COUPLED NATURAL CONVECTION AND ATMOSPHERIC WIND FORCED ADVECTION IN ABOVE GROUND REACTING HEAPS

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ABSTRACT

A CFD code CFX-4.1 has been employed to simulate a flow and pressure field around an above ground heap. Due to porosity of the heap material a wind driven forced gas advection field within the heap will result. If the heap material contains oxidizable material as in mine wastes and coal stockpiles, then natural convection induced by heat of oxidation will also occur. Here we attempt to couple the CFD wind flow model with a model which simulates the heat and mass transfer within heaps containing oxidizable material. This study shows that even under relatively moderate wind flows the traditional assumption that the heaps are immersed in a static atmosphere becomes questionable.

1. INTRODUCTION

Above ground mine waste heaps and coal stockpiles can contain material which when exposed to the atmosphere undergo oxidation. In the case of mine wastes oxidation of sulphidic ores results in the release of heavy metals which are ultimately leached into the environment. The oxidation reaction releases heat resulting in increases in temperatures within the heaps or stockpiles. Temperatures can become sufficiently high as to cause combustion of coal stockpiles.

Oxidation is initiated as atmospheric oxygen enters the heap from the atmosphere/heap interface by the process of molecular diffusion. At this time, the oxidation reactions are confined to the surface layers of the heap and the removal of oxygen from the gas phase and the heat released from the oxidation reaction will cause small changes in the gas density within the heap. This in turn will induce a convective air current within the heap and in so doing could significantly increase the rate of atmospheric oxygen transport into the heap and the global oxidation of the heap.

Earlier models (Pantelis and Ritchie, 1991; 1992) focussed on the processes of natural convection in heaps as a result of the oxidation of sulphides. These models were based on the assumption that the heaps are immersed in a static atmosphere. It is becoming apparent now that a moderate wind flowing over the heap can set up pressure gradients which are of the order of those associated with natural convection. Thus wind induced forced gas advection within the heaps will have a significant effect on the overall flow field within the heap. In this study we shall attempt to couple the model of heap oxidation with a CFD model for the wind flow over the heap.

2. MATHEMATICAL MODEL

2.1 Heap Interior

The interior of the heap is a multiphase system. If each α-phase ($\alpha = g, l, s$) is comprised of N_α species, and ω_i^α ($i = 1, ..., N$) represents the mass fraction of the species i in the α-phase, then the mass balance for each of the species $i = 1, ..., N_\alpha$ is given by

$$\frac{\partial \rho_\alpha \omega_i^\alpha}{\partial t} + \nabla \cdot \vec{F}_i^\alpha = -S_i^\alpha, \quad \alpha = g, l, s \quad (1)$$

where S_i^α is the consumption rate of the species i in the α-phase, ρ_α is the bulk density of the α-phase and is related to the intrinsic density ρ^α by $\rho_\alpha = \epsilon_\alpha \rho^\alpha$ where ϵ_α is the volume fraction of the α-phase. The species mass flux $\vec{F}_i^\alpha$ is given by

$$\vec{F}_i^\alpha = \rho_\alpha \vec{v}^\alpha \omega_i^\alpha - \rho_\alpha D_i^\alpha \nabla \omega_i^\alpha, \quad \alpha = g, l \quad (2)$$

where we set $\vec{F}_i^s = 0$. Here D_i^α represents the effective diffusion coefficient for the species i through the α-phase (dispersion is omitted) and $\vec{v}^\alpha$ is the Darcian velocity of the α-phase.

If we sum (1) over the species we obtain the mass balance equations for each phase

$$\frac{\partial \rho_\alpha}{\partial t} + \nabla \cdot (\rho_\alpha \vec{v}^\alpha) = \sum_i S_i^\alpha, \quad \alpha = g, l, s \quad (3)$$

where we assume a rigid solid phase (i.e. $\vec{v}^s = 0$). For the gas and liquid phases the phase velocity $\vec{v}^\alpha$, is related to the phase specific discharge by $\vec{q}^\alpha = \epsilon_\alpha \vec{v}^\alpha$ which is described by Darcy's Law

$$\vec{q}^\alpha = -\frac{K_\alpha(\epsilon_\alpha)}{\mu_\alpha}[\nabla P^\alpha + \rho^\alpha g \vec{e}_z] \quad \alpha = g, l \quad (4)$$

where P^α is the pressure of the α-phase, K_α is the permeability of the α-phase which is a function of the volume fraction of that phase and $\vec{e}_z$ is the unit vector in the vertical.

