CHAPTER FIVE – DISCUSSION ON SULPHUR, MINERALS, MACERALS AND TRACE ELEMENT OCCURRENCE

The relationships between trace elements, sulphur, mineral matter and macerals are discussed in Section 5.1. and 5.2 through curve fitting comparison, statistical analysis using Principal Component Analysis (PCA) and fundamental investigation. A correlation matrix for all trace elements, forms of sulphur and minerals is given in Table XII and XIII in the appendix.

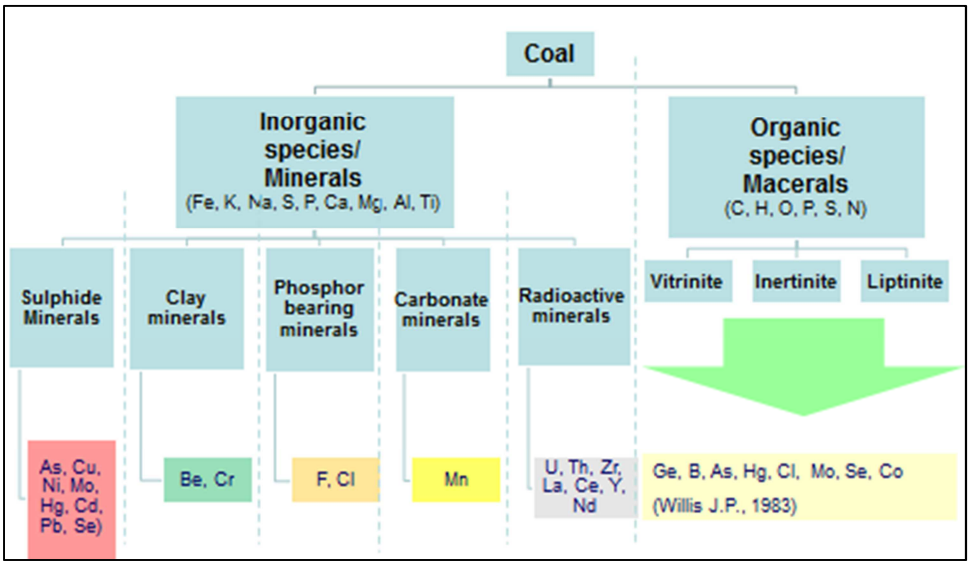

Figure 92: *Trace element origin and associations.*

According to Jolliffe (2002), 'Principal Component Analysis (PCA) is a multi-variate analysis where the central idea of principal component analysis (PCA) is to reduce the dimensionality of a data set consisting of a large number of interrelated variables, while retaining as much as possible of the variation present in the data set'.

In the research undertaken the correlation matrices were derived using *MS Excel*, and for the PCA analysis *Statistica*, which is statistical analysis software, was used.

The sum of squares of the Principle Components (PC) coefficients and factor loadings are normalised to be equal to unity for each factor (Jolliffe, 2002). Typically,

the output from computer packages (like *Statistica*) that implement factor analysis uses the normalisation in which the sum of squares of coefficients in each PC before rotation is equal to the variance (eigenvalue) associated with that PC. The Eigen values are also referred to as empirical orthogonal functions. The latter normalisation is used in Figures 94 etc. The choice of normalisation constraints is important in rotation as it determines the properties of the rotated factors.

5. 1 Relationship between Trace elements, sulphur and mineral matter associations

5.1.1 Witbank Coalfield No. 4 Seam

Figure 93 displays the relationship between Total Sulphur and CV at various low grade export thermal coal quality specifications from 4500 to 6150 kcal/kg.

