

## THE MODELLING OF FLOW AND CHEMICAL REACTIONS IN WASTE PILES

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### ABSTRACT

Software package SULFIDOX (Sulphide ore Oxidation model) has been produced that models flow of air and mineral bearing water within waste mineral piles, together with transport of components undergoing chemical reactions and equilibria, including dissolution or precipitation of mineral phases. The code was developed as a joint project between CSIRO Mathematical & Information Sciences and ANSTO, Managing Mine Wastes Project. The code is based on the general pde package *Fastflo* and is configured as a Toolbox, with a GUI designed ultimately for use by clients such as mining companies. The Toolbox is linked to a powerful local equilibrium model (LEM) previously developed by ANSTO from earlier models.

The key numerical issue is the efficient partitioning of transport and chemical processes, including equilibria.

### NOMENCLATURE

$P^g$	total gas pressure
$p^g$	gas pressure perturbation
$P_{eq}^g$	equilibrium gas pressure
$P_0$	ambient ground gas pressure
$\phi$	total head of liquid phase
$T_0$	ambient temperature
$\theta$	temperature relative to ambient
$\omega_{O}^g$	mass fraction oxygen in gas phase
$\omega_S^s$	mass fraction of reactable sulphur (solid phase)
$\rho^s$	intrinsic density of solid phase
$\rho_0^g$	atmospheric density of gas phase
$\rho^l$	intrinsic density of liquid phase
$g$	acceleration due to gravity
$\mu_g$	viscosity of gas phase
$c^s$	specific heat of solid phase
$c^l$	specific heat of liquid phase
$c^g$	specific heat of gas phase
$D_b^g$	coefficient of diffusion of oxygen in air
$D_h^l$	coefficient of diffusion of solutes in water
$D_h^g$	coefficient of heat conduction for gas phase
$D_h^l$	coefficient of heat conduction for liquid phase
$D_h^s$	coefficient of heat conduction for solid phase

$\beta_g$	mass of oxygen consumed per unit mass of sulphur in the oxidation reaction
$\beta_h$	heat of reaction per unit mass of sulphur
$\omega^i$	mass fraction chemical component no $i$
$R_i$	rate of chemical reaction no $i$
$\nu_{ij}$	stoichiometric coefficient for $j$ -th component in $i$ -th reaction
$M_j$	chemical component no $j$
$K_p$	solubility product of a mineral
$K_i$	formation constant for complex no $i$

### INTRODUCTION

Waste ore piles are susceptible to oxidation of sulphides (e.g. iron pyrites) with the production of sulphuric acid. The acidification can lead to the solubilisation of other trace metals and their transport through the waste pile and into the surrounding environment. There is a need to quantify the environmental impacts of waste ore piles over extended periods of time. Much work has been done in this area but the work described here goes further in that it attempts to combine the modelling of transport processes with chemical reactions, including kinetically controlled ones (slow) and fast chemical equilibria. This paper describes a package – SULFIDOX – designed to model all these processes, together with a graphical user interface (GUI) designed specifically for use by scientists and engineers in this area.

SULFIDOX (Sulphide ore Oxidation model) models flow of air and mineral bearing water within waste mineral piles, together with transport of components undergoing chemical kinetic reactions and chemical equilibria, including dissolution or precipitation of mineral phases. The major chemical process modelled is oxidation of sulphide to sulphuric acid, together with the associated generation and transport of heat. The paper describes the mathematical model used in SULFIDOX to represent the physical and chemical processes, and the numerical algorithms employed to integrate the model through time. The development of the mathematical theory with a description of the physics is presented in a separate document (Stepanyants, 1999). SULFIDOX is a modification of an earlier package FIDHELM (Finite Difference Heap Leaching Model) (Pantelis, 1993) which models the major physical processes involved in the oxidation of mine waste heaps.

