EVALUATION OF ACID BASE ACCOUNTING DATA USING COMPUTER SPREADSHEETS

Michael W. Smith and Keith B.C. Brady

Abstract. Overburden analysis data in the form of acid-base accounting (ABA) can be efficiently and effectively evaluated using spreadsheet programs for personal computers. The Pennsylvania Department of Environmental Resources (PaDER), Bureau of Mining and Reclamation has developed a spreadsheet which calculates several parameters from ABA data including mass-weighted maximum potential acidity (MPA), neutralization potential (NP) and net neutralization potential (NNP). The spreadsheet also summarizes the overburden analysis in terms of the ratio of NP to MPA and the percent sandstone. With the spreadsheet, aggregate overburden characteristics can be summarized for an entire mine site.

Computer spreadsheet software is ideal for performing the numerous repetitive calculations necessary in integrating large quantities of ABA data. The ABA spreadsheet integrates sulfur content and neutralization potential data, as well as sample interval thicknesses, the percentage of each unit spoiled, and overburden unit weights. The area of influence of each drill hole is determined and the actual mass of strata are calculated by taking into account the geometry of the mine site and overburden unit weights. The ABA summary data can be compared using a variety of significance thresholds for NP and percent sulfur, and other factors can readily be changed to review their impact. The spreadsheet approach permits more complex and detailed analysis of overburden data and facilitates comparison between calculation methods.

Additional Key Words: overburden analysis, acid base accounting, computer spreadsheet.

Introduction

Acid base accounting (Sobek et al. 1978) is the most commonly used overburden analysis technique for predicting the water quality likely to result from a coal mining operation. In Pennsylvania, acid base accounting (ABA) has been used since about 1979 and now accompanies approximately fifty percent of current surface mining permit applications. ABA evaluates the maximum potential acidity (MPA) and the neutralization potential (NP) from individual strata and expresses them as tons per thousand tons of calcium carbonate equivalent. As such, it has been used to identify potentially acid-forming or alkaline-forming strata. Although not originally intended for the purpose, ABA is also used to predict postmining water quality. This is done by individually sampling all of the strata within a proposed mine site. The weighted aggregate of all samples are considered together to evaluate the potential of the site to produce acidic or alkaline water following mining.

Using ABA data for prediction of postmining water quality requires the integration of the chemical characteristics of each individual strata in order to characterize the entire mine site. The large volume of ABA data which accompanies a typical permit application makes it all but impossible to accomplish this intuitively. However, the widespread availability of personal computers and spreadsheet software greatly enhance one's ability to quantitatively and objectively evaluate ABA data and to evaluate it using a variety of procedures. This paper discusses a method developed by the Pennsylvania Department of Environmental Resources (PaDER) that offers a reliable and convenient means of summarizing large volumes of overburden data.


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History of Quantitative ABA Evaluation

Early users of ABA data as a predictor of postmining water quality tended to balance the MPA against the NP for an overburden column giving equal weight to the strata at the top and bottom. It was presumed that the postmining water quality would be determined by whichever factor predominated. For example, where NP exceeded MPA, alkaline drainage would result. Issuance of surface mining permits based on this assumption frequently resulted in severe acid mine drainage pollution (Brown and Harburger 1985). Leading to the realization that modifications to ABA review procedures were required for reliable predictions of postmining water quality.

The need for a simple method of computing and summarizing ABA-data became essential in the early 1980’s when coal companies began to propose the addition of supplemental alkaline material as a means of offsetting an NP deficiency (MPA > NP) and the potential for acid production at a mine site. Because of the large number of arithmetic operations required, the concept of using computer spreadsheets for calculating the deficiencies soon followed. Originally, calculations were weighted only according to thickness. However, in most cases the topography is hilly with flat-lying strata so that the uppermost strata are not as aerially extensive as lower strata, making volume or area-weighted calculations more essential. Recent developments in the utility of computer spreadsheet software enabled the PaDER to design more sophisticated spreadsheets which considered mass or volumetric weighting of each overburden sampling interval.