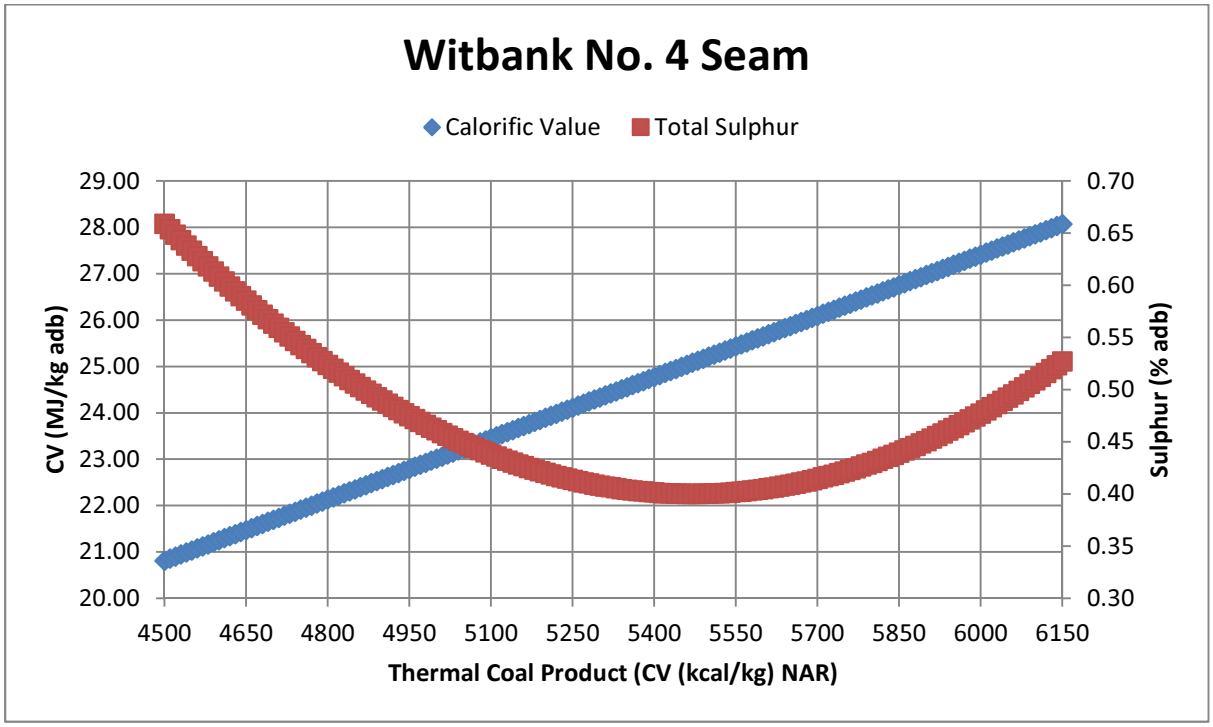

Figure 93: *Total Sulphur distribution at various thermal coal export grades (4000-6000 kcal/kg NAR CV) – Witbank Coalfield No. 4 Seam*

Based on the trend and relationship shown in Figure 93, the next step would be to evaluate the trend and identify the associated trace elements.

The correlation factors between trace elements and various mineral species are given in Tables XII and XIII in Appendix E. The correlation factors are derived from trace element and mineral matter data trends with raw data from Table VII, VIII, IX.

From Figure 94 it can be seen that most of the inorganically associated trace elements falls within the same quadrant as pyrite. The elements closely correlated to pyrite remain Hg, As, Cd, Pb, Mo, Cu, Ni and Co.