The SULFIDOX package is a Toolbox of the commercial software package *Fastflo*, developed by CSIRO Division of Mathematical and Information Sciences. *Fastflo* itself is a general purpose package for solving systems of partial differential equations (pdes) and is based on the finite element method (CSIRO, 1999).

### MATHEMATICAL MODEL

Consider a two-dimensional model of a heap comprised of pyritic ore lying on a relatively impermeable ground surface with sides and upper surfaces which represent the heap/atmosphere interface. The physical model necessarily contains a relatively large number of variables and parameters.

Let  $\mathbf{u}$  denote the vector whose components are the dependent variables to be defined below. The general balance equations for heat and mass transfer in multiphase systems are written in the conservation form

$$\frac{\partial c^i(\mathbf{x}, t, \mathbf{u})}{\partial t} + \nabla \cdot \mathbf{F}^i(\mathbf{x}, t, \mathbf{u}, \nabla \mathbf{u}) = \underline{\sigma}^i(\mathbf{x}, t, \mathbf{u}),$$

$$i = 1, \dots, 5 \quad (1)$$

where  $\underline{\sigma}^i$  is a generic source term and  $\mathbf{F}^i$  usually represents the flux of heat or mass.

For the physical component of the heap oxidation model we have

$$\mathbf{u} = (p^g, \phi, \theta, \omega_O^g, \omega_S^s)^T \quad (2)$$

The five principal physical state variables are defined in the nomenclature section. There are five equations comprising system (1): the first equation describes the gas phase transport; the second equation describes the liquid phase transport; the third equation describes heat flow in the system; the fourth equation describes the transport and consumption of gas phase oxygen; the fifth equation describes the oxidation of solid reactable sulphur.

In the system (1)

$$\mathbf{c} = \begin{pmatrix} 0 \\ 0 \\ \varepsilon^s \rho^s c^s + \varepsilon^l \rho^l c^l + \varepsilon^g \rho^g c^g \\ \varepsilon^g \rho^g \\ \varepsilon^s \rho^s \end{pmatrix}$$

The flux term is written as two components

$$\mathbf{F}^i = \mathbf{U}^i - D^i \nabla u^i, \quad i = 1, \dots, 5$$

where the advective flux is given by

$$\mathbf{U}^i = \begin{pmatrix} \frac{K k_{rg}(\varepsilon^g)}{\mu_g} (\rho^g - \rho_{eq}^g) g e_z \\ 0 \\ (\rho^l c^l \mathbf{q}^l + \rho^g c^g \mathbf{q}^g) \theta \\ \rho^g \mathbf{q}^g \omega_O^g \\ 0 \end{pmatrix}$$

and the diffusivity coefficients are given by

$$D^i = \begin{pmatrix} \frac{K k_{rg}(\varepsilon^g)}{\mu_g} \\ K \\ \varepsilon^s \rho^s D_h^s + \varepsilon^l \rho^l D_h^l + \varepsilon^g \rho^g D_h^g \\ \varepsilon^g \rho^g \Lambda^g(\varepsilon^g) D_b^g \\ 0 \end{pmatrix}$$

The source terms are given by

$$\underline{\sigma} = -(S^g, 0, S^h, -S^g, -S^s)^T$$

The sources  $S^g$  (for gas phase oxygen),  $S^s$  (for reactable sulphur) and  $S^h$  (for oxidation heat) are defined empirically and are directly related (4) to the rate of oxidation of solid phase reactable sulphur.

#### Initial Conditions

The initial conditions are given by

$$\mathbf{u} = \mathbf{u}_0 = (0, \phi_0, 0, \Omega_O^g, \Omega_S^s)^T$$

where  $\phi_0$  is a prescribed initial total head,  $\Omega_O^g$  is the oxygen mass fraction for air and  $\Omega_S^s$  is the initial mass fraction of solid phase sulphur.

#### Boundary Conditions

Boundary conditions for the main physical state variables are stated here.

