and recovery per reagent. (c) One-at-a-time sensitivity of the net value to a 25 percent change of each variable (5 °C for temperature) around the selected recipe, clipped to the search bounds.

Table 3. Best recipe per reagent for the weathered-clay rare earth preset at 25 °C (Fig. 6). C: reagent molarity; r: particle radius; L/S: litres of solution per kilogram of ore; t: contact time; reagent: consumed plus unrecycled free reagent. Price of TREO 40 USD kg⁻¹; reagent prices as in the package database.

Reagent	C (mol L ⁻¹)	r (mm)	L/S	t (h)	Recovery (%)	Reagent (kg t ⁻¹)	Net value (USD t ⁻¹)
ammonium sulfate	0.31	1.1	1.0	2.5	84	9.0	21.53
magnesium sulfate	0.47	1.9	1.0	13.8	83	12.0	21.17
sulfuric acid	0.19	0.8	1.0	2.1	79	19.1	19.42
hydrochloric acid	0.38	1.9	1.2	2.2	79	16.4	17.97
nitric acid	0.15	2.0	1.2	2.1	67	11.1	13.61
citric acid	0.04	2.5	1.2	1.1	37	9.5	0.01

6.2 Projecting to the plant

With the recipe fixed and the particle radius set to 5 mm for run-of-mine ore, Fig. 7a projects a 6 m lift irrigated at 8 L m⁻² h⁻¹. Recovery reaches 84 percent after 90 d if the solution wets all of the ore, and 50 percent with a contact efficiency of 0.6; the contact efficiency scales the curve and does not change its shape, because for this exchange-dominated ore the limit is the delivery of salt through the lift, not the exchange itself. Halving the irrigation rate stretches the time to 99 percent of the plateau from 22 to 44 d for the same reason. For in-situ recovery (Fig. 7b) the same recipe in a 30 m well pattern with a sweep

efficiency of 0.8 reaches 67 percent after 365 d, which is the batch recovery of 84 percent times the sweep efficiency to within 0.1 percentage points. A wider spread of travel times between fast and slow paths changes only how early the plateau is approached. Figure 7c is the hydraulic feasibility map behind every in-situ projection: the pressure needed to inject a given flow, as a function of permeability. For a 10 m thick ore layer and 30 m well spacing, the 1.5 MPa injection limit is crossed below $3.4 \times 10^{-14} \text{ m}^2$ at $2 \text{ m}^3 \text{ h}^{-1}$ and below $1.7 \times 10^{-13} \text{ m}^2$ at $10 \text{ m}^3 \text{ h}^{-1}$. That is the permeability range of many clay-rich regoliths, for which this map decides whether wells are an option at all.