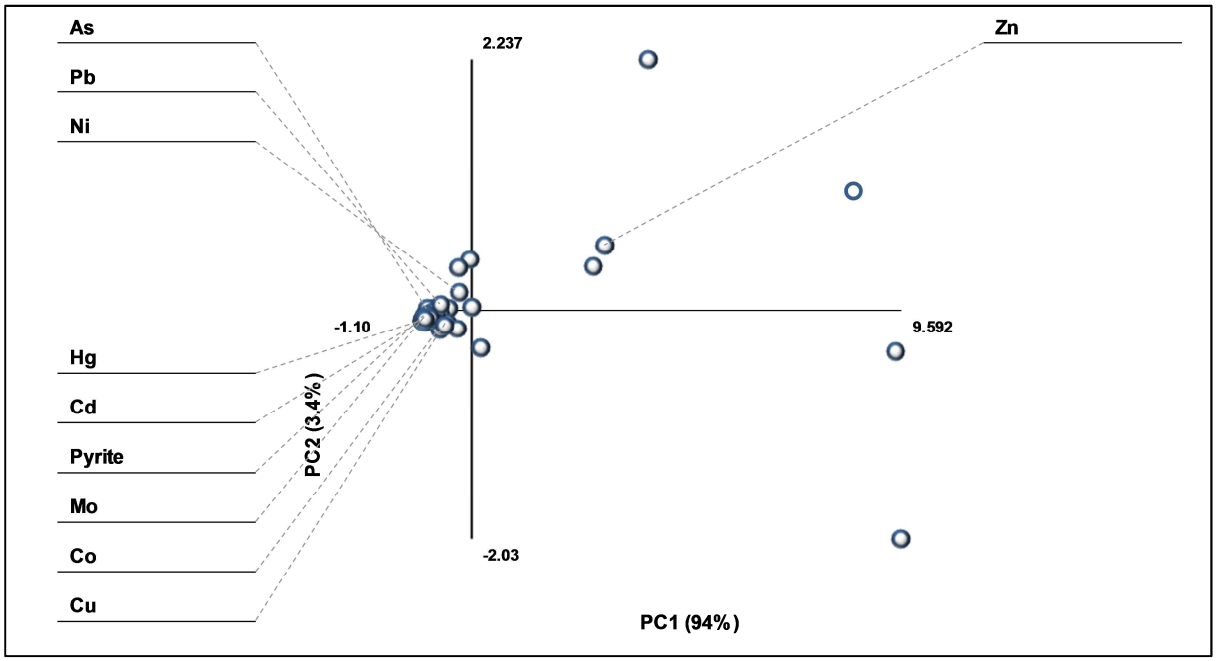

Figure 94: *Witbank Coalfield No. 4 Seam Pyrite Association*

From Figure 94 it can be seen that Cr, Sc and Sb fall within the same quadrant. Most of the trace elements with high organic affinity are also associated with kaolinite. This is likely due to the distribution of fine clay in the organic matrix. In Figure 95, 'PC1' and 'PC2' refers to the Principal Component association factors with correlating and non-correlating components respectively.