The gas pressure perturbation  $p^g$  is set to zero on the upper surfaces of the heap (atmospheric pressure); a condition of zero gas phase discharge is imposed at the bottom of the heap (impermeable to gas flow).

The total liquid phase head  $\phi$  is set to a fixed value ( $\phi_0$ ) at the base of the heap; a gradient condition is set on the upper sides consistent with an imposed irrigation rate ( $Q^l$ ).

The relative temperature  $\theta$  is set to zero (ambient) on the upper surfaces of the heap and for the example presented later in this paper an insulating boundary condition is imposed at the base. The user can impose a more general condition here, such as a Newton cooling law.

The gas phase oxygen fraction  $\omega_O^g$  is set to the value appropriate for air on the upper sides of the heap ( $\Omega_O^g$ ). A

condition equivalent to zero flux of oxygen is imposed at the base of the heap (impermeable). No boundary conditions are required for the solid phase sulphur mass fraction  $\omega_s^f$ .

The physical model is driven by the imposed irrigation rate, gravity and the rate of oxidation of reactable sulphur, (supplied as empirical functions of oxygen concentration, mass of reactable sulphur and temperature) and the associated rate of release of heat.

## CLOSURE

The system in the preceding section is closed by a number of formulae which are functions of the dependent variables. We divide these into two sets; (i) constitutive equations which will be regarded as independent of the heap system under consideration and hence are fixed in the model and (ii) empirical relationships which may be modified for each heap system considered and are supplied by the user.

### Constitutive Equations

The gas pressure  $P^g$  is defined by

$$P^g = p_0^g + p^g + p_{eq}^g$$

where  $p_{eq}^g$  is the equilibrium gas pressure and is given by

$$p_{eq}^g = P_0 e^{-gz/(R_0 T_0)}$$

$P_0$  is the ambient ground gas pressure given by

$$P_0 = R \rho_0^g T_0$$

and  $p^g$  is the pressure perturbation. The ambient ground gas density  $\rho_0^g$  and the ambient temperature  $T_0$  are supplied by the user. The equilibrium gas density is given by

$$\rho_{eq}^g = \rho_0^g e^{-gz/(RT_0)}$$

and the gas density given by

$$\rho^g = P^g / (RT)$$

where  $T = T_0 + \theta$ , which defines  $\theta$  as the relative temperature. Here  $R$  is the gas constant for the gas mixture.

By definition the volume fractions must satisfy  $\epsilon_s + \epsilon_l + \epsilon_g = 1$ , and this constraint is incorporated in the model.

The phase specific discharges are given by Darcy's Law

$$\mathbf{q}^\alpha = \frac{K k_{r\alpha}}{\mu_\alpha} (\nabla P^\alpha + \rho^\alpha g \mathbf{e}_z) \quad \alpha = g, l \quad (3)$$

Note:

1) the gas phase specific discharge is calculated from the gas pressure perturbation so that (3) is modified

$$\text{to } \mathbf{q}^g = \frac{K k_{rg}}{\mu_g} (\nabla p^g + (\rho^g - \rho_{eq}^g) g \mathbf{e}_z)$$

the liquid phase specific discharge is calculated from the the total head  $\phi$  rather than the liquid phase pressure  $P_l$ . They are related by  $P^l = \rho_g^l (\phi + z)$ .

## Empirical Relationships

There are a number of empirical formulae which are required to be defined by the user. The SULFIDOX package is designed to give greater flexibility in the choice of these formulae. Some care should be exercised here since they may influence the efficiency of the numerical algorithm.

