PyriteOxidation

Sulfide oxidation and acid generation in mine tailings – in-browser app • Hydrogeological Repository

What it does

PyriteOxidation estimates how fast sulfide minerals oxidise in an unsaturated tailings impoundment, and what that releases. Oxygen diffuses down from the atmosphere into the air-filled pore space; where it reaches unreacted pyrite or pyrrhotite it is consumed; and the model tracks the oxidation front through the profile together with the **sulfate, ferrous iron, acidity, nickel and zinc** released.

It is the source term an acid rock drainage assessment needs before any of it can be routed anywhere: the input to a reactive transport model, a load balance, or a closure-cover evaluation.

It applies the same principles as the PYROX model of **MD Wunderly** and **DW Blowes**, Institute for Groundwater Research, University of Waterloo. The original is a DOS-era Fortran program driven by a fixed-format text file; this is the same class of calculation in a browser, with the profile edited as a table and the results plotted as they are produced.

Everything runs in your browser

No installation, no account, and no dataset to download. A 26-node, 20-year run finishes in about 10 milliseconds on your own machine, so changing a moisture profile and re-running is immediate – and nothing about the site you are assessing is transmitted anywhere.

What you get

Output	Detail
Oxygen profile	Normalised oxygen concentration against depth, one curve per printed time. The first thing to check against measured porespace oxygen.
Sulfide remaining	The unreacted fraction against depth, so what is left to oxidise can be read directly rather than inferred.
Reaction front	When the oxidation front reached each depth. Nodes it never reached are left off the plot rather than drawn at zero.
Diffusion coefficient	The effective diffusivity derived for each element from porosity, moisture and temperature, on a log axis.
Loads against time	Cumulative sulfate, iron, acidity, nickel and zinc per square metre of tailings surface.
Run comparison	Up to eight runs overlaid, which matters because D_2 is a fitting parameter rather than a measurement.
Exports	CSV for the profiles, loads, element table and reaction front; the original program's .DAT and .out layouts; and chart images.

How the estimate is built

The unsaturated zone is divided into nodes from the tailings surface down to the water table. Properties between two nodes are the mean of the pair, so a layer boundary needs a node on each side of it. Oxygen is held at atmospheric concentration at the surface, and the base is closed.

Step	What sets it
Bulk oxygen diffusivity	Air-filled porosity and temperature, by the empirical relation for tailings of Reardon and Moddle (1985). Porosity itself does not enter – only how much of it is air.
Oxygen transport	Time-dependent diffusion down the profile, with a sink wherever unreacted sulfide remains.
Grain oxidation	Shrinking core: an unreacted centre inside a growing rim of oxidation products that oxygen must diffuse through, so each grain slows as its rim thickens.
Rate of rim growth	D_2, the grain radius, and the sulfide packed into the solid phase – more grains share the available oxygen, so each retreats more slowly.
Products	Pyrite gives 2 sulfate, 1 ferrous iron and 2 acidity per mole; pyrrhotite gives 1 sulfate and 1 iron, with no net acidity in this formulation.

Moisture content, and D_2, decide almost everything. Oxygen diffuses roughly ten thousand times faster through air than through water, so how wet the tailings are sets how deep oxygen reaches and therefore how fast anything oxidises. The profile entered must represent the average through the months when oxidation happens; a wet-season or dry-season snapshot will give a rate that is wrong by a wide margin, and nothing later in the calculation will reveal it.

D_2, the diffusion coefficient through the oxidised rim, cannot be measured. It is a fitting parameter: you adjust it until the modelled oxygen profile matches what was measured in the field. A run that has not been matched against field oxygen data is an assumption, not an estimate – which is why the app keeps several runs side by side rather than presenting one.

How a run works

Step	What happens
1. Material	Mineral, grain radius, starting radius, D_2, any nickel or zinc, and the run timing. Worked examples load with one click, or open an existing .DAT file.
2. Profile	The node table: sulfide sulfur, porosity, moisture, temperature and bulk density down the profile. Air-filled porosity is shown per row, and rows the diffusion floor will catch are marked while you edit.
3. Run	The solve, with anything that stops it or is worth knowing reported before the numbers.
4. Profiles	Oxygen and sulfide against depth, plus the reaction front and the diffusion coefficient.
5. Loading	Cumulative release per square metre, by species.
6. Results	The numbers behind the plots: profile at a chosen time, loads, element table, or front arrival.
7. Compare	Saved runs overlaid, for fitting D_2 against field data.
8. Export	CSV, the original .DAT and .out layouts, and chart images.

Limitations worth knowing

- This is the oxidation source term only. It does not route water, does not transport the products away, does not buffer acidity against carbonate or silicate minerals, and does not predict a pore-water chemistry. What it reports is what a reactive transport model or a load balance takes as input, not what a seepage sample would show.

- The diffusion relation has no root once air-filled porosity falls below about 0.05. Very wet layers are held at a floor value, and the app marks them: there the diffusion coefficient is a limit of the formula, not a property of the tailings.
- Grains are one size and one mineral, spherical, and evenly distributed within each layer. A real tailings mass is none of those things, and a wide grain size distribution will oxidise differently from its mean.
- Temperature affects oxygen diffusion through the profile but not the rim-limited rate at the grain, and there is no explicit temperature dependence on reaction kinetics. Bacterially catalysed oxidation, which can dominate in the field, is not represented at all.
- Moisture content, porosity and temperature are fixed for the whole run. Seasonal wetting and drying, a rising or falling water table, and consolidation over decades are all outside the model.
- The starting radius must be below 1. With no rim there is no resistance to oxidation and the rate at the first instant would be unbounded; 0.99 is the usual choice.

Checked against the original program, on its own worked examples. The four sample profiles distributed with PYROX – spanning 20 to 85 nodes, both minerals, uniform and sharply layered sulfide, and profiles wet enough to reach the diffusion floor – were run through both. Oxygen concentrations agree to within 0.006 of a normalised unit and typically to within 0.0005; the original reports them to four decimals, so that is at or near the limit of what can be compared. Cumulative sulfate agrees to about 1%. This is a differential equation solved on a grid rather than a table lookup, so exact equality is neither achievable nor meaningful – the original itself moves by about 0.02% when its own time step is refined tenfold.

Credit

The PYROX model is the work of **MD Wunderly** and **DW Blowes** at the Institute for Groundwater Research, University of Waterloo, with the coupled oxidation and reactive transport formulation published by Wunderly, Blowes, Frind and Ptacek in *Water Resources Research* (1996). The bulk oxygen diffusion relation for tailings is that of **EJ Reardon** and **PA Moddle** (1985). This app is an independent implementation of those published principles and claims no authorship of the method.

Beta. PyriteOxidation is published for evaluation and feedback. Check any figure you rely on against an independent calculation before using it in a design or an assessment.