As the use of ABA for postmining water quality prediction became more widespread, the spreadsheet was also used to summarize the data numerically for comparison with postmining water quality. Again, this required a quantitative summary of the data which took into account the actual volume or mass of each overburden sampling interval. Two recent studies by diPietroco and Rauch (1988) and Erickson and Redin (1988) have compared numerical summations of ABA data with postmining water quality. Because of the large number of nine sites required for studies of this type and the effort required to make the area of each stratigraphic interval, precise volumetric calculations were not performed. diPietroco and Rauch calculated volume-weighted summary values by assuming an idealized right-triangle shaped area to be mined. Erickson and Redin used essentially the same method. This assumption was easily applied to single core log data where the coal was not steeply dipping. However, it can only be considered as an approximate technique for volumetric adjustment of ABA data. In these studies, aggregate MPA and aggregate NP were calculated. These volumes were then used to determine the net neutralization potential (NMP = NP - MPA) of the aggregate overburden volume and the NP/MPA ratio. Since the strata are represented more realistically, they found that volume-weighted calculations yielded better results than a columnar (equal unit-volume for all strata) approach.

Methodology

The current spreadsheet program used by the PaDER includes several important parameters useful in summarizing aggregate overburden characteristics. These include mass weighting using selected unit weights according to rock type, the percentage of a unit that is spilled, and threshold significance levels for NP and sulfur content. The current spreadsheet program calculations are undertaken over the past several years. The concepts presented here could be adopted with almost any commercial spreadsheet software.

Figure 1 is a printout of the overburden calculation spreadsheet used by PaDER, showing the layout of the input data and calculated results. Data input is designed to mimic ABA reports currently in use. Manual data input from the keyboard is kept to a minimum. The only required input are bottom depth, rock type, sulfur, and fize. All other values are either calculated or can use predetermined defaults.

Area of Influence

The spreadsheet is designed to analyze ABA data for individual drill holes. Where only one drill hole is available to characterize the overburden at a given mine site, quantitative analysis is simplified, although a single hole may not be representative of the entire mine site. In most cases, the information available from surface mining permit applications in Pennsylvania is complete enough such that a more rigorous approach to quantitative evaluation of overburden data can be undertaken. Virtually every site in the state has two (and usually more) overburden holes. Using the outcrop boundary and the limits of mining as delineated in the permit application, the area of influence of each drill hole can be approximated using the Thiessen polygon method (Davis 1973 and Brasington 1988). An example Thiessen polygon construction at a hypothetical mine site is shown in Figure 2. The area within each polygon are closer to the data point (drill hole) in the center of the polygon than they are to any other data point. In brief, the polygons are constructed by drawing lines between each drill hole. Each line is then bisected with a perpendicular and the perpendiculars are extended to form polygons. The area of each polygon can be calculated using a planimeter and this value can be used as a factor in determining actual volume or mass or for applying relative weights to each drill hole. Although there are other more elaborate methods which could be employed, they usually require many data points and lengthy, complex calculations. The Thiessen method is more representative than simple arithmetic.
The document contains a table and several paragraphs of text discussing overburden analysis and calculation methods. The table appears to be a spreadsheet listing various data points for different sample intervals, including thickness, rock type, sulfur content, deficiency/excess, acreage, and more. The text explains the process of determining overburden volume and provides a formula for calculating volumetric calculations.