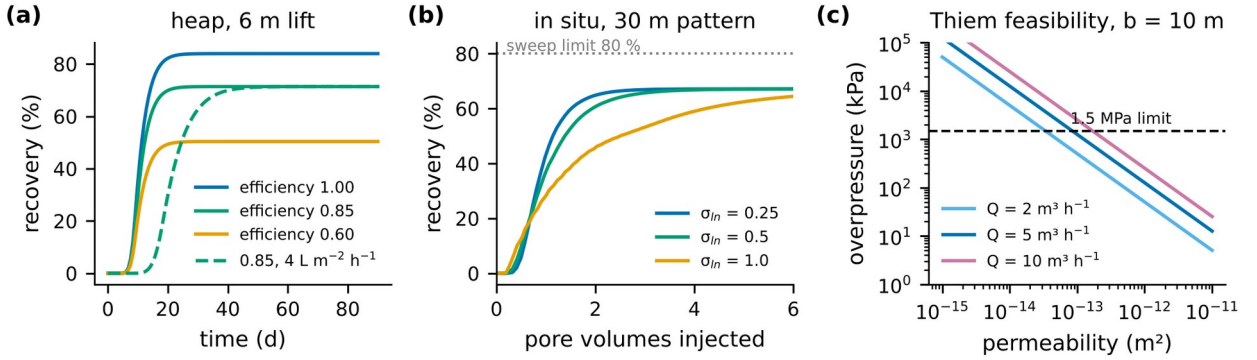


Figure 7. Plant-scale projections with the recipe of Fig. 6 and 5 mm particles. (a) Heap, 6 m lift, $8 \text{ L m}^{-2} \text{ h}^{-1}$, three solution-ore contact efficiencies, and $4 \text{ L m}^{-2} \text{ h}^{-1}$ at 0.85. (b) In-situ recovery in a 30 m pattern, 10 m thick, $5 \text{ m}^3 \text{ h}^{-1}$, permeability 10^{-12} m^2 , sweep efficiency 0.8, for three log-normal spreads of streamtube travel time; the horizontal axis is in pore volumes of the pattern. (c) Thiem injection overpressure as a function of permeability for three injection rates, 10 m formation, 30 m spacing, 0.1 m well radius, against a 1.5 MPa limit.

6.3 Closing the loop from the image

Figure 8 runs the whole chain on the three synthetic sample images, generated as packings of circular grains at three porosities, at a nominal $1 \mu\text{m}$ per pixel. The permeability scales with the square of the pixel size, so this choice places the three images in the 10^{-13} m^2 range of consolidated weathered rock; the same clay image at $4 \mu\text{m}$ per pixel gave $7.1 \times 10^{-12} \text{ m}^2$ in Fig. 2. The ore layer is 5 m thick, the wells are 30 m apart and the design flow is $10 \text{ m}^3 \text{ h}^{-1}$. The fine, open packing ($\phi = 0.47$) gives $k = 4.4 \times 10^{-13} \text{ m}^2$ and needs 1139 kPa, which is within the limit. The dense packing ($\phi = 0.37$) gives $k = 1.9 \times 10^{-13} \text{ m}^2$ and would need 2695 kPa, so the flow is cut to $5.6 \text{ m}^3 \text{ h}^{-1}$ and the median travel time between wells rises from 9 to 12 d. The coarse packing ($\phi = 0.34$, $k = 3.7 \times 10^{-13} \text{ m}^2$) needs 1367 kPa. The recipe is the same in all three cases. Because the exchange is limited by equilibrium, all three reach the same 67 percent within the year. What the image changes is how fast they get there, and whether the well design works at all. Half of the final recovery is reached after 5.9 d in the coarse packing, 7.8 d in the fine one, and 11.2 d in the dense one at its reduced flow (Fig. 8c). This is the practical content of an image-informed design. A tight ore shows up as an unworkable well field before any chemistry is run, and the design flow, the well spacing or the layer thickness can be changed at the screening stage.

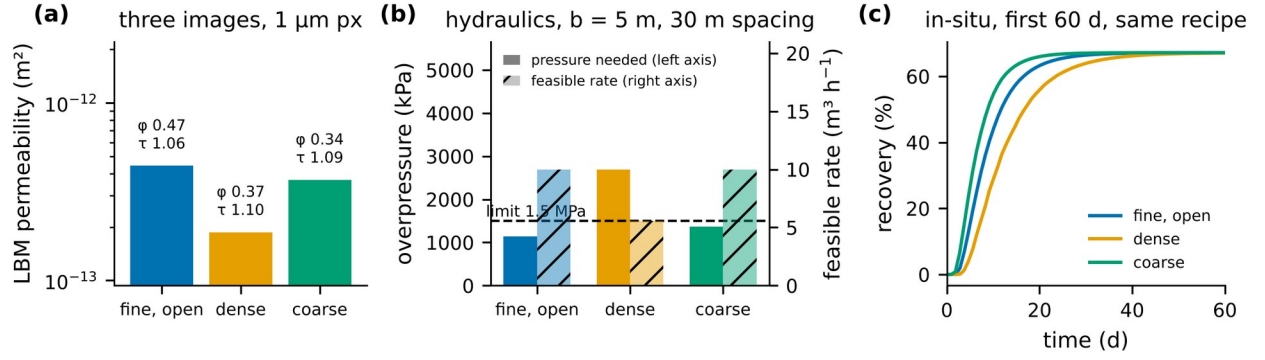


Figure 8. From image to plan on three synthetic sample images at $1 \mu\text{m}$ per pixel. (a) Lattice Boltzmann permeability with porosity and tortuosity. (b) Injection overpressure needed for $10 \text{ m}^3 \text{h}^{-1}$ in a 5 m thick formation (solid bars, left axis) against the 1.5 MPa limit, and the feasible rate after the cut (hatched bars, right axis). (c) In-situ recovery over the first 60 d with the recipe of Fig. 6 and the same sweep efficiency.