- The liquid phase volume fraction  $\epsilon^l(P^l, P^g)$  is related to the gas and liquid phase pressure through the relationship  $p^{cap}(\epsilon^l) = P^g - P^l$ , where  $p^{cap}$  is the capillary pressure and is an empirical function of  $\epsilon^l$ . Inversion of this relationship gives  $\epsilon^l(P^l, P^g)$ .
- The relative permeabilities  $k_{r\alpha}$  ( $\alpha = l, g$ ) of the liquid and gas phases need to be supplied as functions of the phase volume fractions. On the basis of Darcy's Law, for  $\alpha = l$  (3) should have the expression  $\mathbf{K} = K k_{rl} / \mu_l$  ( $K$  is the intrinsic permeability) to the immediate left of the bracketed expression. However, the Darcian description of water flow through porous materials such as found in mine waste heaps is still controversial. There is good reason to believe that this relationship will not hold and that the water infiltration through the ore body may depart from the traditional Darcian flow regime (a discussion of this may be found in (Stepanyants, 1999)). In the absence of a more reliable liquid phase transport model we allow the user to specify  $K$  as a function of the liquid volume fraction  $\epsilon^l$  without the restriction just mentioned.
- The sources  $S^g$  (for gas phase oxygen)  $S^s$  (for reactable solid phase sulphur) and  $S^h$  (heat of oxidation) are given by  $S^g = \beta_g S_{max} S$ ,  $S^s = S_{max} S$ ,  $S^h = \beta_h S_{max} S$  (4) where  $S$  is the normalized intrinsic oxidation rate which is supplied as a function of  $\omega_o^g$ ,  $\omega_s^f$  and  $\theta$ , and  $S_{max}$  is the maximum oxidation rate.
- The tortuosity factors  $\Lambda^\alpha$  ( $\alpha = l, g$ ) are supplied as functions of  $\epsilon^\alpha$  ( $\alpha = l, g$ ).

## CHEMISTRY

The system (1) already contains some chemistry through the components oxygen and sulphur, ( $i=4,5$  in (1)). Despite this we shall refer to the model described above as the physical component of the SULFIDOX model. The system is augmented by a module which can include the chemical transport in the liquid phase. This module is meant to be separate from the physical model and is activated by the user if required.

To distinguish between the physical and chemical components we augment the dependent variable vector

$$\mathbf{u} = (\mathbf{u}_{phys}, \mathbf{u}_{chem})^T \quad (5)$$

where  $\mathbf{u}_{phys}$  is given by (2) and

$$\mathbf{u}_{chem} = (\omega_1^l, \dots, \omega_N^l)^T$$

where  $\omega^1, \dots, \omega^N$  denote the mass fractions of the  $N$  chemical components which may exist in the liquid phase. A set of chemical components is a minimal basis for representation of all dissolved chemical species in a system. The basis is not uniquely defined. Two conventions are commonly used: (1) a component is the total concentration of all liquid phase species involving a given element, or (2) a component is taken to be a master species representative of the element. The second convention is used in the LEM module. Individual species concentrations can be determined from the mass action equilibria for the liquid phase.

The system (1) is augmented with the system defined by

$$c^i = \epsilon^i \rho^l, \quad \mathbf{U}^i = \rho^l \mathbf{q}^i u^i, \quad D^i = \epsilon^i \rho^l \Lambda^i D_b^i, \\ i = 6, \dots, N-5 \quad (6)$$

The extra equations describe the transport of each of the  $N$  components by advection and diffusion processes, in addition to the concomitant chemical reactions. The  $\sigma^i$  ( $i=6, \dots, N-5$ ) are sources describing the reaction kinetics. The initial conditions are denoted

$$\omega_i^l = \Omega_i^l, \quad t = 0$$

where the  $\Omega_i^l$  are user supplied. These values are also used as boundary values on the upper sides of the heap; in addition, zero flux conditions are imposed at the base of the heap.

If the  $N$  components are involved in  $M$  reactions then there will exist  $M$  rate terms  $R_i$  ( $i=1, 2, \dots, M$ ). In terms of the generic source term defined above we have for  $j = 1, \dots, N$

$$\sigma^{5+j} = \sum_{i=1}^M v_{ij} R_i \quad (7)$$

where  $v_{ij}$  represents the stoichiometric coefficients for the  $j$ -th component in the  $i$ -th reaction.