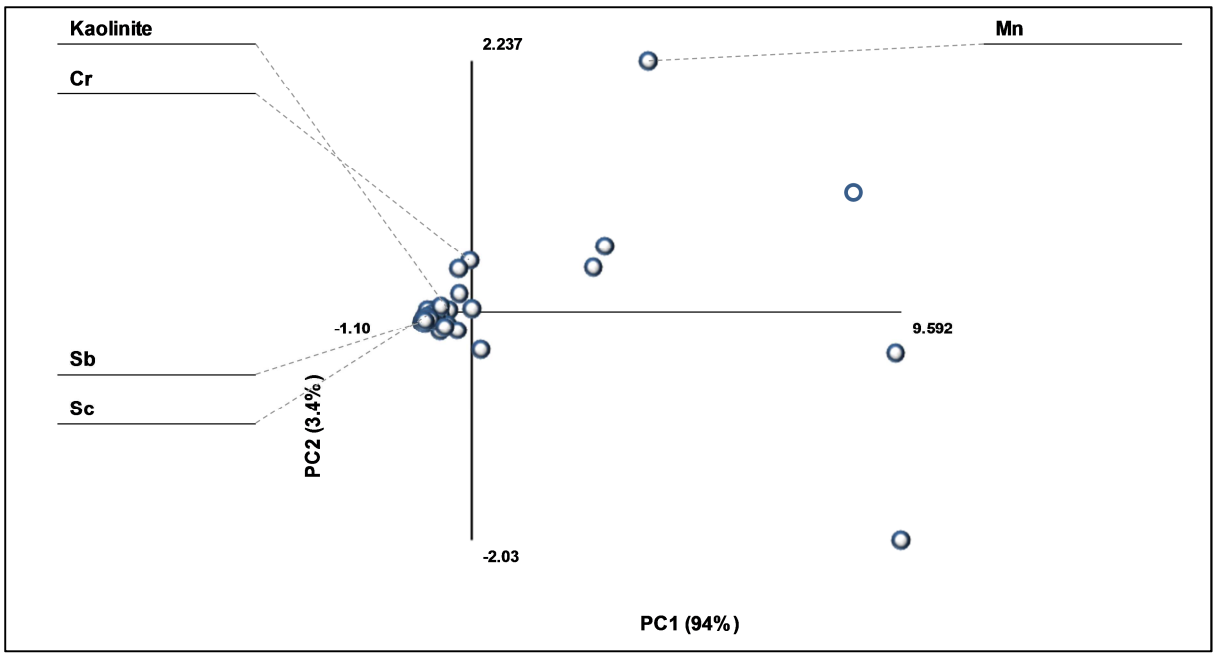

Figure 95: *Witbank Coalfield No. 4 Seam Kaolinite Association*

In Figure 96 it can be seen that the organic sulphur, vitrinite and Ge content fall within the same quadrant and have a 93.8 % correlation coefficient factor.

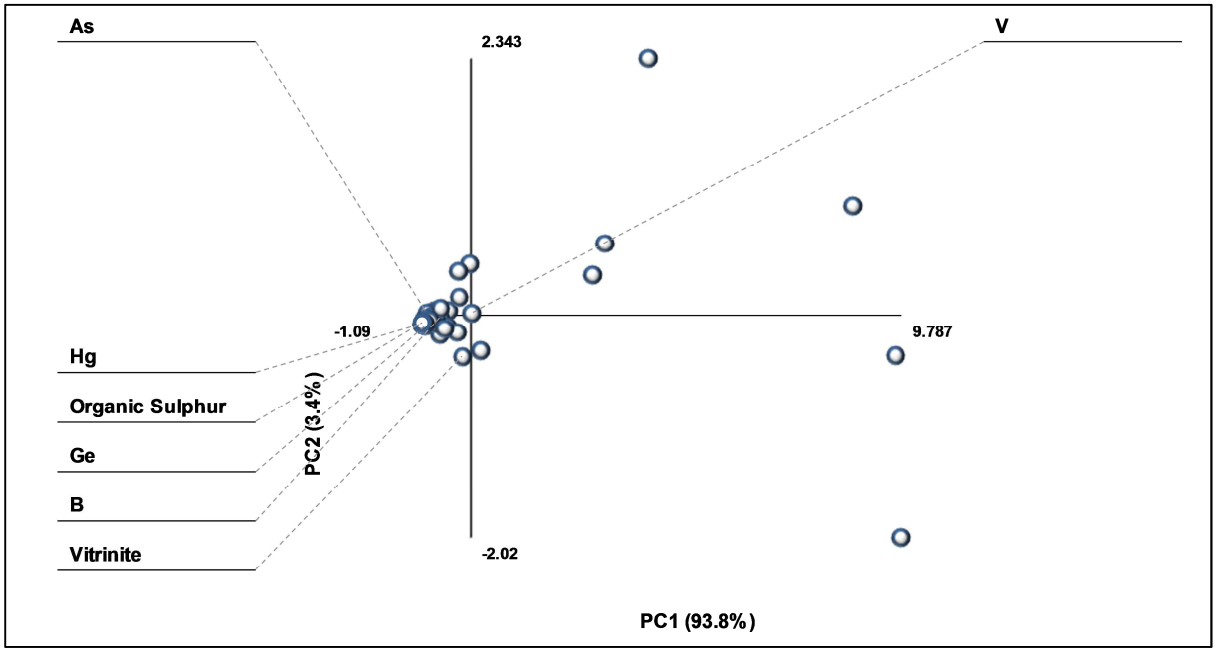

Figure 96: *Witbank Coalfield No. 4 Seam Vitrinite & Organic Sulphur Association*

It addition it is also shown in Figure 96 that there is a strong association between the organic sulphur, vitrinite, As and Hg data.

