An object-oriented particle tracking code for pyrite oxidation and pollutant transport in mine spoil heaps

C. J. Gandy and P. L. Younger

ABSTRACT

A physically based contaminant transport model, POTOMAC (Pyrite Oxidation products Transport: Object-oriented Model for Abandoned Colliery sites), has been developed to simulate the pyrite oxidation process in mine spoil heaps and the subsequent transport of the reaction products. This is believed to represent the first particle tracking model created using object-oriented technology and has proved capable of simulating the large time scales (on the order of centuries) required for this application. The model conceptualises a spoil heap as a series of 'columns', each representing a portion of the unsaturated zone, where active weathering and precipitation of secondary minerals takes place. The columns are then connected to a saturated zone, beneath the water table, where the contaminants are transported to the heap discharge. A form of particle tracking, the 'random walk method', is used to transport both the oxidant, oxygen, and the products, ferrous iron and sulfate. The subsequent oxidation of ferrous iron and precipitation of ferric oxyhydroxide is incorporated to provide an iron 'sink', where iron is effectively removed from the transport process. The application of POTOMAC to a case study, the Morrison Busty spoil heap in County Durham, UK, has produced encouraging results.

Key words | mine water, object-oriented programming, particle tracking, pollutant transport, pyrite oxidation, spoil heaps

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NOTATION

V	Average linear groundwater velocity (m/d)
D_L	Coefficient of longitudinal hydrodynamic dispersion (m^2/d)
x	Space dimension (m)
t	Time (d)
R_d	Retardation factor
C	Concentration of solute (mg/l)
C_sQ	Source or sink function having a concentration C_s (mg/l) and a flux rate Q (m^3/d), leading to a loading rate
K	Hydraulic conductivity (m/d)
n	Mean effective porosity
$(\partial h/\partial x)$	Head gradient
α_l	Longitudinal dispersivity, which is taken to be a 'characteristic length' of the porous medium (m)
D_D	Coefficient of molecular diffusion (m^2/d)
D_a^0	Diffusion coefficient for oxygen in air (m^2/s)
D_w^0	Diffusion coefficient for oxygen in water (m^2/s)
S_w	Relative water saturation
H	Henry's constant
μ	Mean of the distribution
σ	Standard deviation of the distribution
Z	A normally distributed random variable with zero mean and unit variance

ACRONYMS

OOP	Object-Oriented Programming
POTOMAC	Pyrite Oxidation Products Transport: Object-oriented Model for Abandoned Colliery sites

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INTRODUCTION

Surface spoil heaps can be potential long-term sources of contamination for local water courses and groundwater systems due to the significant quantities of sulfide minerals, particularly pyrite, which they often contain (Strömberg & Banwart 1999; Younger *et al.* 2002). Oxidative weathering and dissolution of these minerals releases metals (e.g. iron, zinc, copper), sulfate and, in the case of pyrite, acidity into percolating waters, which then discharge into the wider environment, coating stream beds with orange precipitates of iron hydroxides and oxyhydroxides ('ochre') (Younger 1995, 1998).

Pyrite, which is widespread in coal measures strata, is the principal sulfide mineral responsible for contamination in coal spoil heaps. Oxidation of pyrite by dissolved oxygen occurs when oxygen enters a spoil heap, either dissolved in infiltrating rainwater or in its gaseous form (which subsequently dissolves in the pore water):

$$FeS_{2(s)} + \frac{7}{2}O_{2(aq)} + H_2O_{(aq)} \rightarrow Fe^{2+}_{(aq)} + 2SO^{2-}_{4(aq)} + 2H^{+}_{(aq)}. \quad (1)$$

The ferrous iron (Fe^{2+}) released by pyrite oxidation is subsequently picked up by percolating water and is itself oxidised by dissolved oxygen to the ferric state (Fe^{3+}):

$$Fe^{2+}_{(aq)} + \frac{1}{4}O_{2(aq)} + H^{+}_{(aq)} \rightarrow Fe^{3+}_{(aq)} + \frac{1}{2}H_2O_{(aq)}. \quad (2)$$

Upon hydrolysis, the ferric iron spontaneously precipitates as ferric oxyhydroxide ($Fe(OH)_3$) and releases more protons (acidity):

$$Fe^{3+}_{(aq)} + 3H_2O_{(aq)} \leftrightarrow Fe(OH)_{3(s)} + 3H^{+}_{(aq)}. \quad (3)$$

The effective remediation of these polluting discharges requires an understanding of their long-term evolution. However, at present there is no comprehensive method to predict either the longevity of contaminant sources, or the evolution of their strength over the contaminating lifetime of a spoil heap (Younger 2000), although contaminant concentrations have long been shown to follow an exponential decline with time (Frost 1979; Glover 1983; Younger 1997). Such estimates are essential for an optimum choice of remediation options. Where contaminant loadings are high early in the life of a discharge, the predicted time scale for the depletion of source minerals in the active weathering zone will dictate whether long-term remediation must involve expensive techniques, such as chemical dosing, or whether less costly 'passive treatment' methods, using, for example, constructed wetlands, will eventually suffice (Wood *et al.* 1999).

A physically based contaminant transport model, POTOMAC (Pyrite Oxidation products Transport: Object-oriented Model for Abandoned Colliery sites), has been developed to predict the long-term contamination potential of mine spoil heaps. The latest object-oriented techniques have been employed in the development of POTOMAC to produce a computationally fast model capable of simulating large time scales, on the order of centuries.

