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COMPUTATIONAL MODELLING OF REACTIVE MULTIPHASE FLOWS IN HYDROMETALLURGICAL PROCESSES

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ABSTRACT

This paper describes the development of a 3D modelling environment for the treatment of complex multiphase reactive transport in porous media. The principle application has been in hydrometallurgy, the analysis of heap leaching as a tool for recovering metals such as copper and gold from primary ores, although the techniques are also relevant to processes such as in situ leaching and pressurized leaching, and environmental problems such acid mine drainage and water treatment. These processes offer considerable challenges in the development of effective computational models due to the wide range of physical phenomena present. These phenomena include a series of interacting physico-chemical processes, including, in stockpile leaching, the transport of a leaching solution and air through the porous stockpile, a sequence of highly inter-dependent gas-liquid-solid reactions, the impact of the bacterial population as a catalyst of the reaction sequence, and the generation and transport of thermal energy.

Typically such problems concern large heaps (width and depth of hundreds of meters) of low grade ore reacting over timescales that may, particularly in the case of acid drainage, be measured in years. Even experimental tests, such as the commonly used column leach tests, can take months or even years to complete. This means that it is very difficult to evaluate the impact of process design and control systems on the operation of the heap in a reliable fashion. Computational modelling of such processes offers the possibility of carrying out large numbers of tests in a comparatively insignificant time, and, although it can never completely remove the need to carry out some physical experiments for the purposes of calibration, can hugely reduce the cost. In addition by modelling whole or large sections of heaps phenomena can be studied that do not occur in the laboratory.

The model builds on existing computational fluid dynamics techniques to provide a comprehensive set of tools for modeling the full set of physical phenomena present in these systems. It incorporates a number of algorithms including

- Variably saturated flow models using a variation of Richard’s equation.
- Transport of multiple chemical species

- Chemical reactions in different phases and mass transport between those phases, including oxygen consumption, water evaporation and condensation, precipitation and dissolution of various salts, and dissolution reactions between the active leaching agents and the mineral substrate.
- Shrinking core models to allow for the effect of diffusion and mineral consumption over time for multiple soluble species and multiple particle size classes
- Growth, death and transport of lithotropic bacteria, and their catalytic effects on key chemical processes in sulphide leaching.
- A comprehensive heat balance allowing for heat generation and consumption through reactive chemistry, evaporation and condensation, and external boundary conditions including prevailing weather and time of day.

Unsurprisingly, a large number of parameters are required to accurately represent the complex physics involved in reactive transport, and so parameter estimation and validation are key issues. A sophisticated optimization procedure has been developed to estimate model parameters against laboratory column data. This procedure is embedded within a software tool and used to determine key model parameters and evaluate their sensitivity against experimental data. The validation procedure for this complex model is then described.

Finally, since the computational model can be applied to complex 3D geometries representing full scale heaps, a careful case study will demonstrate how the model is applied in the analysis of industrial scale heaps.