Volumetric Calculations

In contrast to thickness weighting and volume weighting using the triangle approximation of dIPerelon, the overburden analysis spreadsheet uses actual measured acreages of the area to be mined. For most uses it is impractical to measure the area for each sample (stratigraphic) interval, which would be necessary for precise volumetric calculations. As an alternate and much simpler method, the acreage for the uppermost unit and lowermost unit can be determined, with the spreadsheet interpolating the areas for each intervening sample interval. In most instances, this method will provide acceptable volumetric calculations under a wide range of topographic conditions. The area covered by each sample interval is estimated by determining its depth in the drill hole at the middle of the interval. This technique is illustrated in Figure 3. The spreadsheet calculates this value using the equation:

\[ h_I = h_T + \left[ ((D_{TOP}^2 - D_{BOT}^2) / 2) / D_{TOP} \right] \times (A_B - A_T) \]  

Where:  
- \( h_I \) = Acreage at sample (stratigraphic) interval  
- \( h_T \) = Acreage represented by the middle of the uppermost sample interval  
- \( h_B \) = Acreage represented by the middle of the lowermost sample interval  
- \( D_{TOP} \) = Drill hole total depth  
- \( D_{TOP} \) = Depth at top of sample interval  
- \( D_{BOT} \) = Depth at bottom of sample interval
Figure 2. Typical mine plan map showing Thiessen polygon method of defining area of influence for each drill hole. Dashed lines are construction lines drawn between drill holes. Polygons are constructed by bisecting the construction lines with perpendiculars. Outer limits of polygons are defined by mining limits and coal outcrop boundary. Interior polygons (1 and 2) are calculated as columns (top acreage - bottom acreage). Remaining polygons calculated using different top and bottom acreages.

This equation provides a reasonable approximation of acreages covered by each sample interval provided that the strata are not steeply dipping and that the topography, if viewed in cross section, is not markedly convex, concave or irregular. It can be appropriately applied to area mines, contour mines, and mountaintop removal mines and works equally well in steep or gentle topography. The data input requirements are minimal. The acreage represented by the lowermost unit (usually measured as the coal outcrop limit) and the uppermost unit must be provided. Where no acreages are provided, the default value of 1.0 is used for all intervals and the spreadsheet performs column (thickness-weighted) calculations. If the drill hole is located to represent maximum cover, then the top acreage is very small and the default value of 1.0 acre is probably appropriate.

If the drill hole is located where overburden thickness is at a maximum, then the modeled geometry resembles a cone and the calculated results should approximate those using diPretoro's method. However, for most applications where the uppermost unit covers a significant acreage but less than the lowermost unit, the site geometry is modeled as a truncated cone. Area mines are represented with nearly equal top and bottom acreages. For multiple drill hole sites, a combination of geometries may be most appropriate. For example, where interior polygon sections which are bounded by other polygons rather than the coal outcrop limits exist, they are best represented as area mine sections with the bottom acreage equal to the top acreage.

Where unusual topography occurs which renders the linear interpolation method inaccurate, the overburden analysis can be divided into two or more sections. Measured acreages are used for the upper and lowermost units of each section and the values are interpolated between measured units.

Actual volumes are calculated by multiplying the unit thickness by its area. But ABA data are expressed as tons per thousand tons of overburden. Therefore, it is more appropriate to evaluate the data in the same units. The importance of using weight rather than volume units is intensified where the unit weights of the rock types vary significantly. ABA values are expressed in terms of absolute quantities by multiplying their volumes by unit weights. The spreadsheet includes default unit weight values for each rock type. Unit weights typical of Allegheny group rocks in western Pennsylvania were obtained from Geyer and Wilshusen (1982). Coal and carbonolith (carbonaceous sedimentary rock) unit weights were determined from PaDIR file data. Through a series of nested "IF" operators, the appropriate unit weight is selected according to the rock type specified. The unit weight for any particular rock type can be changed by entering the desired value in the unit weight table.

Most ABA reports include the "pavement" or underlying strata, which can vary in thickness. Although this material will not be mined, it is presumed that at least the uppermost portion of it will be disturbed by mining and that it will have some impact on mine drainage chemistry. For most applications, it is appropriate to include the upper foot of pavement material as the lowermost sample interval in the spreadsheet.