The transport routine within POTOMAC is based on a particle tracking technique, the 'random walk method', whereby solute mass is simulated by a set of moving particles, each of which contains a proportion of the total mass of solute. The resulting particle (or mass) distribution is easily converted to a concentration distribution when required. This has the major advantage of avoiding numerical dispersion, a common problem in other solutions to the advection–dispersion equation. The method is also easily implemented in an object-oriented framework since each particle can be considered as an 'object' and, although demonstrated here in the field of pollutant transport in mine spoil heaps, it may be applied to other solute transport applications.

Application to the Morrison Busty spoil heap in County Durham, UK, has enabled predictions to be made on the contaminating lifetime of the spoil heap.

CONCEPTUAL MODEL

A mine spoil heap can be conceptualised as a series of columns (Gandy 2003), which represent an unsaturated zone where oxidative weathering of pyrite takes place, draining into a saturated zone beneath the water table, which may be within the spoil, effectively producing a perched aquifer, or within the underlying bedrock (Figure 1). This conceptual

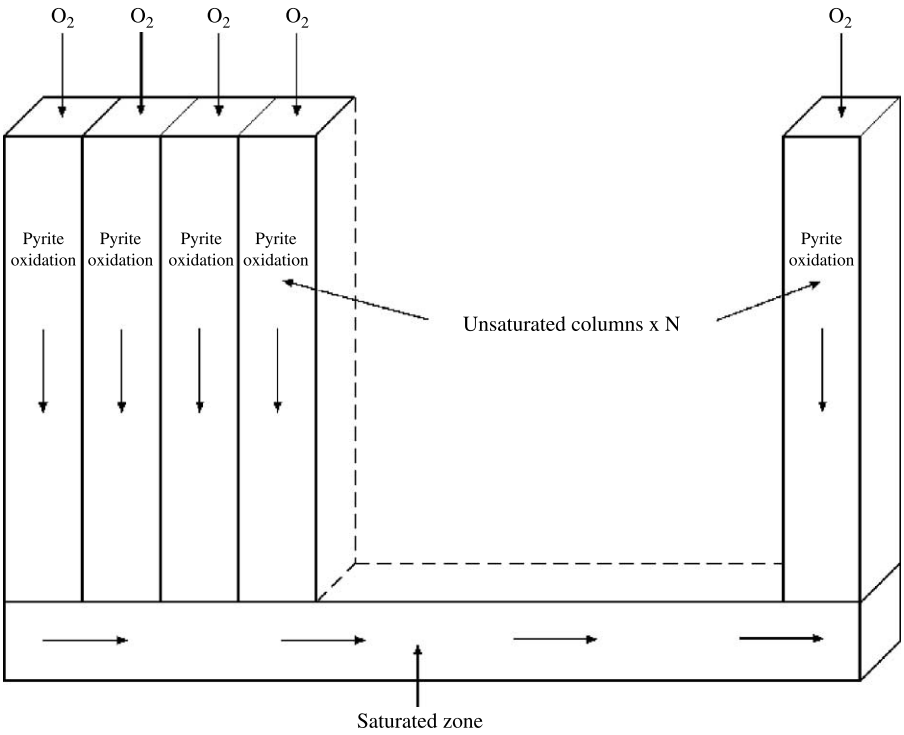

Figure 1 | Conceptual model of a mine spoil heap.

model represents a pseudo-two-dimensional approach to modelling contaminant transport in spoil heaps, with flow in a vertical direction within the columns and in a lateral direction in the saturated zone.

Within the conceptual model, oxygen, in both its gaseous form and dissolved in infiltrating precipitation, enters each column at the spoil surface and is transported vertically, reacting with any pyrite present within the unsaturated spoil (Equation (1)). On reaching the saturated zone, oxygen is removed from the model system since it is assumed that no pyrite oxidation takes place within the saturated zone due to the lack of availability of gaseous oxygen. The contaminants resulting from the pyrite oxidation process in the unsaturated zone, i.e. ferrous iron and sulfate, are added to the percolating groundwater and are transported vertically through each column. There is assumed to be no lateral movement of water or gas between columns. The columns are unsaturated and, as such, the pore space within the spoil is assumed to be partly water-filled and partly air-filled. Oxidation of ferrous iron by dissolved oxygen (Equation (2)), and the subsequent precipitation of ferric oxyhydoxide (Equation (3)), produces a 'sink' for iron and results in its effective removal from the model. It is assumed there is no sink for sulfate. On reaching the saturated zone, each chemical constituent is transported laterally to the spoil heap discharge.

SOLUTE TRANSPORT

The transport of dissolved components within POTOMAC is based on a particle tracking technique, the 'random walk method', which has been used successfully for many years to simulate conservative and reactive transport in porous media (e.g. Prickett *et al.* 1981; Kinzelbach 1988; Valocchi & Quinodoz 1989; Tompson & Gelhar 1990; Kinzelbach & Uffink 1991). The fundamental idea is to simulate the concentration distribution of chemical constituents by a finite number of discrete particles, each of which is moved by groundwater flow and is assigned a mass which represents a fraction of the total mass of chemical constituent involved.