7 Model performance

Table 4 and Fig. 9 give wall-clock times on one core of a cloud virtual machine (Python 3.13, numpy 2.5). The geometry of a 256×256 image takes 44 ms. The lattice Boltzmann permeability of the same image, run to the 10^{-7} convergence criterion, takes 223 s; it is the slowest single step and it is optional. A batch evaluation costs 44 ms for the exchange-dominated clay and 331 ms for the three-host fly ash at 85°C , where the fast calcium phase forces short sub-steps early on. The search therefore completes 480 evaluations over six reagents in 5.7 s, and its time grows linearly with the budget (Fig. 9b). A 48 h laboratory column with 40 cells takes 190 ms, a 120 d heap 1.0 s, and a one-year in-situ projection with five streamtubes 15 s. A complete image-to-plan run takes 20 to 60 s without the lattice Boltzmann step and a few minutes with it. That is fast enough to screen a catalogue of feedstocks, or to run the loop many times inside an uncertainty analysis.

Table 4. Wall-clock times of the stages on one core.

Stage	Setting	Wall-clock time (s)
pore geometry	256×256 image	0.044
pore LBM permeability	256×256 image, to 10^{-7} convergence	222.8
batch, clay	exchange host, 4 h	0.044
batch, fly ash	three dissolution hosts, 85°C , 4 h	0.331
column	40 cells, 48 h	0.190
heap	24 cells, 120 d	0.98
in situ	5 streamtubes $\times$ 20 cells, 365 d	15.5

Stage	Setting	Wall-clock time (s)
search	480 evaluations, 6 reagents	5.7

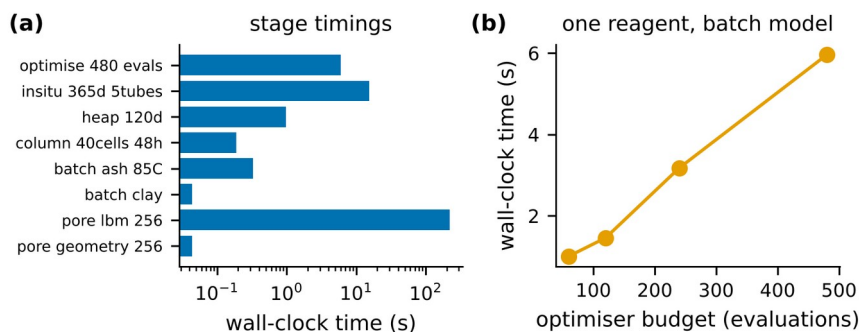


Figure 9. Computing cost. (a) Wall-clock time of each stage (Table 4). (b) Search time against its evaluation budget for one reagent on the batch model.

8 Limitations and outlook

Lixa is a screening tool, and its limits should be stated plainly. The pore stage works on a two-dimensional slice and computes geometry and flow only. Permeability and tortuosity from a slice are not those of the volume, a slice connects less readily than a volume, so it can report a blocked pore space where the rock conducts, and the tortuosity is a 4-connected path measure. There is no pore-scale solute transport or reaction; the chemistry runs at the reactor scale with the pore numbers as parameters. A three-dimensional image stack, a D3Q19 solver and a pore-scale advection-diffusion-reaction solver on the same lattice are the natural extensions, and the pipeline already accepts properties computed elsewhere through the same interface. The built-in chemistry is lumped: there is no speciation, no complexation and no precipitation, and the exchange affinity does not depend on temperature. Gypsum formation in sulfate systems and iron hydroxide precipitation at rising pH, both of which matter for red mud and fly ash, are outside the model; the PHREEQC bridge exists to check a recipe against a full equilibrium model. The rate constants in the presets are indicative values from the literature, two of the five presets have been checked against the data they were built from and three have not. They are meant to be re-fitted to one bottle-roll test per ore, and a calibration mode that fits k_{ref} , D_{eff} and the host shares to a measured recovery curve is the next planned feature. The heap and in-situ models carry no unsaturated flow, no heat balance and no interference between wells; they rank options and size the problem, and they do not replace a site flow model. The economics leave out the downstream steps (solvent extraction, precipitation), wells, permitting, water and the neutralisation of effluent, so the net value is a ranking metric and not a margin.