Fraction Spoiled

Previous quantitative evaluations of ABA data invariably discounted the coal, presuming that its recovery in the mining operation was 100% complete. Typically this is not the case, and pit losses in the order of 5 to 20% can be expected. The spreadsheet includes a column to indicate the fraction of
material to be returned to the backfill. For overburden, this will be 1.0 (i.e., 100%) since all of the overburden will be returned. Thus, the default value is set at 1.0. For coals which will be removed, a fraction representing pit losses can be entered (such as 0.90). This permits the calculation to reflect the retention of potentially acid forming pit cleanings and coal rejects. It may also be possible that various alternate mining schemes are proposed, such as removal of some overburden strata either for commercial purposes or to minimize acid formation. The fraction spoiled column can be used to reflect this.

NP and MPA

For each stratigraphic (or sample) interval the maximum potential acidity (MPA) and neutralization potential (NP) are calculated and expressed as total tons CaCO₃ equivalent using the following equations:

\[
\text{MPA} = \frac{8 \times \text{Sulfur}}{31.25} \times \frac{T_t}{A_t} \times A_t
\]

\[
\text{NP} = \frac{\text{NP} \times T_t}{A_t} \times \text{Unit wt.} \times \text{Fraction Spilled}
\]

Where: \(T_t\) = Thickness of sample (stratigraphic) interval (feet) 
\(A_t\) = Acreage covered by sample interval

These two values represent the total amount of potential acidity and neutralization potential for a single interval. In this sense, the spreadsheet goes one step beyond volumetric adjustment of the acid base accounting data by using actual densities to calculate total tonnages. Then, for each interval, the net NP (NNP) is determined by subtracting MPA from NP. The total tons of overburden for a sample interval is calculated by multiplying thickness times unit weight times area. This number will be used for subsequent summary parameters.

Alkaline Addition Rate

For mine sites where off-site alkaline materials will be imported, the impact of the additional alkaline material, in terms of ABA summary parameters, can be examined by including it in the ABA calculations. A spreadsheet entry (labeled ALK ADD) in Figure 1 is used. The "alkaline addition" rate is entered in units of tons CaCO₃/acre. If a different material or impure limestone will be used, it must be converted to CaCO₃ equivalent. Since the acreage of the bottom sample interval equals the total surface acreage represented by this drill hole, the alkaline addition rate per acre is multiplied by this number to obtain the total quantity of imported alkaline material as CaCO₃. This value is added to the column of NP values and is reflected in the total NP. It is also added to the total overburden weight for calculation of NP and MPA in tons/1000 tons.

Summary Parameters

The principal purpose of the overburden spreadsheet is to provide useful parameters which summarize the aggregate overburden characteristics. The summary parameters calculated by the spreadsheet, along with their formulas, are listed in Table 1. The most obvious parameters are calculated total tonnages of MPA, NP, NNP, and total tons of overburden. They represent absolute amounts expressed in tons and are calculated by summing the value for each individual stratigraphic interval. Total tons MPA, NP and NNP are also expressed as tons per thousand tons of overburden representing the entire overburden volume as if it were a single homogeneous sample.