The governing equation for solute transport in porous media, the advection–dispersion equation, can be written (in one dimensional form) as

$$\frac{\partial}{\partial x}\left(\frac{D_L}{R_d}\cdot\frac{\partial C}{\partial x}\right)-\frac{V}{R_d}\cdot\frac{\partial C}{\partial x}\pm C_sQ=\frac{\partial C}{\partial t} \tag{4}$$

Solute transport is governed by two fundamental processes: advection and dispersion. Advection is defined as the movement of solutes by the bulk motion of the flowing groundwater, at the same rate as the average linear velocity of the groundwater (Anderson & Woessner 1992), where the average linear velocity (V) can be defined as

$$V=\frac{K}{n}\left(\frac{\partial h}{\partial x}\right). \tag{5}$$

Hydrodynamic dispersion refers to the spreading of the contaminant due to the fact that not all of it actually moves at the same speed as the average linear velocity of the groundwater (Anderson & Woessner 1992). It is therefore the spreading of the contaminant in excess of the displacement attributable to advection alone (Fetter 1999). The spreading of the solute in the direction of bulk flow is known as longitudinal dispersion, while spreading in directions perpendicular to the flow is called transverse dispersion. The longitudinal dispersion coefficient (D_L) in Equation (4) is a term which includes both mechanical mixing and molecular diffusion and is given by

$$D_L=\alpha_l V+D_D \tag{6}$$

For the transport of solutes within POTOMAC, molecular diffusion is considered to be negligible, so the longitudinal dispersion coefficient is assumed to be simply a product of mechanical mixing. However, diffusion plays an important role in the transport of gaseous oxygen within the air-filled pores. Pyrite oxidation reactions consume oxygen (Equations (1) and (2)) and the resulting change in concentration with depth is referred to as the oxygen concentration gradient. This gradient is the driving force for the diffusive transport of oxygen through the spoil heap (Gerke *et al.* 1998). The effective diffusion coefficient for oxygen in the air phase is calculated using the approaches of Elberling *et al.* (1993) and Gerke *et al.* (1998) and is given by

$$D_a=0.273D_a^0(1-S_w)^{3.28}+\frac{S_wD_w^0}{H}. \tag{7}$$

Once calculated, the oxygen diffusion coefficient is incorporated into the transport routine by way of Equation (6), in place of the coefficient for molecular diffusion (D_D), while the mechanical mixing term is taken to be zero. Therefore:

$$D_L=D_a. \tag{8}$$

The random walk method has the major advantage of not involving numerical dispersion, a problem encountered with many other methods of solving the advection–dispersion equation (e.g. Method of Characteristics), since concentration distributions are calculated only when required (Marsily 1986). It solves Equation (4) by routing particles at the average linear groundwater velocity to represent advection, then adding a random displacement, tending to the normal distrbiution, for dispersion. Sorption and decay are incorporated by adjusting the velocity of the particles and the mass carried by the particles. The direct result of the random walk model is the particle (mass) distribution. The conversion of particle clouds to concentration distributions is achieved by spatial discretisation and summing of particles in the appropriate cell (Kinzelbach 1988).

The basic concepts of the random walk method have been reviewed by several authors: Prickett *et al.* (1981), Uffink (1985, 1988), Kinzelbach (1986, 1988), Marsily (1986), Ackerer (1988), Valocchi & Quinodoz (1989), Tompson & Gelhar (1990), Kinzelbach & Uffink (1991), Kitanidis (1994), Zheng & Bennett (2002), LaBolle *et al.* (1996), Wen & Kung (1996) and others. It can be demonstrated by a simple one-dimensional transport problem where the concentration distribution resulting from an instantaneous injection of mass, M, at location $x=0$ in an infinite column of porous medium in which there is uniform flow at a velocity, V, yields the concentration distribution at time t:

$$C(x,t)=\frac{1}{\sqrt{4\pi\alpha_l Vt}}\exp\left[\frac{-(x-Vt)^2}{4\alpha_l Vt}\right]. \tag{9}$$

Equation (9) is equivalent to the probability density function, $n(x)$, of a normally distributed (Gaussian) random variable X:

$$n(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[\frac{-(x-\mu)^2}{2\sigma^2}\right]. \quad (10)$$

Equations (9) and (10) can thus be equated to establish the following relationships:

$$n(x) = C(x,t) \quad (11)$$

$$\mu = Vt \quad (12)$$

$$\sigma = \sqrt{2\alpha_l Vt}. \quad (13)$$

In terms of solute transport, advective movement therefore represents the mean of a normally distributed random variable (μ) and dispersive movement of the deviation from the mean (σ) (Zheng & Bennett 2002). The process is shown diagrammatically in Figure 2 for a particle moved in the x direction in a single time step. The path length is normally distributed with mean μ, represented by the advective displacement, and standard deviation σ, represented by the dispersive displacement. It is important to note that the random movement to represent the effects of dispersion can be in the positive or negative x direction but is shown here in the positive direction.

Each particle is therefore moved over a distance x during a single time step of length t (Kinzelbach 1986) according to

$$x = Vt + Z\sqrt{2\alpha_l Vt} \quad (14)$$

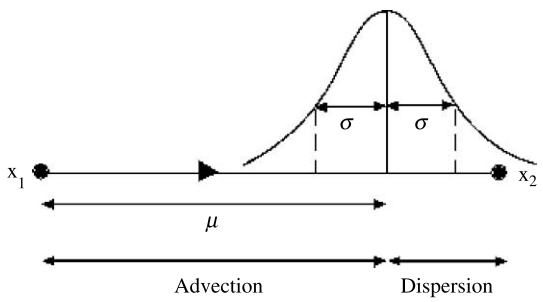

Figure 2 | Transport of a particle in the x direction in a single time step, where X_1 is the initial particle position and X_2 the new particle position.

where Z is a normally distributed random variable with zero mean and unit variance. The resulting path lengths are normally distributed with mean Vt and standard deviation $\sqrt{2\alpha_l Vt}$.