Assuming that locally the phases are at thermodynamic equilibrium we write the heat equation as

$$\sum_\alpha \frac{\partial}{\partial t}[\rho_\alpha c^\alpha T] + \sum_\alpha \nabla \cdot \vec{F}_h^\alpha = S_h \quad (5)$$

where T is the temperature, c^α is the specific heat capacity of the α-phase and S_h is the heat source/sink term. The phase heat flux $\vec{F}_h^\alpha$ is given by

$$\vec{F}_h^\alpha = \rho_\alpha c^\alpha \vec{v}^\alpha T - \rho_\alpha D_h^\alpha \nabla T \quad (6)$$

where D_h^α is the coefficient of heat conduction of the α-phase.

The system of equations (1)-(6) are supplemented by the following identities:

$$\sum_{1 \le i \le N_\alpha} \omega_i^\alpha = 1, \quad \sum_{\alpha = g,l,s} \epsilon_\alpha = 1 \quad (7)$$

For the gas phase we assume the ideal gas law

$$P_i^g = R_i \rho_i^g T, \qquad 1 \le i \le N_g \quad (8)$$

where P_i^g is the partial pressure, R_i is the gas constant and ρ_i^g is the density of the species i in the gas phase. By definition $\omega_i^g = \rho_i^g / \rho^g$. The gas phase pressure P^g is given by

$$P^g = \sum_{1 \le i \le N_g} P_i^g \quad (9)$$

The above system of equations are further supplemented with empirical formulae for the source terms and appropriate boundary conditions. The solution method is based upon finite differences and the details follow similar lines to those outlined in Pantelis and Ritchie (1991; 1992).

0.1 Atmospheric Wind Flow

The atmospheric wind flow calculations were performed using the multi-purpose CFD code CFX-4.1 which is developed and marketed by CFDS, Harwell Laboratory (CFX-Release 4.1, 1995). The model domain around the heap can be easily fitted into a computational grid, on which discrete values of the velocity, pressure etc. are calculated. The code solves the basic set of equations for conservation of mass and momentum and, in a non-isothermal flow energy, which are called the Navier Stokes equations. The code uses a non-staggered grid to solve the equations of turbulent flow in complex geometries.

The problem is solved by finding the steady-state, incompressible, turbulent flow around the heap. The turbulence model of k-ϵ was chosen, together with log-law wall functions. This choice of turbulence model was made because it has been proved to be successful when applied to a wide range of engineering flows and in establishing the pressure distribution around a building (McCaughey and Fletcher, 1993) which is very similar to this type of problem.

A typical heap with a height of 20 m and 100 m in horizontal base length was considered. The sides of the heap have a slope of 30 degrees in towards the centre of the heap. The heap was located within a computational region which was 800x520 m. On the left hand side of the flow domain, the inlet velocity was specified as the inlet boundary condition. On the right hand side of the flow domain, the pressure gradient was set to zero. At the top of the flow domain, the constant velocity boundary condition was used (far field wind velocity). Continuity of mass flux of gas across the atmosphere/heap interface is a required condition. However, given that the gas flow in the heap is orders of magnitude smaller relative to the gas flow in the atmosphere, we assume that the impact of the flow field in the heap is very small on the atmospheric wind flow. Therefore, a no slip boundary condition along the atmosphere/heap interface was chosen when solving for the wind flow over the heap. As a consequence of this assumption the calculations of the wind flow model and heap interior were executed separately. The outlet boundary condition was applied sufficiently far downstream (500 m) such that the flow has become fully developed. The density and viscosity of the fluid were set to the values of 1.242 $kg\ m^{-3}$ and $1.77 \times 10^{-5}\ Ns\ m^{-2}$, respectively; these being typical values of air.

The computational grid was generated by splitting the flow domain into five blocks with each block containing 50 x 50 cells. The cell sizes were chosen in such a way that the cells were sufficiently close to the block and so that the cell sizes expand smoothly away from the block with a geometrical progression with a ratio 1.2.

The equations of mass and momentum conservation, together with the equations for turbulent kinetic energy and the dissipation rate, were solved using an iterative method. The SIMPLEC method was used to perform the pressure correction calculations. All physical equations were solved using Stone's method with an under-relaxation factor set to 0.2.