### Table 1. ABA spreadsheet summary parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tons overburden</td>
<td>total weight of overburden</td>
<td>(\Sigma) tons overburden for each sample interval</td>
</tr>
<tr>
<td>MPA (tons)</td>
<td>total maximum potential acidity</td>
<td>(\Sigma) MPA for each sample interval</td>
</tr>
<tr>
<td>MPA (tons/thousand)</td>
<td>maximum potential acidity</td>
<td>(\Sigma) MPA (tons/thousand) overburden</td>
</tr>
<tr>
<td>NP (tons)</td>
<td>total neutralization potential</td>
<td>(\Sigma) NP for each sample interval</td>
</tr>
<tr>
<td>NNP (tons/thousand)</td>
<td>total net neutralization potential</td>
<td>(\Sigma) NNP (tons) - MPA (tons)</td>
</tr>
<tr>
<td>Overburden volume (acres/ft)</td>
<td>total volume of overburden</td>
<td>(\Sigma) (thickness x acreage x fraction spoiled) for each interval</td>
</tr>
<tr>
<td>Percent sandstone</td>
<td>total volume - weighted percent sandstone</td>
<td>(\Sigma) (thickness x acreage x fraction spoiled) for each sandstone interval/overburden</td>
</tr>
<tr>
<td>DSR ratio</td>
<td>KP to MPA ratio</td>
<td>NNP (tons) / MPA (tons)</td>
</tr>
<tr>
<td>DiPretoro ratio</td>
<td>(\bar{C} \text{P} / \text{MPA} / \text{TONS})</td>
<td>NNP (tons) / MPA (tons)</td>
</tr>
<tr>
<td>Total/acre required</td>
<td>CaCO₃ equivalent</td>
<td>(\Sigma) CaCO₃ equivalent required for DSR Ratio = 1.0</td>
</tr>
<tr>
<td>Tons/acre NP required</td>
<td>(\Sigma) CaCO₃ equivalent</td>
<td>NNP (tons) / acreage at bottom sample interval ((0 = \text{excess} \times \frac{x}{\text{deficiency}}))</td>
</tr>
</tbody>
</table>

1 For diPretoro method, calculated as described by diPretoro 1988.
2 Includes NP from alkaline addition.

For comparison, the same parameters are calculated using diPretoro's (1988) triangle-volume weighting method. As part of a study on the effectiveness of alkaline addition in ameliorating acid mine drainage (Brady et al. 1990), the spreadsheet was used to characterize overburden conditions for ten different mine sites. The results using the acreage interpolation method and diPretoro's method are expressed as aggregate NNP and as the NNP/MPA ratio and are compared in Table 2. Although they always differ slightly, the results from both methods are usually fairly close, especially the NNP/MPA ratio. In most of these cases, the diPretoro method calculated a somewhat lower NNP. This apparently results from the diPretoro triangle-approximation method which tends to underestimate upper, generally higher NP strata where the mine site configuration resembles a truncated cone or where overburden holes were not drilled at maximum cover.

Tons per acre NP required

Especially where alkaline addition requirements are to be determined, it is useful to know the limestone application rate which would be required to fulfill any net neutralization potential deficiency. In practical terms, this amount is expressed as the required tons per acre. It is the total tons NNP divided by the total acreage represented by the drill hole (i.e., the acreage of the bottom sample interval). Positive NNP values are indicated as an excess. Negative NNP values are indicated as deficiencies. Of course, this does not presume that merely bringing the NNP to zero indicates a suitable alkaline addition rate. It is presented only as a summary parameter to be used in
the review of ABA data. Also, where this parameter is used in combination with the significance threshold values discussed below, the limestone requirement may be very different than for a straightforward balance of total NP versus total MPA.

If an alkaline addition rate has already been specified in the spreadsheet input data, it will be reflected in all of the applicable summary parameters. Therefore, the amount required is in addition to the specified value. By comparing the same spreadsheet with and without alkaline addition or at various alkaline addition rates, the impact of the alkaline addition on the ABA summary parameters can easily be observed. In most cases, only very large (500 tons/acre or more) alkaline addition rates have a noticeable impact on these values.

NP/MPA Ratio
diPretoro (1988) used the ratio of aggregate neutralization potential to maximum potential acidity as an ABA summary parameter. When this ratio equals 1, the NP and MPA are theoretically equal. This parameter is calculated by dividing the total tons NP by total tons MPA. diPretoro found that mine sites with a ratio less than 2.4 generally resulted in acid mine drainage, whereas mine sites with ratios above 2.4 usually produced alkaline drainage. For comparison, both the numbers derived from the areal interpolation (labelled as the DDR ratio on Figure 1) and the diPretoro triangle method (labelled diPretoro ratio) are shown.

Percent Sandstone
Several studies have found (diPretoro and Rauch 1987, Williams et al. 1982, Brady et al. 1988, Kanai et al. 1989) that where overburden is mostly composed of sandstone, acid drainage predominates. Consequently, a summary value showing the percentage of sandstone overburden was incorporated into the spreadsheet. This is a volume percentage calculated by summing the volume of each sample interval identified as sandstone and dividing this by the total overburden volume.