For gaseous oxygen particles, advection is taken to be zero so that the distance x over which an oxygen gas particle moves in a single time step of length t is taken to be

$$x = Z\sqrt{2D_a t}. \quad (15)$$

For all particles, the random number Z is taken to lie between -6 and $+6$, to give possible locations of particles out to 6 standard deviations either side of the mean. This is felt to be practical since it is unlikely that a particle will move beyond that distance (Prickett *et al.* 1981). Z is generated from a pseudo-random number sequence. Such numbers are not truly random since their pattern recurs cyclically. However, the sequence has been initialised using the system clock so that a different starting point occurs at the beginning of each simulation.

OBJECT-ORIENTED MODEL DESIGN

Object-Oriented Programming (OOP) is often referred to as a new paradigm (Budd 1991). It is a technology that has become increasingly popular over the past ten years and involves concepts that are fundamentally different to those employed in conventional procedural programming techniques (Murray & Kutija 2000). The major advantages of the approach are the ability to re-use code, so saving valuable time, and the ease with which code can be extended (Graham 2001).

POTOMAC has been written in a fully object-oriented style, incorporating the main features of OOP, such as inheritance, polymorphism and encapsulation. Each physical element within the conceptual model is assigned to an object, which contains the properties and methods associated with that physical element. It is believed to represent the first particle tracking model, or indeed solute transport model, created using object-oriented technology. The physical system and the relation of its objects is shown in Figure 3.

Each one-dimensional column is assigned to an object which is an instance of the class *TPorousMedium* while the

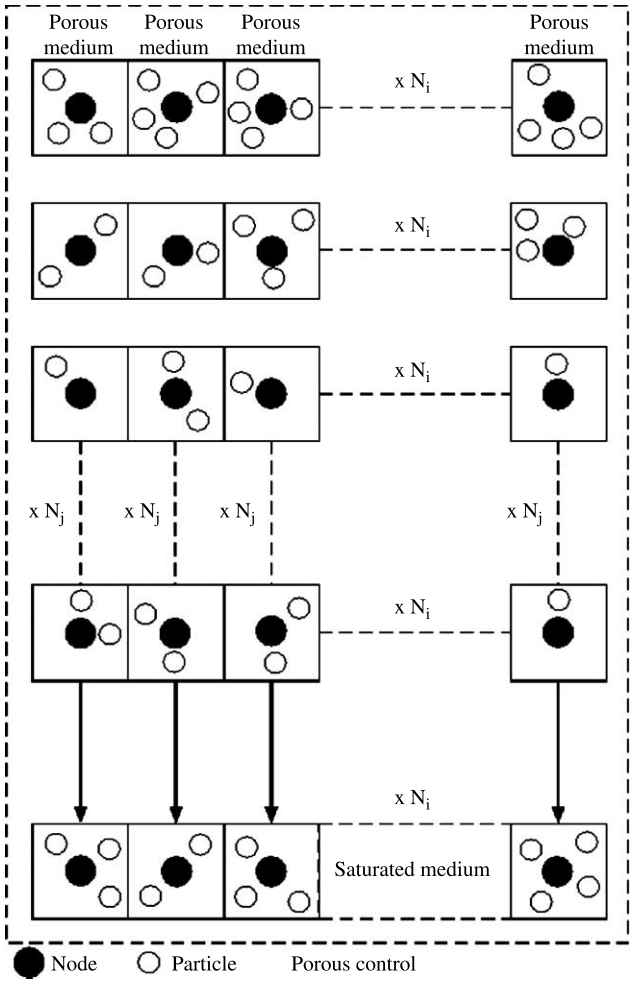

Figure 3 | The overall structure of the physical system showing all the objects involved in N_i columns each containing N_j cells.

saturated zone is assigned to an object which is an instance of the class *TSaturatedMedium*. These objects hold the input variables and methods associated with the unsaturated and saturated zones, respectively. Although several methods held within both classes have identical names, the calculations performed within them are specific to each class and may vary. For example, the calculation of velocity in each column cell is different to that in each saturated zone cell. In a column, the inflow to each cell is based only on the outflow from the cell above, whereas in the saturated zone it is based on the outflow from the corresponding column as well as the outflow from the adjoining cell.

Nodes are located at the centres of each cell in the finite difference grid and each is assigned to an object which is an instance of the class *TNode*. This object stores variables describing the physical properties of the cell and allows between-cell variations in physical properties to be easily implemented since each node is assigned to a separate object which can store different values.

Particles are unique entities which hold a proportion of the total mass of a particular chemical constituent and are transported throughout the model domain. There are three classes which describe particles: *TParticle*, *TOxygenParticle* and *TOxygenDiffusionParticle*. Each class represents a different chemical constituent. Particles are moved vertically through each column before being transferred to the corresponding cell in the saturated zone (Figure 3), where they are transported laterally to the discharge point.

The classes representing nodes and particles are part of the same class hierarchy (Figure 4), where some of the best examples of object-oriented programming features can be found, such as inheritance and encapsulation. The *TCPoint* class is an abstract class, i.e. a base class from which subclasses are created but no direct instances. The child classes created from the *TCPoint* parent class are *TNode* and *TParticleType*. The *TParticleType* class is itself another abstract class as it is only used to create further subclasses describing the different types of particle. The class hierarchy is designed in this way as many properties are required by both the nodes and the particles.

In addition, at the beginning of each simulation one object is created from the *TPorousControl* class, which represents the outer core of the model and, in effect, acts as a manager (Figure 3). This object stores most inputs to the model and passes them to the objects created from the other classes, where the variables are required in the central algorithms.