The user must supply the stoichiometric coefficients  $v_{ij}$  along with  $R_i$  ( $i=1, 2, \dots, M$ ) as functions of the variables  $\mathbf{u}^l$ , i.e.  $R_i$  can be expressed as an explicit function of the physical and chemical variables defined in the solution vector  $\mathbf{u}$  defined by (5). Since the components are quantified by mass fractions the dimensions of the right hand side of (7) must be  $\text{kg m}^{-3} \text{s}^{-1}$ .

#### Local Chemical Kinetics

Consider the  $i=1, \dots, M$  stoichiometric reactions involving  $N$  chemical components,  $M_j$  ( $j=1, 2, \dots, N$ )

$$\sum_j v_{ij} M_j = 0$$

where  $v_{ij}$  are the stoichiometric coefficients for the  $j$ -th component in the  $i$ -th reaction. The rates  $R_i$  for each reaction is given by (no summation on repeated indices)

$$R_i = \frac{1}{v_{ij}} \frac{d[M_j]}{dt}$$

Observation suggests the rate law

$$R_i = k_i \prod_{j=1}^N [M_j]^{\gamma_{ij}} \quad (8)$$

where the coefficients  $k_i$  and the exponents  $\gamma_{ij}$  are determined by experiment. In SULFIDOX one may supply

a formula for the  $R_i$  which may differ from (8). In the chemistry literature the  $[M_j]$  are usually expressed in dimensional units involving moles. However, in the transport equations the components are quantified by mass fractions (i.e. mass of component per mass of phase medium). The  $R_i$  must be supplied in dimensions consistent with those described in the previous section.

Having defined the local chemistry the SULFIDOX formulation incorporates the  $N$  chemical components in  $N$  transport equations as outlined in the previous subsection.

In the current version of SULFIDOX there are  $N=5$  components assumed and  $M=3$  reactions. These limits will be extended in later versions.

#### LOCAL EQUILIBRIUM MODEL

In addition to the chemical model described in the preceding section the SULFIDOX model contains a complete LEM package, MODPHRQ, a geochemical speciation program developed at ANSTO. MODPHRQ is based on HARPHRQ (Brown et al, 1991), a program developed at the Harwell Laboratory, UKAEA; HARPHRQ was itself developed from the U.S. Geological Survey code PHREEQE. MODPHRQ is a very advanced geochemical speciation program; it is coded in FORTRAN.

MODPHRQ has been incorporated into the *Fastflo* Toolbox SULFIDOX by means of special interfacing routines. This enables the individual speciation of each chemical component in the aqueous phase to be tracked in every cell (finite element) through every time step. In the absence of precipitation or dissolution of chemically related mineral phases the component concentrations are conserved.

For modelling purposes the details of individual speciation are not intrinsically significant. The main reason for including the LEM capability in SULFIDOX is to track changes in component concentrations due to precipitation and dissolution of related mineral phases. Thus in addition to the above  $N$  chemical components suppose there are  $N_S$  mineral phases and  $N_H$  heterogeneous equilibria of the form.

$$\sum_{j=1}^J b_{pj} \log(a_j) \leq \log(K_p) \quad (9)$$

for each mineral phase  $p$  ( $1$  to  $N_g$ ). Here  $a_j$  is the chemical activity of the  $j$ -th species involved,  $b_{pj}$  is the associated coefficient and  $K_p$  is the solubility product. If the mineral phase is present equality applies in (9), otherwise inequality (solution undersaturated with respect to this phase). In addition there will be a set of liquid phase equilibria of the type

$$\log(a_i) = \log(K_i) + \sum_{j=1}^J c_{ij} \cdot \log(a_j) \quad (10)$$

one for each associated complex, where  $K_i$  is the formation constant of the  $i$ -th such complex.