5.1.2 Waterberg Upper Ecca

The distribution of the sulphur and the CV of the Waterberg Upper Ecca in Figure 97 indicates an inverse relationship.

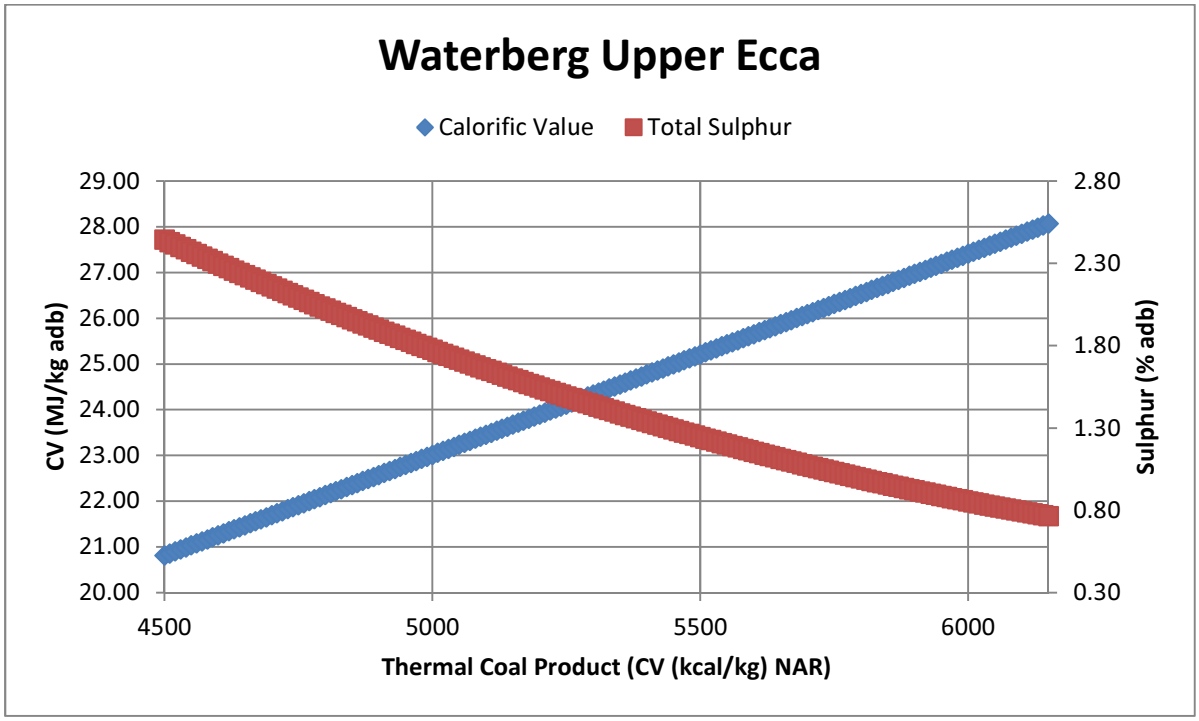

Figure 97: *Sulphur distribution at various thermal coal export grades (4000-6000 NAR) - Waterberg Upper Ecca*

In Figure 98 a clearer association of pyrite and its associated trace elements can be observed as they appear orthogonal in the same quadrant. These trace elements include Hg, As, Co, Cd, Pb, Cu, Sb and U.