OVERVIEW OF A MODEL SIMULATION

The initial step in a model simulation is the creation of an object from the *TPorousControl* class to store the input data

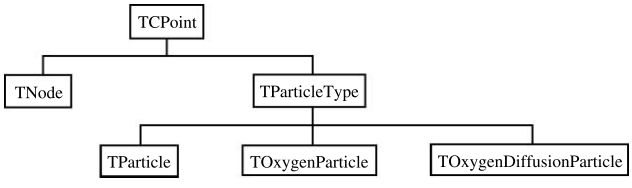

Figure 4 | Class hierarchy for nodes and particles.

and set up the physical system. Once the input parameters are entered, a model simulation can be carried out, which involves three stages, all of which are methods of the *TPorousControl* class: Simulation Preparation; Calculation; Finish Simulation.

The Simulation Preparation method is concerned with the establishment of the physical system in preparation for the main calculations. It is only performed once, at the beginning of each simulation, in contrast to the Calculation method which is carried out during each time step. The first stage in the Simulation Preparation method is the creation of objects to represent the saturated zone (from the *TSaturatedMedium* class), each unsaturated column (from the *TPorousMedium* class) and the nodes within each cell (from the *TNode* class). The model inputs they require as variables are passed from the object of the *TPorousControl* class. Various lists are also created at this point to store the objects representing the columns (within the *TPorousControl* object) and the objects representing the nodes and particles, both within the *TSaturatedMedium* object and each *TPorousMedium* object. The only methods carried out during the Simulation Preparation stage are those which calculate the values of properties which remain constant throughout a simulation, e.g. delta x (distance between nodes) and calculation of velocity in each cell.

The Calculation method is the core of the simulation where the main calculations are carried out. In a single time step, the model performs all the calculations concerning the unsaturated zone, looping through each column in turn, then deals with the saturated zone (Figure 5). The whole process is repeated for each remaining time step.

The addition of particles is the initial step in the Calculation method. Dissolved and gaseous oxygen particles are added to the uppermost cell in each column and, for each particle added, an object of either the class *TOxygenParticle* or *TOxygenDiffusionParticle* is created. These objects then enter their respective lists in that column's object of the *TPorousMedium* class. The user chooses the number of particles to add. The greater the number added, the more accurate the simulation, since the mass is distributed between more particles so after their random movement there should be a greater distribution of chemical constituent throughout the column rather than a concentration in one place.

The next step is to oxidise any pyrite present within each cell according to the amount of available oxygen. Therefore, the mass of both dissolved oxygen and gaseous oxygen is determined for each cell in turn and, if there is oxygen present within a particular cell, it reacts with any pyrite in that cell according to Equation (1), creating further particles to store the resulting ferrous iron and sulfate masses. These particles are objects of the *TParticle* class and are added to the relevant list in the column's object of the *TPorousMedium* class. The initial position of each new particle is set as the position of the node in the cell in which oxidation has taken place. The mass of pyrite in that cell is adjusted accordingly, depending on the amount of mineral dissolved by the oxidation process, and similarly the mass of oxygen in each particle is adjusted. The model then checks to see if any dissolved or gaseous oxygen particles have no remaining mass and any such particles found are removed from the model.

This process is then repeated for the oxidation of ferrous iron (Equation (2)). The mass of both oxygen and ferrous iron in each cell is determined and, if both are present in a particular cell, ferrous iron oxidation is carried out there. The mass of ferrous iron and oxygen stored in each particle is adjusted according to the amount lost during the oxidation process and the model again checks to see if any particles containing either dissolved oxygen or gaseous oxygen have no remaining mass and any found are removed from the model.

After the chemical reactions have taken place, the simulation progresses to the transport of the remaining particles. Each particle is moved separately according to Equations (14) and (15), depending on the type of particle. The particle's velocity is determined by its position. The velocity has already been calculated for each cell during the Simulation Preparation stage of the simulation and stored in the corresponding node. The particle takes its velocity from the node in the cell in which it resides. The particle's position is adjusted within its object after it has been moved.

During the transport process, some particles may have moved out of the base of the column so these have to be removed from their respective lists in the columns and transferred to the corresponding list in the saturated zone. The objects of the classes *TOxygenParticle* and *TOxygenDiffusionParticle* are destroyed at this point since it is assumed there is no oxygen present in the saturated zone.