Calculations were performed for a typical case with the wind velocity of 10 $km\ h^{-1}$. The main requirement is the knowledge of the distribution of the pressure perturbation around the heap and the pressure distribution obtained is shown in Figure 1. The figure shows the high pressure on the front face of the heap where the air flow is brought to rest. The pressure becomes negative on top of the heap where the flow is directed and then levels off at a small negative value in the recirculation region. The pressure distribution obtained in this case shows a large similarity with the pressure distribution obtained experimentally and computationally around a model building (McCaughey and Fletcher, 1993).

3. CASE STUDY

The heap material is assumed to have an intrinsic permeability of $10^{-8}m^2$, which is high for typical mine waste heaps but possibly approaching those of some coal stockpiles. For heaps comprised of mine wastes the intrinsic oxidation rate (IOR), under fully oxygenated conditions, are typically of the order of $10^{-8}kg(sulphur)m^{-3}s^{-1}$ whereas in bio-oxidation heaps where the winning of metals is the goal the IOR can be as high as $10^{-6}kg(sulphur)m^{-3}s^{-1}$. For this study we use a maximum IOR of $10^{-6}kg(sulphur)m^{-3}s^{-1}$. In mine wastes the presence of microorganisms are involved as catalysts for the oxidation of the sulphides

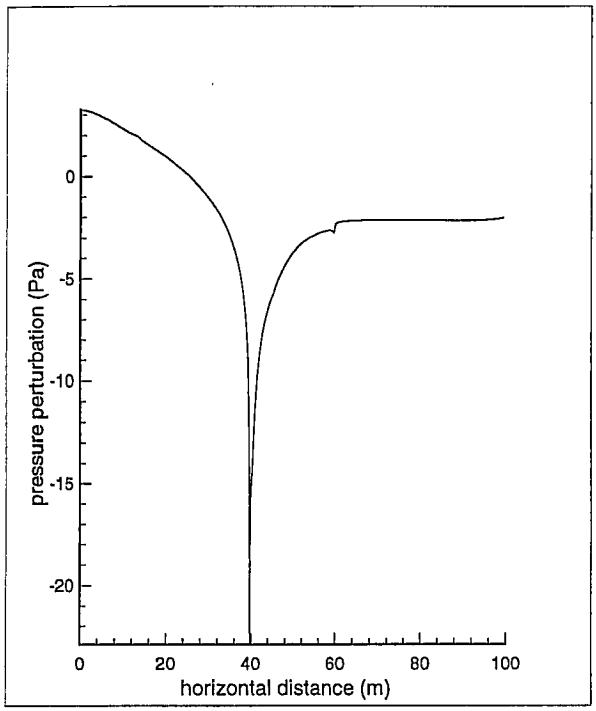

Figure 1: The pressure perturbation along the atmosphere/heap interface as a result of a wind flow over the heap of wind velocity 10 $km\ h^{-1}$. The heap is 20 m in height and 100 m in horizontal base length. The sides of the heap have a slope of 30 degrees in towards the centre of the heap.

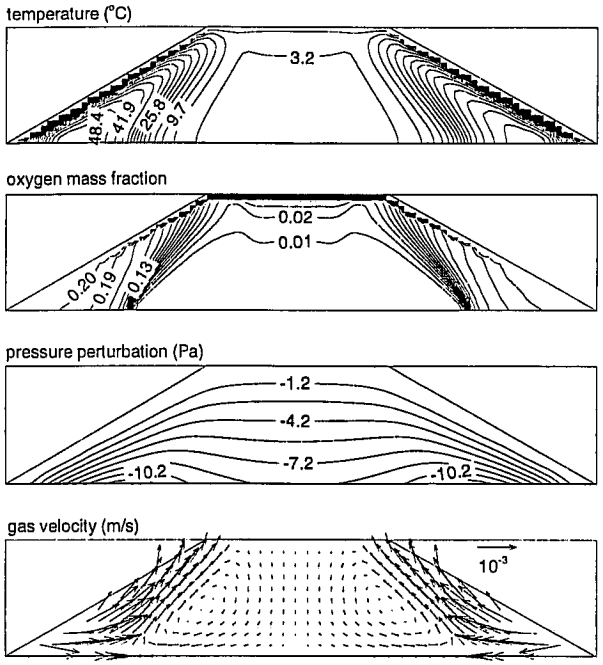

Figure 2: Contours for the oxygen mass fraction, temperature, gas pressure and the gas velocity vector field in an oxidizing heap at 1/5 year. The heap is 20 m in height and 100 m in horizontal base length. The sides of the heap have a slope of 30 degrees in towards the centre of the heap.

up to some temperature ceiling. In this study we shall deliberately ignore this temperature ceiling in order that some similarities can be drawn with coal stockpiles. The latter are predominantly associated with the oxidation of carbonaceous material, however, we note that the IOR may be different to that associated with sulphidic material.