Two directions follow from the design. Because the batch model is cheap and its inputs form a small validated vector, Lixa runs are a natural training set for a surrogate model. A neural operator of the kind built for pore-scale reactive transport (Jung et al., 2023) could return a recipe for a new image in milliseconds. And because every stage is a function with typed inputs, the loop can be wrapped by an agent that proposes bench tests, reads their results and updates the presets, which would close the loop with the laboratory and not only with a simulator.

9 Conclusions

Lixa v0.1.2 turns an image of a critical-mineral ore into a leaching recipe and a plant-scale projection through one chain. The pore stage reads porosity, connectivity, surface, tortuosity and permeability from the image with a verified lattice Boltzmann solver. The kinetics turn those numbers and a recipe into metal released and reagent spent, with an exact mass balance. The search evaluates hundreds of recipes on the batch model and keeps the one with the highest net value within the limits. The plant stage carries that recipe to a heap or a well field with the same kinetics and takes its hydraulics from the image. The numerical parts reproduce exact solutions to 0.12 percent for flow, 0.004 for transport and better than one part in a thousand for kinetics. The shipped presets for clay-hosted rare earths and coal fly ash are consistent with the published recovery ranges they were built from. For weathered-clay rare earths the search returns the salt and the concentration used in industry, in seconds. The question the domestic critical-minerals effort faces is not whether a given ore can be leached. It is which of many dilute, unconventional feedstocks deserves a bench programme, and under what recipe. Lixa answers that question on one consistent basis, reproducibly, in minutes.

Appendix A: A complete run on a weathered-clay ore

This appendix follows one run of the pipeline from the command line to the plan, with every number taken from the files the run wrote (paper/data/example_run/). The case is the running example of the paper: a weathered granite clay with adsorbed rare earths, to be leached through wells rather than mined. The purpose is to show what the user supplies, what each stage returns, and how the output is read.

A1 The question and the inputs

A deposit of weathered granite clay has been drilled and assayed at 800 ppm TREO. One image of its pore space is available at 1 μm per pixel; here it is the synthetic clay image of Fig. 2a, which stands in for a micro-tomography slice (Fig. A1a). The operator wants to know which reagent to use, at what strength and for how long, whether the clay is permeable enough to be leached in place through wells, and what that would be worth for a 500 kt block. Strong acids are to be avoided, because the solution would be injected into the ground. The user supplies three things: a sentence describing the ore, the image, and the tonnage. Everything else takes the package defaults, which are listed in Table A1 so that the reader can see what the result rests on.

Table A1. Inputs of the worked example. Defaults are the values shipped with Lixa v0.1.2 and can be changed on the command line or in a YAML file.

Input	Value	Source
ore description	weathered granite clay with adsorbed rare earths, 800 ppm, in-situ wells, no strong acid	user
image	clay_regolith_porous.png, 256 $\times$ 256 pixels, 1 μm per pixel (synthetic)	user
ore tonnes	500 000	user

Input	Value	Source
ore preset matched	Ion-adsorption clay (regolith-hosted REE); hosts: exchangeable rare earths on clay (share 0.90), refractory minerals (share 0.10)	interpreter
reagents searched	ammonium sulfate, magnesium sulfate, citric acid (the three acids excluded by the description)	interpreter
search bounds	concentration 0.01 to 2 mol L ⁻¹ ; 25 °C; particle radius 0.5 to 5 mm; L/S 1 to 5; time 1 to 24 h	default
evaluation budget	480 batch simulations	command line
well pattern	spacing 30 m, ore thickness 10 m, injection 5 m ³ h ⁻¹ per pattern, pressure limit 1500 kPa, sweep efficiency 0.7	default
leach duration	365 d	command line
prices	TREO 40 USD kg ⁻¹ ; ammonium sulfate 0.20 USD kg ⁻¹ , 80 percent recycled; other operating cost 3 USD t ⁻¹ ; discount rate 8 percent	default

