

the sample mass (or sample volume) is large enough to represent the original site (the local segment being sampled); (3) whether assay portion is prepared well enough to depict the initial sample. Sample numbers are dictated by the confidence level, the variance of population and the acceptable estimation error as well as the homogeneity and the spatial continuity of population. For a homogeneous  $\sqrt{2}S_2/\sqrt{2}\alpha$  population, sample numbers can be calculated by the formula:  $n=Z/2$  the function of Normal  $\alpha$  (where  $n$  represents the sample number required;  $Z$ , distribution for given confidence level;  $S_2$ , the variance of samples; and  $r$ , the estimation error). Sample mass depends on the grain size of the sample, the heterogeneity constant of the material of interest and the fundamental variance. It can be calculated by the formula:  $M=C*d^3/s^2$  (where  $M$  represents the sample mass required;  $C$ , the heterogeneity constant of the material of interest;  $d$ , the grain size of the coarsest top 5% of the sample;  $s$ , the fundamental error of sampling). In order to minimize the sample preparation errors, designing and implementing a good sample preparation procedure is very important, which includes employing suitable equipment and responsible personnel. A case study has been conducted using the geochemical data of the gold mine tailings related to acid rock drainage in the Witwatersrand Basin, South Africa, and the results indicate that if sampling much more than necessary, we would waste the costly resources and if sampling fewer than required, we would get an incorrect conclusion. Thanks are given to the Water Research Commission (WRC) in South Africa for funding this project (WRC Project Number 1624) and giving permission to publish the results.

**Key words** geochemical sampling; environmental risk assessment; sample number; sample mass; sample preparation error

## Chemical origin of acid mine drainage and its computer simulation with Phreeqc—A case study of Zibo coal mining district

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Research on the origin of acid mine drainage (AMD) is helpful to find a way to avoid and remediate AMD and its pollution. AMD is mainly from pyrite (FeS<sub>2</sub>)-containing minerals (such as coal and ore) during mining process and reproduction, and is common and dangerous to water environment in the world. The results of research showed that ions of calcium and magnesium in AMD came mainly from calcite and dolomite. To my knowledge, other sources (such as chlorite) for the ions and their chemical origin were not studied. In this paper, the AMD in the Zibo coal-mining district as a case, its chemical characteristics and its origin were determined. And based on the analysis of the regional geological conditions, Phreeqc was used to stimulate the AMD's chemical origin. The results showed that acidification and neutralization are two processes, and the characteristics depended upon chemical reactions that occurred in the two processes. In the AMD, sulfate ion came from FeS<sub>2</sub> and is an indicator of acid process, and ions of calcium and magnesium originated from calcite and chlorite and were indicators of neutral process. Dissolved silica (SiO<sub>2</sub>) was rich in the AMD, and it is a specific characteristic feature of the AMD in the Zibo coal mining district, for chlorite was involved in its origin.

**Key words** acid mine drainage (AMD); chemical thermodynamics simulation; Zibo coal mining district; chlorite; phreeqc

## Geochemical characteristics of acid mine drainage and sediments from coal mines, Shanxi Province, China

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In this study, geochemical characteristics of acid mine drainage (AMD) and its sediments from the Malan and Sitai coalmines, Shanxi Province, China, were investigated. Many analytical approaches such as IC, ICP-MS, XRD, XRF, and modeling calculation of hydrogeochemistry using PHREEQCI software were employed. The AMD is characterized by higher concentrations of iron and sulfate, a low pH, and elevated concentrations of a wide variety of heavy metals. The results of modeling calculation by PHREEQCI software demonstrate the metals in AMD are present mainly as  $Me^{n+}$  and  $MeSO_4^{n-2}$  species. The sediments of AMD are composed mainly of iron-bearing minerals such as goethite and schwertmannite, which are controlled by pH, Fe and SO<sub>4</sub><sup>2-</sup> concentrations. The schwertmannite mineral has been found for the first time in China.