The first simulation of the heap interior was run for a time of 1/5 year which is sufficient time to observe the typical long term behaviour of the gas flow field. Static equilibrium atmospheric conditions are assumed (no wind). Figure 2 shows the contours for the oxygen mass fraction, the temperature, the sulphur oxidation rate and the gas flow fields within the heap at 1/5 year. We see that with the relatively high IOR used here the oxygen cannot penetrate well into the heap from the upper surface where diffusion is the dominant oxygen transport mechanism. Penetration of oxygen into the heap is greater at the sides where gas advection is significant. Gas entering the sides of the heap by natural convection are associated with velocities of the order of $10^{-3} m\ s^{-1}$. What is important to note here is the symmetry of the pressure and gas flow fields about the axis of the heap.

In the second case study we assume the same geometry but ignore any oxidation or heat generated within the heap. We now assume that a prevailing wind of mean velocity of 10 $km\ hr^{-1}$ flows over the heap in the direction of the positive x-axis as described in the previous section.

The pressure distribution arising from the wind flow over the heap sets up a gas flow within the heap as shown in Figure 3. Clearly the pressure field is asymmetric about the axis of the heap. The gas velocity vector field

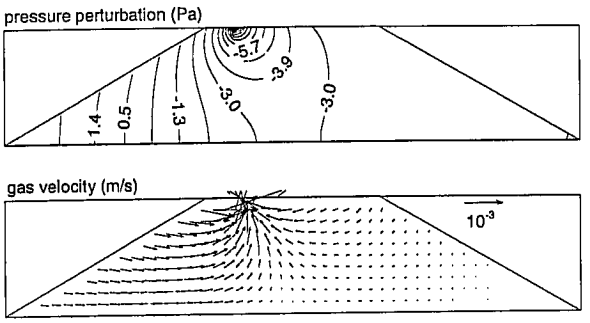

Figure 3: Contours for the gas pressure and the gas velocity vector field in the heap where no oxidation is occurring and a prevailing wind flow exists over the heap with an average speed of 10 $km\ hr^{-1}$ in the direction left to right. The heap is 20 m in height and 100 m in horizontal base length. The sides of the heap have a slope of 30 degrees in towards the centre of the heap.

is shown and typical gas velocities are of the order of $10^{-3} m\ s^{-1}$.

We now examine the situation of a prevailing wind over the heap in combination with internal heat generated by oxidation. The heap parameters are identical to Case 1 with the wind pressure distribution of Figure 1 imposed across the atmosphere/heap interface. The initial gas pressure perturbation within the heap is obtained from the steady state solution of the previous simulation. Figure 4 shows the asymmetry of the contours due to a prevailing wind over the heap at 1/5 year.

The gas velocity field is noticeably different from those of Case 2 although the magnitudes of the velocities are of the same order of magnitude. This is a clear illustration of how natural convection and externally wind driven advection can combine to form a composite flow pattern distinct in appearance from those that appear when the processes act individually. The gas pressure perturbation, oxygen and temperature contours display a clear asymmetry about the heap axis.

It is also instructive to observe the evolution of maximum temperatures in the heaps. Figure 5 shows that the maximum temper-