A2 The command

The whole chain is one command:

```

lixo plan \
  --describe "weathered granite clay with adsorbed rare earths, 800 ppm, in-
situ wells, no strong acid" \
  --image clay_regolith_porous.png --pixel-size 1 \
  --tonnes 500000 --days 365 --evals 480 --lbm --no-llm \
  --out runs/clay_isr

```

--describe is read by the rule-based interpreter (Sect. 2.6), which matched the preset for ion-adsorption clay with a confidence of 0.8, read the grade as 800 ppm, set the route to in situ, and excluded sulfuric, hydrochloric and nitric acid. --image and --pixel-size send the image to the pore stage; --lbm asks for the lattice Boltzmann permeability instead of the Kozeny-Carman estimate. --tonnes and --days size the plant stage. --evals is the search budget, shared equally among the reagents. --no-llm keeps the run fully deterministic. The run took 234 s on one core, most of it in the lattice Boltzmann step, which ran to its convergence criterion. The output folder holds report.md (the plan in one page), result.json (every number) and four figures, which are reproduced here as Fig. A1 to A4.

A3 Pore stage

The segmentation (Fig. A1b) gives a porosity of 0.47, all of it connected (0.47), a specific surface of $1.9 \times 10^5 \text{ m}^2 \text{ m}^{-3}$ and a tortuosity of 1.06. The lattice Boltzmann solver gives a permeability of $4.43 \times 10^{-13} \text{ m}^2$, which is about 0.45 darcy, in the range of a silty sand. Two of these numbers change the chemistry. The

surface seen in the image, $0.14 \text{ m}^2 \text{ g}^{-1}$ of solid, is far below the $20 \text{ m}^2 \text{ g}^{-1}$ at which the preset was fitted, because a $1 \mu\text{m}$ pixel resolves none of the roughness that carries most of a clay's surface; the surface ratio is therefore held at its lower clamp of 0.2 (Sect. 2.2), and the reaction-control rate constant of the refractory host is scaled down by that factor. The ratio ϕ_{eff}/τ is 0.44 against a reference of 0.12, so diffusion into grains is faster than in the preset. Neither matters much for this ore, because 90 percent of its rare earths are held by exchange, which does not depend on either number. The permeability is the number that matters, and it goes to the plant stage.

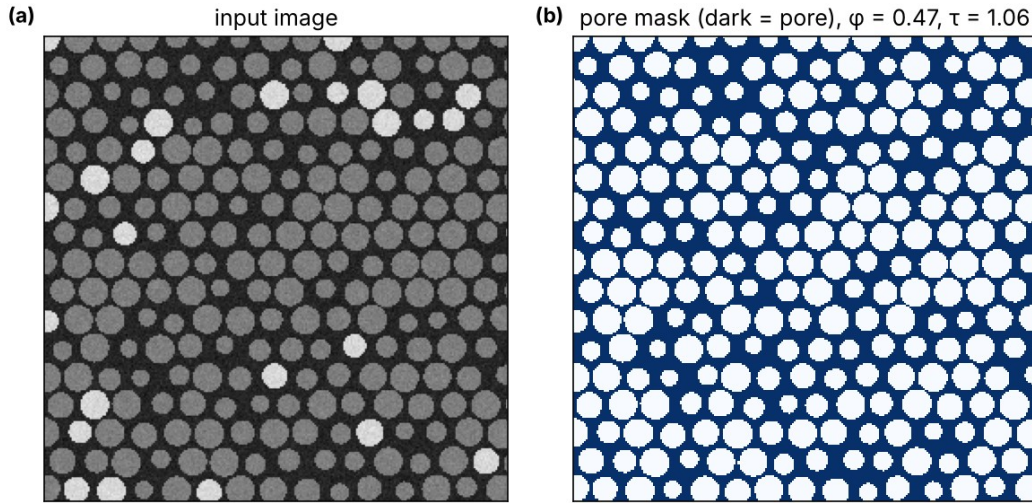


Figure A1. Pore stage of the worked example. (a) Input image at $1 \mu\text{m}$ per pixel. (b) Pore mask after Otsu segmentation; porosity 0.47, tortuosity 1.06, permeability $4.43 \times 10^{-13} \text{ m}^2$ by lattice Boltzmann.