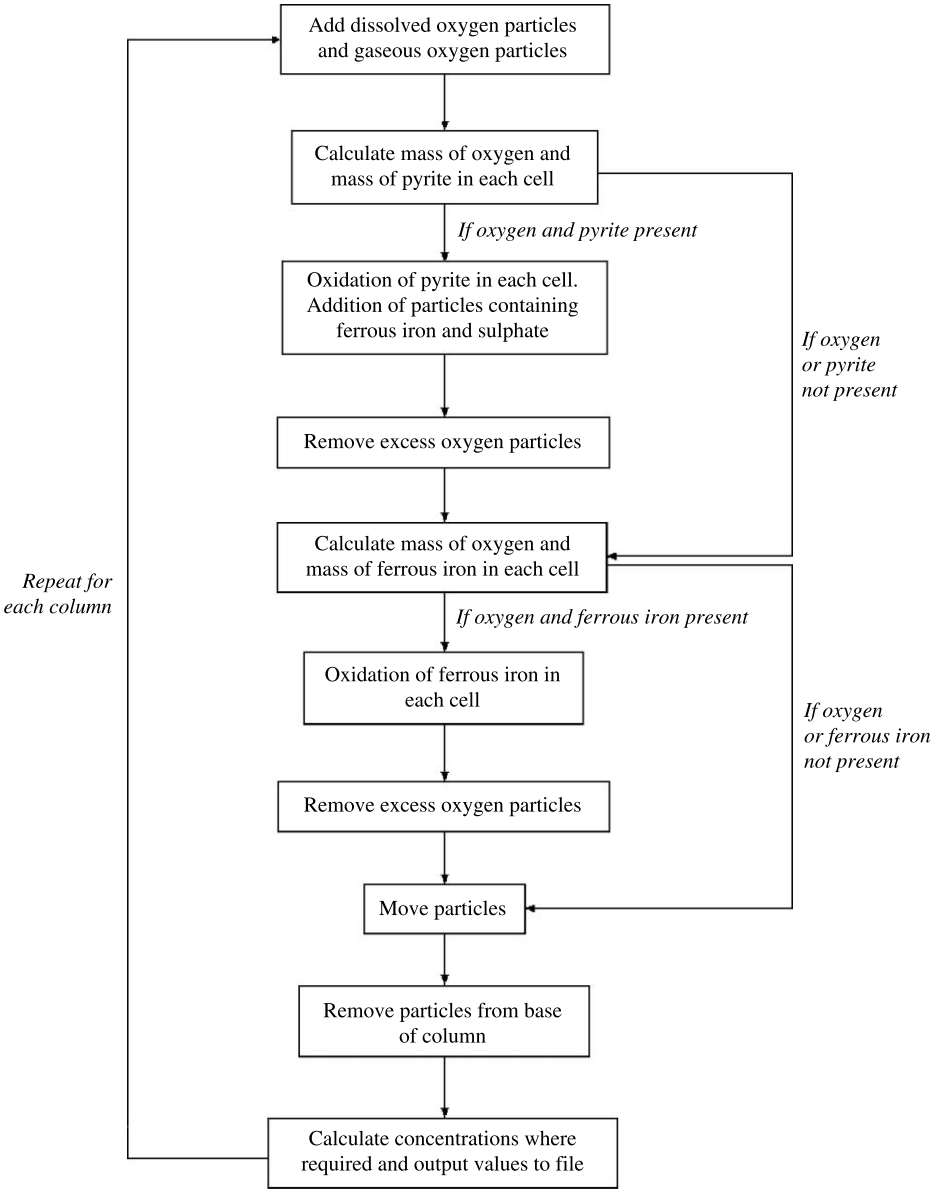

Figure 5 | Flowchart of column calculation loop for a single time step.

Each particle's new position is set as the position of the node in the cell to which it has moved in the saturated zone. Constituent masses are summed and concentrations calculated where required.

The entire process described above for the Calculation method is repeated for each column before the simulation moves onto the saturated zone. The code first checks to see whether there are any particles within the saturated zone and, if any are present, they are moved according to Equation (14). Each particle's position is updated in its object after the transport process. As in the columns, when a particle leaves the saturated zone it is removed from its list in the object of the *TSaturatedMedium* class and added to a temporary list where the total mass of each constituent is determined so that effluent concentrations can be calculated. Constituent masses in each cell are also calculated in the event that their concentrations are required in the output results. If so, the values are output to the relevant files.

The Finish Simulation method takes place after the final time step has been completed and destroys all the objects

that have been created during the simulation. Finally, when the model is closed down, the object of the *TPorousControl* class is destroyed.

APPLICATION OF POTOMAC

POTOMAC has been applied to the Morrison Busty spoil heap, which lies near the village of Quaking Houses in County Durham, UK, in order to predict the contamination potential of the waste material and assess the long-term water quality evolution. The spoil heap covers an area of approximately 35 ha and varies in thickness from 4–10 m. It comprises colliery waste in the form of grey and black weathered shale, ash, coal and coal dust, and overlies glacial clay and sandy drift deposits which in turn overlie Carboniferous Coal Measures beds. A perched water table appears to exist within the heap, above the impermeable clay layer at the base of the spoil, at a depth of approximately 6–9 m, while the most significant discharge enters a local watercourse, the Stanley Burn. Further details on the Morrison Busty spoil heap are given in Gandy & Younger (2003). Since the pollutant-generating part of the spoil heap occupies only a small area, a 500 m by 125 m (62,500 m^2) section of the heap was taken for modelling and the perched water level was kept constant at a depth of 8 m below the spoil surface, producing a saturated zone with a constant thickness of 2 m. For the POTOMAC simulation, the area to be modelled was divided into 20 columns, with each column divided into 8 cells.

Grid discretisation is an important consideration as it affects both the quality of the results and the length of time taken to run a simulation. It is clear that the greater the number of columns, the more computation will be required, so the greater the total simulation time. However, a balance must be achieved in which the simulation time and computational power are not allowed to dominate at the expense of accuracy. The greater the number of columns, the smoother the expected results since more particles are involved in the simulation, resulting in a greater distribution of mass. A Pentium III, 1 GHz computer with 512 MB memory proved capable of running a 500 yr simulation of the Morrison Busty spoil heap in approximately 2 d. However, this simulation used a daily time step and 10 particles of each constituent were added each time step. Since each particle represents an "object", which is assigned to a portion of computer memory, this amounts to considerable memory requirements during the course of the simulation.

Following successful calibration against observed iron and sulfate concentrations in the perched groundwater and discharge from the Morrison Busty spoil heap, a long-term simulation was carried out to predict the contamination over a 500 yr period. Results for the perched groundwater are shown in Figures 6 and 7. An exponential decline in concentration with time can be clearly seen from these figures, with iron and sulfate predicted to persist in both the perched groundwater and heap effluent (not shown) for several centuries, although the latter is predicted to contain lower concentrations than the perched groundwater, probably due to dilution by water of a much higher quality, generated in less contaminated parts of the spoil heap.