Given a set of component values for a cell the attached LEM module will calculate all the species concentrations as well as quantities of mineral phases precipitated or

dissolved (mass of mineral per mass of liquid phase). The LEM module has finite mineral accounting, i.e. the mineral is not assumed to have an infinite supply. The LEM module thus requires the starting quantities of the mineral phases present. It is possible for a mineral to be exhausted, i.e. fully dissolved. The speciation and mineral accounting is done by solving a set of nonlinear equations with constraints: these include the equilibria expressions (9) and (10), as well as mass balance equations and charge balance. The equation set also includes the nonlinear relationship between species activity and concentration. These numerical routines are now highly developed and efficient. The details will not be described here; interested readers should refer to Brown et al (1991) and references cited therein.

The speciation and mineral accounting computation is done for every cell at every time step: to do this component values and the current quantity of each mineral phase in each cell are stored in memory.

To reduce the computational burden MODPHRQ requires that a list of potential mineral phases be nominated, together with the starting quantities. As a preliminary task MODPHRQ constructs from a full thermodynamic database a condensed data set for just the relevant species and phases.

## NUMERICAL METHOD

The augmented system equations (1) plus (6) are solved over the heap domain by stepping through time in a segregated manner (sequential iteration approach). This is virtually obligatory: it is computationally unfeasible to solve these equations in a fully coupled manner. The sequential iteration approach is widely used in hydrogeochemical models (Yeh and Tripathi, 1989). The sequential iteration method readily allows coupling to the LEM module. The cost per step is also relatively low. The obvious disadvantages of the sequential method is that we can expect a strict limit on time step for numerical stability; in practice we have found this to be not too onerous.

Within each time step the principal state variables are updated one at a time. Because the variables are coupled by a variety of terms it is necessary to do this within an iterative loop, which is repeated until a convergence criterion is satisfied. This also takes account of the nonlinearity of the equation set. Within the inner loop time derivatives are represented by second order accurate difference expressions (Crank-Nicolson method).

The sequential iteration method can be described as follows.

*Initiate*

*Advance to next time level*

*loop until convergence:*

update  $p^g$

update  $w_O^g$

update  $\theta$

update  $w_S^s$

update  $\phi$

update of chemical component concentrations

*end loop*

*adjust* chemical component values by running LEM

The LEM procedure appears numerically as a source/sink of chemical components at every time step. It thus has the potential to affect both the accuracy and the numerical stability of the segregated time-stepping scheme. Strictly, the update to the component values caused by the LEM should be incorporated within the inner loop, but this is computationally costly. It is common practice to do the LEM only once per time step at the cost of some loss of accuracy, and we follow this practice.

Aside from the LEM problem, there is a trade-off between time step and the inner iterative loop. If the time step is too large convergence of the inner loop will become too slow or fail altogether. Typically one seeks to have the inner loop converge in less than 15 iterations.

The sequential iteration algorithm is readily coded in the Fasttalk language, including the assembly of the PDEs and specification of the boundary conditions.

## GRAPHICAL USER INTERFACE

SULFIDOX comes equipped with a GUI designed to assist the user with setting up runs. There are a large number of physical parameters to be specified for the model, but most of these are fixed, the remainder have sensible default values assigned. The parameters usually needing to be set by the user are as follows.

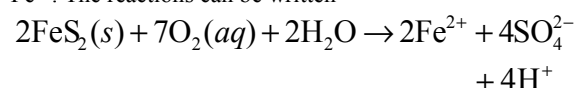
1. Run control parameters
2. Specification of  $K$  as a function of the liquid volume fraction  $\epsilon^l$
3. Specification of rates of chemical reactions as arbitrary algebraic functions of component concentrations
4. Selection of mineral phases from a database

The expressions for the chemical reaction rates can be entered using 'chemical' names, rather than the internal *Fastflo* vector stack references.

The other major input required from the user is a specification of the domain representing the waste pile. This is entered as an ordered list of boundary line segments, in standard *Fastflo* style, usually from a pre-prepared file.