A4 Laboratory stage: the recipe search

The search ran 160 batch simulations for each of the 3 permitted reagents. Figure A2 shows all of them as net value against recovery. The two sulfate salts form one curve: value rises with recovery up to about 80 percent and then drops sharply, because the last few percent of recovery need a much stronger solution and the extra salt costs more than the extra metal is worth. Citric acid scatters below zero; it releases less than half of the rare earths and is too expensive. The best point of each reagent is in Table A2. Ammonium sulfate at 0.23 mol L^{-1} , 1.1 L of solution per kilogram of clay and 2.7 h releases 83 percent of the rare earths with 7.6 kg of salt per tonne, for a net value of 21.91 USD per tonne. Magnesium sulfate reaches 82 percent at 21.48 USD per tonne. The particle radius returned by the search (0.7 mm) has no cost attached for the in-situ route and only a weak effect through the refractory host, so it is reported as the in-place grain size and is not a decision.

Table A2. Best recipe per reagent in the worked example, from `result.json`. Columns as in Table 3.

Reagent	C (mol L^{-1})	r (mm)	L/S	t (h)	Recovery (%)	Reagent (kg t^{-1})	Net value (USD t^{-1})
ammonium sulfate	0.23	0.7	1.1	2.7	83	7.6	21.91
magnesium	0.43	2.2	1.1	3.4	82	12.1	21.48

Reagent	C (mol L ⁻¹)	r (mm)	L/S	t (h)	Recovery (%)	Reagent (kg t ⁻¹)	Net value (USD t ⁻¹)
sulfate							
citric acid	0.04	0.8	1.0	1.1	39	8.9	1.41

This recipe differs in its details from the one in Sect. 6.1 (0.31 mol L⁻¹, 2.5 h), and the two net values differ by 0.39 USD per tonne. The objective is flat along a ridge: once the concentration is on the plateau of the Langmuir curve, above about 0.2 mol L⁻¹, and the contact time is past the first two hours, further changes move the value by a few cents per tonne, and two searches with different reagent lists, routes and random seeds land at different points on that ridge. The sensitivity test (Fig. A3) says the same thing in numbers. Changing the concentration, the time or the particle radius by 25 percent moves the value by at most 0.11 USD per tonne. Temperature was fixed at 25 °C in the search bounds, so its bars are zero by construction; the exchange equilibrium in this model does not depend on it in any case. The one variable with leverage is the liquid-to-solid ratio: 25 percent more liquid removes 0.34 USD per tonne, and the downward step, clipped at the bound of 1 L kg⁻¹ (11 percent less liquid), adds 0.15, because the unrecycled salt charged to a tonne of clay is proportional to the liquid volume while the recovery barely changes. The practical reading is that the bench programme should fix the liquid-to-solid ratio and the salt concentration first, and need not study temperature or contact time beyond two hours.

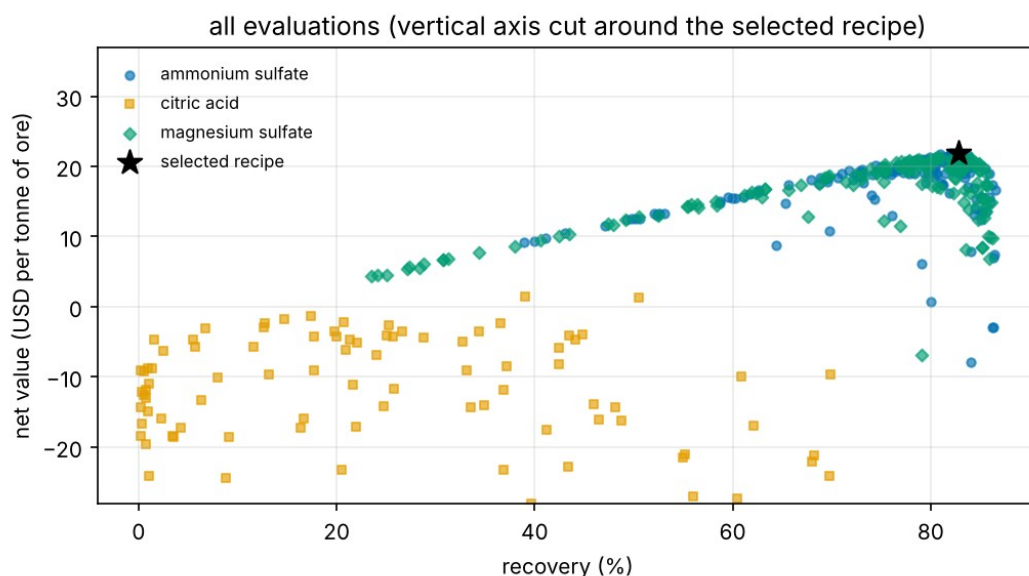


Figure A2. All 480 evaluations of the worked example: net value against recovery, by reagent. The star is the selected recipe. The vertical axis is cut to the region around the optimum.