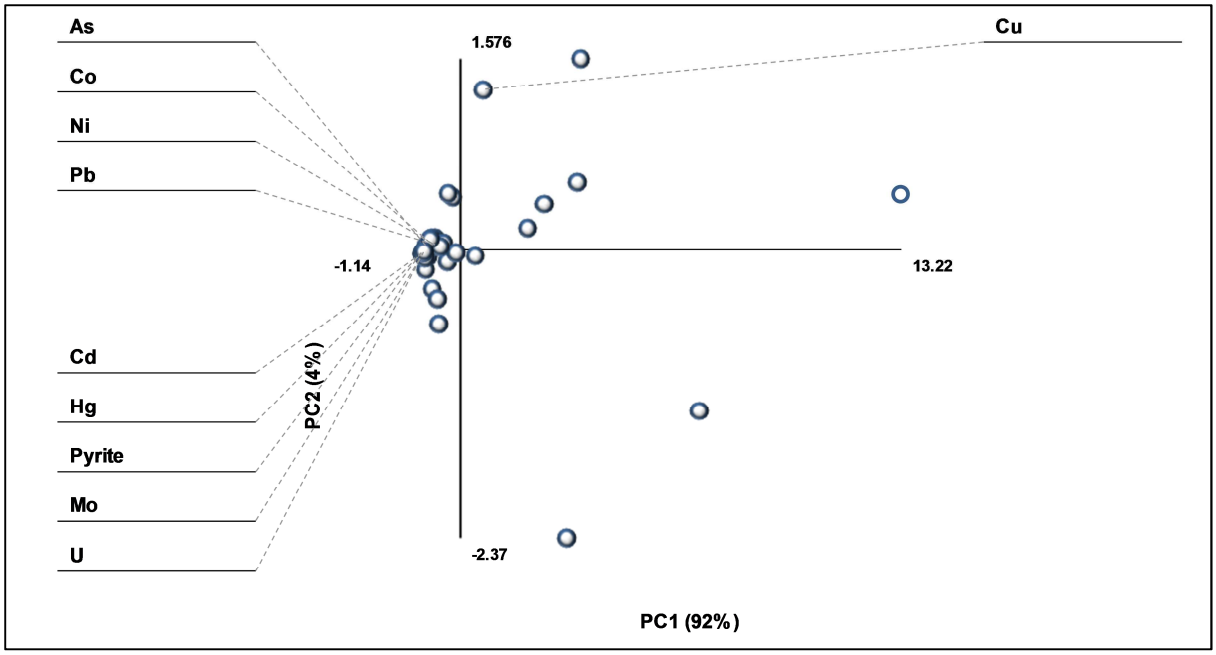

Figure 98: *Waterberg Upper Ecca Pyrite Association*

In Figure 99 in the case of the Waterberg Upper Ecca a similar distribution to the Witbank No. 4 Seam and association is observed in terms of kaolinite and its associated trace elements based on the PCA analysis. Sn and Sb fall within the same quadrant. Most of the trace elements with high organic affinity is also associated with Kaolinite.