## EXAMPLE

An example simulation is briefly described here. The physical model is as described above. In addition, two kinetically controlled chemical reactions are included, representing oxidation of iron pyrites (solid phase) to dissolved  $\text{Fe}^{2+}$ , and further oxidation of  $\text{Fe}^{2+}$  to dissolved  $\text{Fe}^{3+}$ . The reactions can be written



The two processes lead to net consumption of oxygen and production of  $\text{H}^+$ , i.e. an increase in acidity. The chemical components are  $\text{Fe}^{3+}$ ,  $\text{Fe}^{2+}$ ,  $\text{H}^+$  and  $\text{SO}_4^{2-}$ . The first reaction proceeds at a rate essentially that of the overall sulphide oxidation rate (proportional to  $S$ ). The second reaction is

modelled as first order in  $[O_2(aq)]$  and second order in  $[H^+]$ . No fast equilibria are modelled in this example and the LEM module is not used.

The heap geometry is modelled in two dimensions (vertical slice) as a symmetrical trapezoid as shown in the figures below. The base of the heap is 100 m and the height is 20 m. For this example a fairly coarse mesh of 400 nodes and 718 linear triangular elements has been used. The simulation is taken over a 6 month period using a fixed time step of a thousandth of a year for a total of 500 steps. Within each time step the nonlinear iteration achieves convergence in 3-4 iterations for the great majority of the simulation; up to 11 iterations are needed in the early phase.

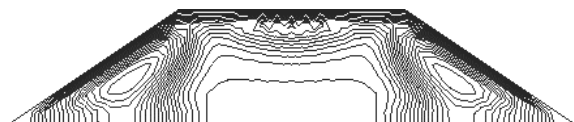
After 6 months the system has settled to a pseudo steady state. We briefly describe the main features of this state.

Figure 1 shows a contour diagram for the mass fraction of oxygen in the gas phase. Clearly oxygen diffuses in from the upper boundaries of the heap and is consumed in the interior by oxidation of reactable sulphur. The mass fraction ranges from 0.22 on the upper boundaries to essentially zero in the interior.



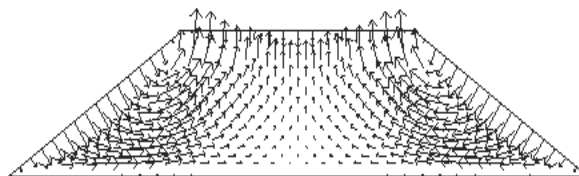
**Figure 1:** Contour diagram of mass fraction of oxygen in gas phase. Contour interval is 5% of total range (0 to 0.22).

Figure 2 shows the corresponding diagram for temperature. There are two maxima, one in each of the tapered sections of the heap. These peaks correspond to the regions of peak oxidation rate. The maximum temperature in the heap is 2.6 °K above ambient. High concentrations of  $H^+$  and dissolved Fe (not shown here) also occur in these high temperature regions. There is also a shallow maximum (1.3 °K above ambient) of temperature in the central top region.



**Figure 2:** Contour diagram of temperature. Contour interval is 5% of total range (0 to 2.6 °K above ambient).

The gas phase velocity is shown in an arrow diagram in Figure 3. Air penetrates the heap through the side walls and escapes through the top with two convection plumes at either end, associated with the regions of peak heat production. Maximum velocity is  $8.6 \times 10^{-6} \text{ m s}^{-1}$ .



**Figure 3:** Arrow diagram for gas phase velocity. Maximum velocity is  $8.6 \times 10^{-6} \text{ m s}^{-1}$ .

## CONCLUSION

The SULFIDOX package is as versatile package for modelling a wide variety of physico-chemical processes important to the simulation of acidification and leaching of heavy metal species from waste ore heaps. The package is computationally efficient and is equipped with an appropriate GUI targeted to the mine waste management community. The *Fastflo* environment has enabled this powerful and flexible package to be assembled with relative ease, including the incorporation of the advanced LEM MODPHRQ.

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