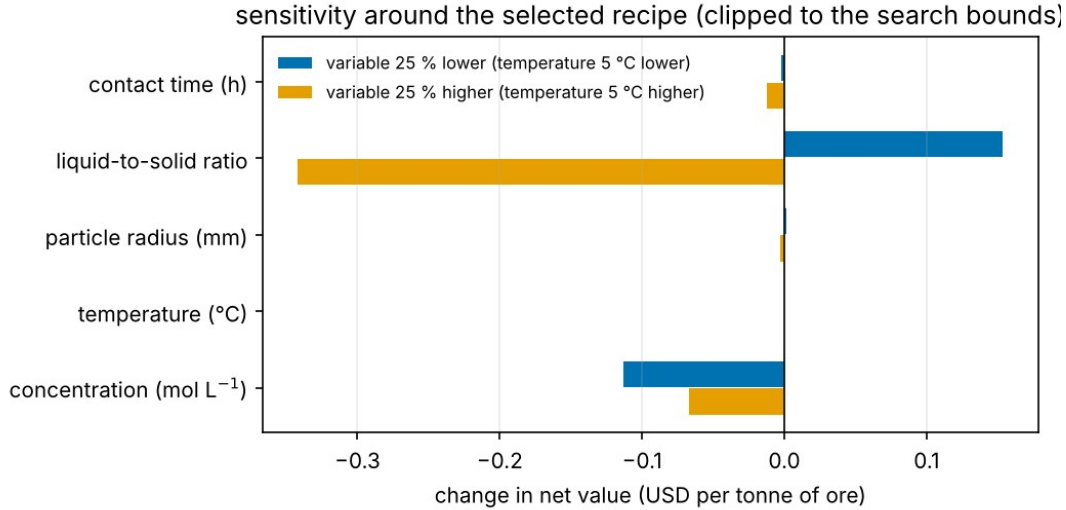


Figure A3. One-at-a-time sensitivity of the net value around the selected recipe: each variable changed by 25 percent (temperature by 5 °C) in both directions and clipped to the search bounds; temperature is fixed in this search, so its bars are zero.

A5 Plant stage: the well field

The in-situ projection first checks the hydraulics (Eq. 9). Injecting $5 \text{ m}^3 \text{ h}^{-1}$ into a 10 m thick layer of permeability $4.43 \times 10^{-13} \text{ m}^2$ through wells 30 m apart needs 285 kPa at the well, well under the 1500 kPa limit, so the design flow is accepted without a cut. The pore volume of one pattern divided by the flow gives a median travel time of 35 d between the wells, and over the year 10.5 pore volumes of solution pass through the pattern. The 500 kt block corresponds to 37 patterns of 13.5 kt each. The recovery curve (Fig. A4b) rises as the first solution reaches the recovery wells, passes 26 percent after 30 d and 56 percent after 90 d, and stays within one percentage point of its final value of 58 percent from day 111 onwards. The plateau is the laboratory recovery of 83 percent multiplied by the sweep efficiency of 0.7, which gives 58 percent; the chemistry is not the limit, the fraction of the ore that the solution reaches is. Reagent per tonne at the plant is 20.5 kg of salt: 0.56 kg consumed by the exchange and the rest the unrecycled fifth of the 100 kg t^{-1} injected over the year. That is the number the economics use, and it is larger than the laboratory figure because the solution keeps flowing through the pattern after the exchange has levelled off.