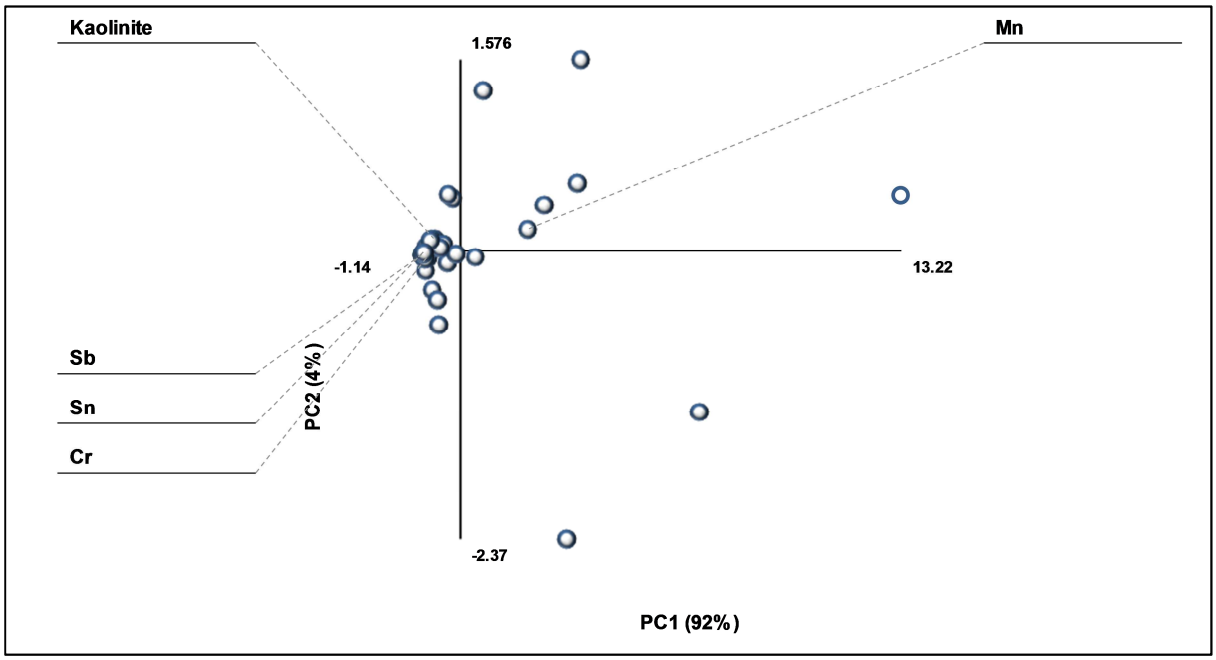

Figure 99: *Waterberg Upper Ecca Kaolinite Association*

In Figure 100 it can be seen that the organic sulphur, vitrinite, V and Ge content fall within the same quadrant and have a 98.87 % variant correlation coefficient factor on the plane.