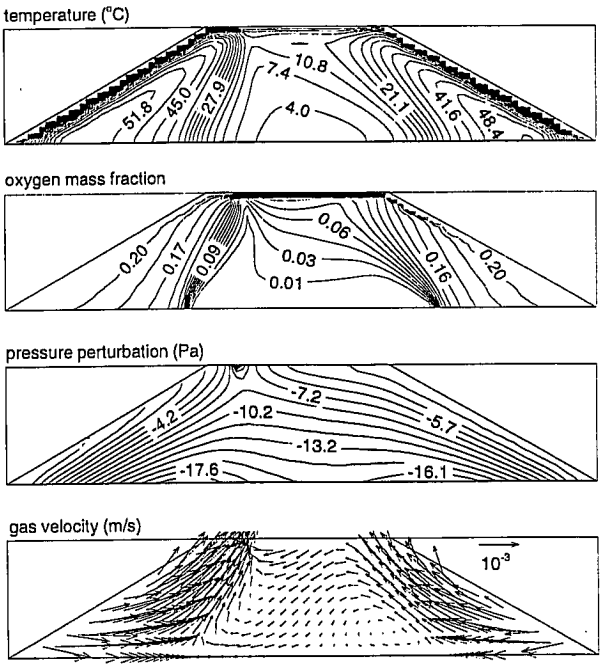

Figure 4: Contours for the oxygen mass fraction, temperature, gas pressure and the gas velocity field in the heap at 1/5 year. A prevailing wind flows over the heap of average speed of 10 $km\ hr^{-1}$ in the direction left to right. The heap is 20 m in height and 100 m in horizontal base length. The sides of the heap have a slope of 30 degrees in towards the centre of the heap.

atures are higher when wind flows are involved. A series of simulations were also carried out using the lower intrinsic permeability of $10^{-9}\ m^2$. The general temperature and flow fields display similar patterns to those presented here for the higher permeability. Figure 5 also shows that the differences in the maximum temperatures are significantly magnified at this lower permeability although their magnitudes are lower. The temperatures involved for the higher permeability case clearly exceed the temperature ceiling associated with the oxidation of sulphides. The simulations do demonstrate, however, that for reactions not involving a temperature ceiling the temperatures can rise unchecked with a greater rate when wind flows are involved.

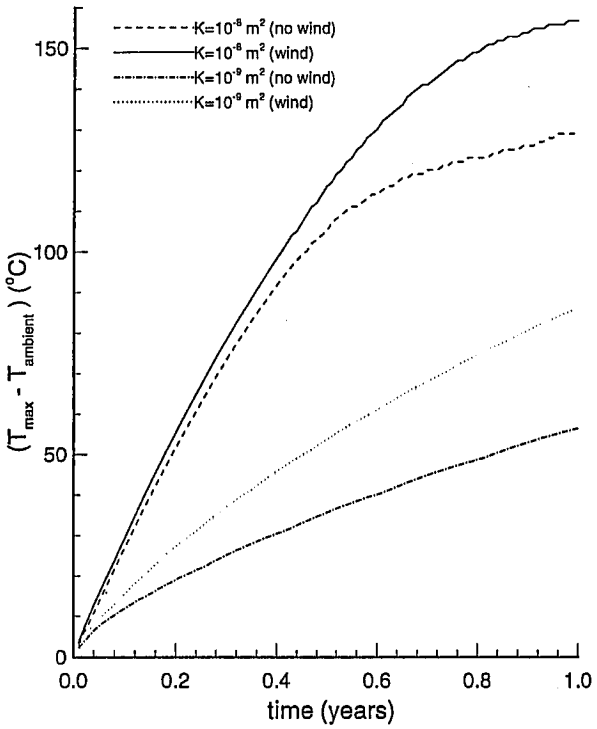

Figure 5: Evolution of maximum temperatures in heaps under no wind and wind conditions for two intrinsic permeabilities, $K = 10^{-8}$ and $K = 10^{-9}\ m^2$.

4. CONCLUSION

This study suggests that the models attempting to simulate heat and mass transfer in above ground mine waste heaps or coal stockpiles should take into account the external nonequilibrium atmospheric conditions. Thus any model describing the internal mechanisms of the heap should be coupled to a CFD model to simulate the atmospheric flow field around the heap. We have demonstrated by simulation that the pressure gradients on the atmosphere/heap interface induced by a relatively moderate wind can be of the order of magnitude as the pressure perturbation associated with natural convection.

The simulations presented here are rather more associated with the oxidation of mine waste heaps than coal stockpiles. In the latter heat generated by oxidation of the carbonaceous material could raise temperatures to sufficiently high enough values to initiate combustion of the coal itself. The coupled model presented here could explain the initiating period leading to the combustion of coal stockpiles in cases where natural convection is insufficient to raise the temperatures required for combustion.

The coupling of the CFD and the interior heap model has been simplified here and only a steady state wind flow was considered. Future simulations should take into account the transient atmospheric conditions and a more detailed coupling of the models should be examined. Therefore efforts should be continued to reduce the numerical intensity of the CFD models, especially if the nonsteady wind flows are to be modelled.

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