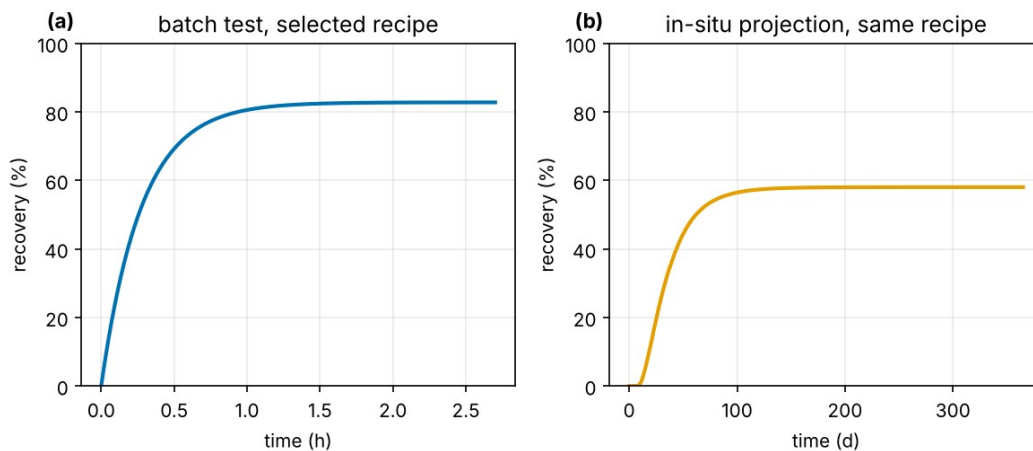


Figure A4. Recovery in the worked example. (a) The batch test with the selected recipe, in hours. (b) The in-situ projection of the same recipe, in days; the plateau is the laboratory recovery times the sweep efficiency of 0.7.

The economics (Table A3) follow from these numbers. The block holds 400 t of TREO; 58 percent of it, 232 t, reaches the solution and is worth 9.3 M USD at 40 USD kg⁻¹. Salt costs 2.05 M USD and other operating costs 1.5 M USD; there is no crushing. The cost of production is 15.3 USD per kilogram of TREO, against a price of 40 USD, and the net present value, with the one-year cash flow discounted once at 8 percent, is 5.3 M USD. These figures exclude solvent extraction, precipitation, wells, permitting and water treatment, so they rank options rather than state a margin, as Sect. 8 says.

Table A3. Economics of the worked example, from result.json. Screening level; excludes downstream processing, wells, permitting and water treatment.

Item	Value
TREO in the block	400 t
TREO recovered in 365 d	232 t (58 percent)
revenue	9.28 M USD
reagent cost	2.05 M USD (20.5 kg t ⁻¹ at 0.20 USD kg ⁻¹)
crushing	0 (in situ)
other operating cost	1.50 M USD (3 USD t ⁻¹)
cost per kg TREO	15.29 USD
net present value, one year at 8 percent	5.31 M USD

A6 Reading the plan

The plan answers the three questions the operator asked. Use ammonium sulfate near 0.2 mol L^{-1} at room temperature, with as little liquid per kilogram as the hydraulics allow; magnesium sulfate costs a few cents more per tonne and is the alternative if ammonium in groundwater is a concern. The clay is permeable enough for wells at the planned flow, with a wide margin on injection pressure. The block is worth working at the assumed price, with recovery limited by sweep rather than by chemistry, so money spent on better well placement buys more than money spent on reagent. The next step is one bottle-roll test at the recommended recipe. If it returns a recovery within about ten percentage points of the prediction, the preset stands; if not, the two exchange parameters of the preset (K_{ex} and X_{max}) are re-fitted to that test and the plan is re-run, which takes a few minutes. A second image from a tighter part of the deposit, run through the same command, would show whether the injection margin holds across the block.

Code and data availability

Lixa v0.1.2 (source code, ore and reagent databases, sample images, tests, and the quick-start, user-guide and science documents) and the material behind this paper are available from the author on request by email (shahram.asgari@uga.edu). That material comprises `scripts/make_figures.py`, which regenerates every figure and every number quoted in the text from the package, one CSV file per plotted series, `results.json`, the figures in PNG and PDF, and the complete output of the worked example of Appendix A.

Author contributions

SA conceived the framework, designed the models and the closed-loop workflow, implemented the code, carried out the verification, comparison and application runs, and wrote the paper.

Competing interests

The author declares no competing interests.

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