The exponential decline in concentration shown by Figures 6 and 7, as well as the results for the heap discharge (not shown), reflect the progressive decrease in the rate of pyrite oxidation as the surface area of pyrite crystals is reduced. At the end of the simulation, after 500 yr, iron and sulfate concentrations in the perched groundwater are predicted to be approximately 23 mg/l and 120 mg/l, respectively, with calculated half-lives in excess of 500 yr for iron and on the order of 84 yr for sulfate. Similarly, for the spoil heap discharge, the development of asymptotic levels results in predicted concentrations after 500 yr of approximately 7.5 mg/l and 37 mg/l for iron and sulfate, respectively. The calculated half-life for iron in the discharge is again in excess of 500 yr while that for sulfate is on the order of 85 yr.

IMPLICATIONS OF AN OBJECT-ORIENTED PARTICLE TRACKING APPROACH

The application of POTOMAC to the Morrison Busty spoil heap has shown the extent of pollution which can be expected from such systems. In order to plan optimally for remediation of polluting discharges from spoil heaps, it is desirable to have an indication of the longevity of contaminant sources and the evolution of their strength over the contaminating lifetime of the heaps. Existing techniques for making the necessary analyses are limited

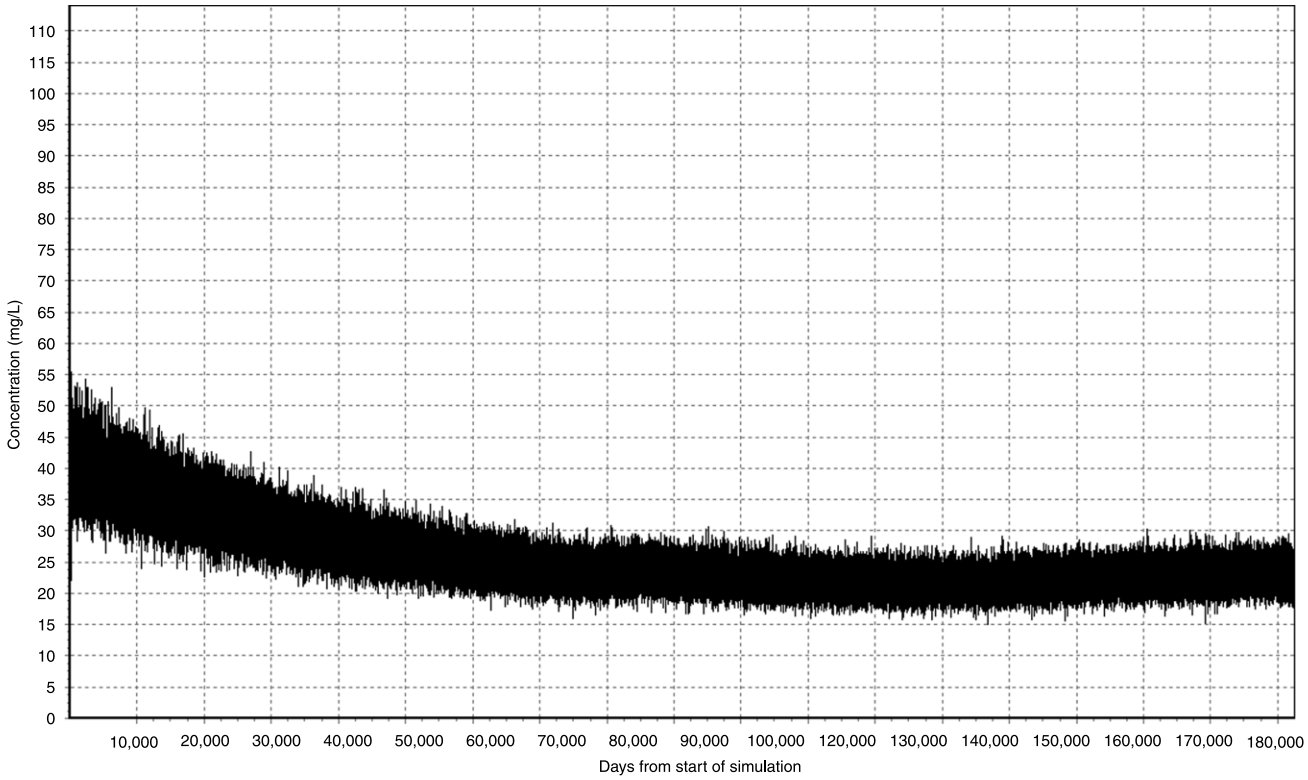

Figure 6 | Predicted iron concentration in perched groundwater of Morrison Busty spoil heap over a 500 yr period.

in that they do not consider temporal changes in key variables and provide little information relevant to the prediction of field contaminant concentrations.

POTOMAC has been developed to predict the long-term quality of discharges from surface spoil heaps undergoing pyrite oxidation. The latest techniques in OOP have been used to create a computationally fast model capable of simulating the large time scales (on the order of centuries) required for this application. POTOMAC uses a particle tracking technique (the random walk method) to simulate transport of both the reactants and the reaction products. This approach is easily implemented using OOP since each particle is assigned to an object which transports a mass of a particular contaminant throughout the model system. Similarly, the series of one-dimensional columns representing the unsaturated zone of a spoil heap, as well as the saturated zone and the nodes located at the centres of each cell within the finite difference grid, are assigned to objects. These objects store the various physical and chemical properties relevant to each and enable heterogeneities to be easily modelled since each node is assigned to a separate object which can store different values for a particular physical parameter.