Significance Thresholds
Brady and Hornberger (1989) suggested threshold values of NP = 30 tons/acre, MPA with "fizz" and percent sulfur = 0.5 as reasonable guidelines to define potentially alkaline or acid-producing strata, respectively. Overburden calculations for alkaline addition were made using this scheme, such that CaCO$_3$ requirements were based only on strata with sulfur contents and NPs exceeding these thresholds. The spreadsheet was designed to perform these or similar calculations. Threshold values for sulfur content, NP, and fizz rating are defined near the top of the spreadsheet. Through a series of "IF" operators, MPA and NP values are only calculated for sample intervals which equal or exceed the threshold values. Using threshold values of 0.5% sulfur, NP = 30, and fizz = 1, for example, MPA will be determined only if the sulfur content equals or exceeds 0.5%. Where sulfur < 0.5%, MPA = 0. NP will only be calculated where the sample NP equals or exceeds 30 and fizz is greater than or equal to 1. Therefore, where NP < 30 or fizz = 0, MPA = 0.

Presumably, this method can be used to eliminate the NP or MPA contribution from strata which are insignificant in terms of the production of acidity or alkalinity. Of course, if no threshold calculation is desired, then zero is entered for the threshold values. Any combination of thresholds can be used. In this manner, the summary parameters can be readily calculated for a variety of threshold values.

Sulfur Content - Carbonate Equivalence
Crovatto and others (1990) have suggested that by using a stoichiometric equivalence factor of 31.25 to compare percent sulfur (MPA) to NP, the actual neutralization requirements may be understated by a factor of two. The alternate equivalence factor to convert percent sulfur to MPA is 62.5. Accordingly, the spreadsheet also reflects this alternate method. All of the summary values are calculated using both the 31.25 and 62.5 equivalence factors.

Summary and Discussion
Computer spreadsheets are an effective means of summarizing and evaluating ABA overburden analysis data. Volumetric and mass-weighted calculations based on actual mine site geometry and overburden unit weights can easily be performed. Underlying assumptions can be readily changed and the spreadsheet automatically performs any recalculation. Through the use of summary parameters, ABA data from an entire mine site can be integrated to form a conceptual picture of the site's aggregate overburden conditions. Moreover, the spreadsheet can be used to perform various quantitative calculations such as alkaline addition requirements.

A study by Brady et al. (1990) used the spreadsheet method of overburden analysis computation to evaluate the effectiveness of alkaline additives to surface mines in preventing pollution from acid mine drainage. Because it considered mass, the fraction spoiled, and a closer approximation of actual site geometry, the spreadsheet offers a better representation of actual field conditions than previous summary methods.

<table>
<thead>
<tr>
<th>SITE NO.</th>
<th>Net NP (tox thousand)</th>
<th>NP/MPA Ratio</th>
<th>Spreadsheet</th>
<th>diPretoro difference</th>
<th>Spreadsheet</th>
<th>diPretoro difference</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>6.10</td>
<td>6.94</td>
<td>2.33</td>
<td>+0.84</td>
<td>2.35</td>
<td>+0.52</td>
</tr>
<tr>
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<td>0</td>
<td>-0.02</td>
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<td>4.64</td>
<td>-2.10</td>
</tr>
</tbody>
</table>

The recent availability of extensive database capabilities and geographic information systems (GIS) provides new uses for summarized ABA data. In many cases, computer analysis data is functionally irretrievable and can be used only by initiating a very laborious file search and data compilation effort. Computer storage of summarized ABA data through such a database and retrieval system could greatly facilitate its use for cumulative hydrologic impact analysis (CHIA) and comparison of overburden quality with postmining water quality. The computer spreadsheet discussed herein or its modifications could readily support such a system.

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Literature Cited