The 500 yr simulation of the Morrison Busty spoil heap represents a huge numerical model containing a large number of particles, with the possibility of up to 2000 particles being added to the model in a single time step. Although each particle represents an object which is assigned to a portion of computer memory (so the memory requirements for such a simulation are considerable), a 1500 yr simulation of this spoil heap has been carried out on a Pentium IV, 2.5 GHz computer in only 18 h. It is believed that it would be almost impossible to run a simulation of this size with a model developed using traditional, procedural programming techniques, due to the time it would take for manipulation of such large arrays and record structures and the passing of a vast number of parameters. However, no direct comparison is available for testing.

The object-oriented style of development also allows the code to be easily extended, in particular to include additional minerals and chemical processes, and perhaps more importantly the approach to be adapted for use in

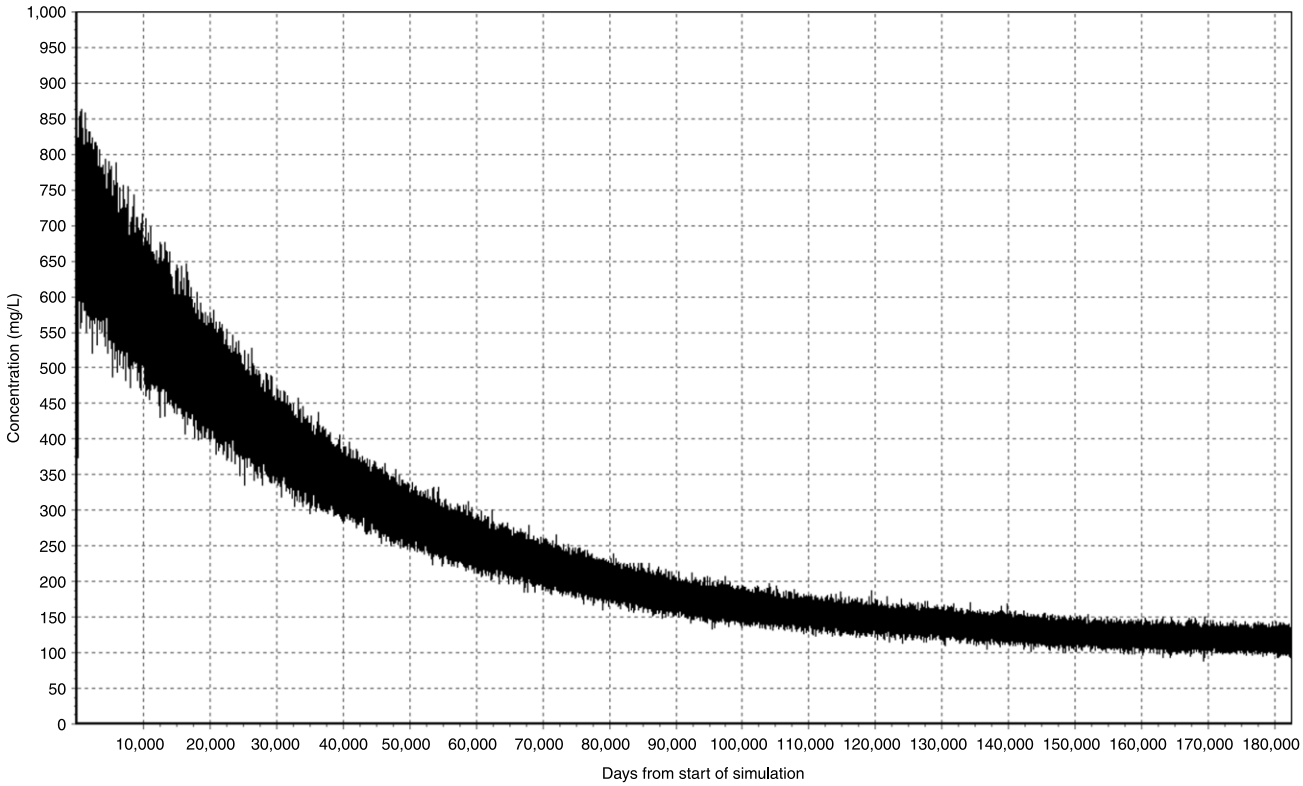

Figure 7 | Predicted sulphate concentration in perched groundwater of Morrison Busty spoil heap over a 500 yr period.

other studies. Some examples include application to contaminated land and to saturated porous medium bioreactors for the treatment of various forms of pollution. The success of POTOMAC in its application to mine spoil heaps vindicates the adoption of an object-oriented approach and suggests that particle tracking codes written in this manner have great future potential for a wide range of hydrogeological and environmental engineering applications.

CONCLUSIONS

POTOMAC is a physically based pollutant transport model which has been developed using the latest object-oriented techniques to produce a computationally fast model capable of simulating the large time scales (on the order of centuries) required to predict the long-term quality of discharges from surface spoil heaps undergoing pyrite oxidation. A particle tracking technique, the "random walk method", is used to simulate the transport of the pyrite oxidation products, ferrous iron and sulfate, and the oxidant, oxygen, while reaction kinetics are included to govern the rate of pyrite and ferrous iron oxidation.

Application of POTOMAC to the Morrison Busty spoil heap in County Durham, UK, has enabled a prediction to be made of the contaminating lifetime of the spoil material and the pattern of pyrite depletion. Results reveal that the spoil heap could remain polluting for many centuries. A knowledge of the expected longevity of contamination is necessary for the planning of remediation strategies for such polluting discharges in order to develop the most efficient treatment system. Therefore, models such as POTOMAC are invaluable for the eradication of polluting discharges from surface spoil heaps.

The OOP techniques used within the design of POTOMAC enable the particle tracking approach to be easily implemented. It also allows for future expansion of the code in order to model additional reactions or easy adaptation to model other systems.

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