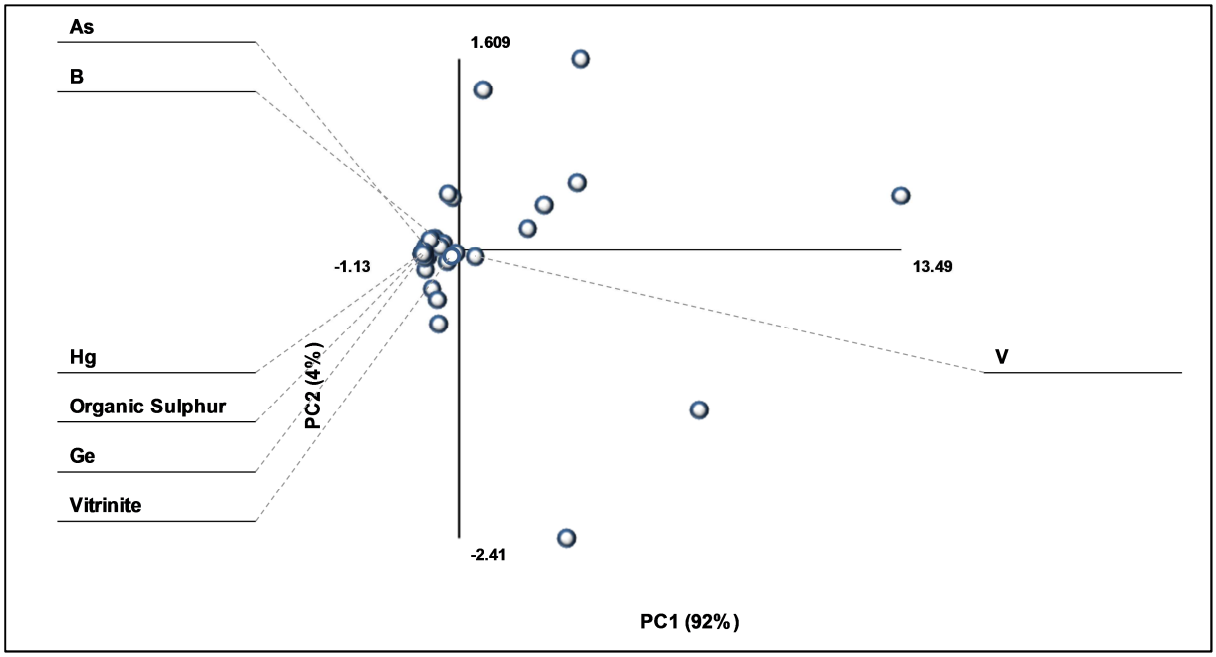

Figure 100: *Waterberg Upper Ecca Vitrinite & Organic Sulphur Association*

From the PCA plot in Figure 100 it is also shown that there is a strong correlation between the organic sulphur, vitrinite, As and Hg data. This could be due to organically bound Hg and As, or the occurrence of fine pyrite nodules in these fractions.

5.2 Modelling of trace element reduction by dense medium beneficiation

The distributions of arsenic and mercury are illustrated in Figure 101 for Witbank Coalfield No. 4 Seam and Figure 102 for Waterberg Upper Ecca. Due to the liberation of pyrite and vitrinite they have distinct washability characteristics.

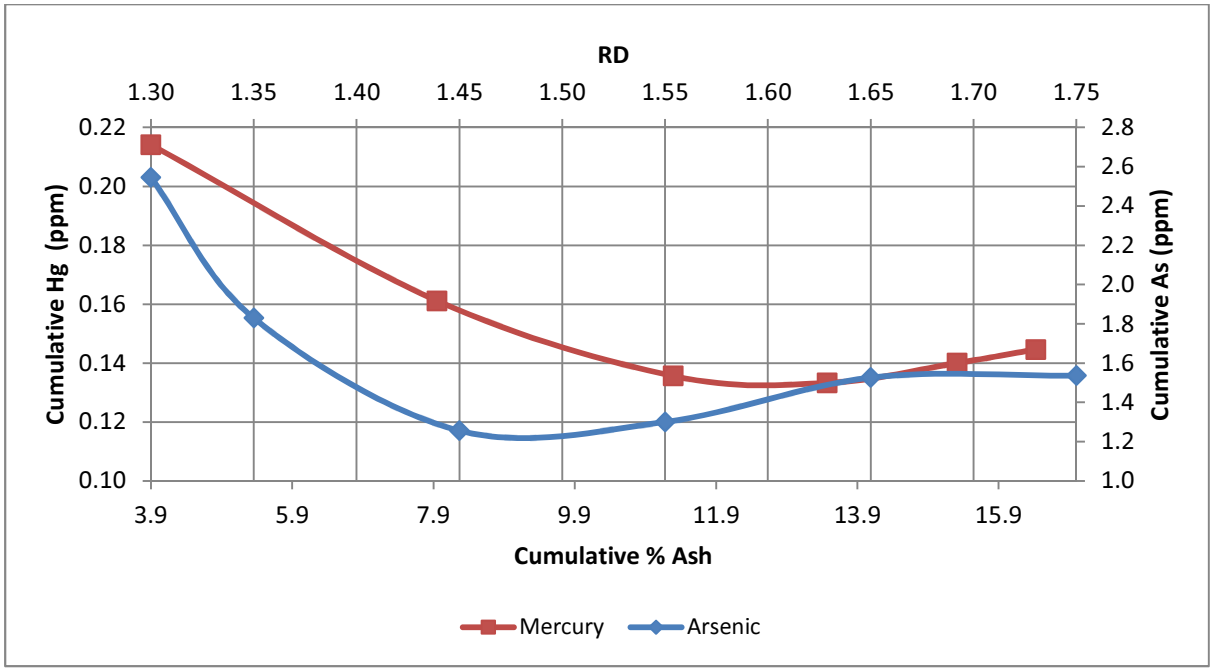

Figure 101: *Washability of Hg and As in Witbank Coalfield No. 4 Seam*

In Figure 101 it can be seen that both As and Hg have a strong organic affinity and decrease with an increase in ash content. This was confirmed through the PCA analysis, see Figure 96. Tables XII and XIII contains the data for the trace element content modelling at various cutpoint RD's.

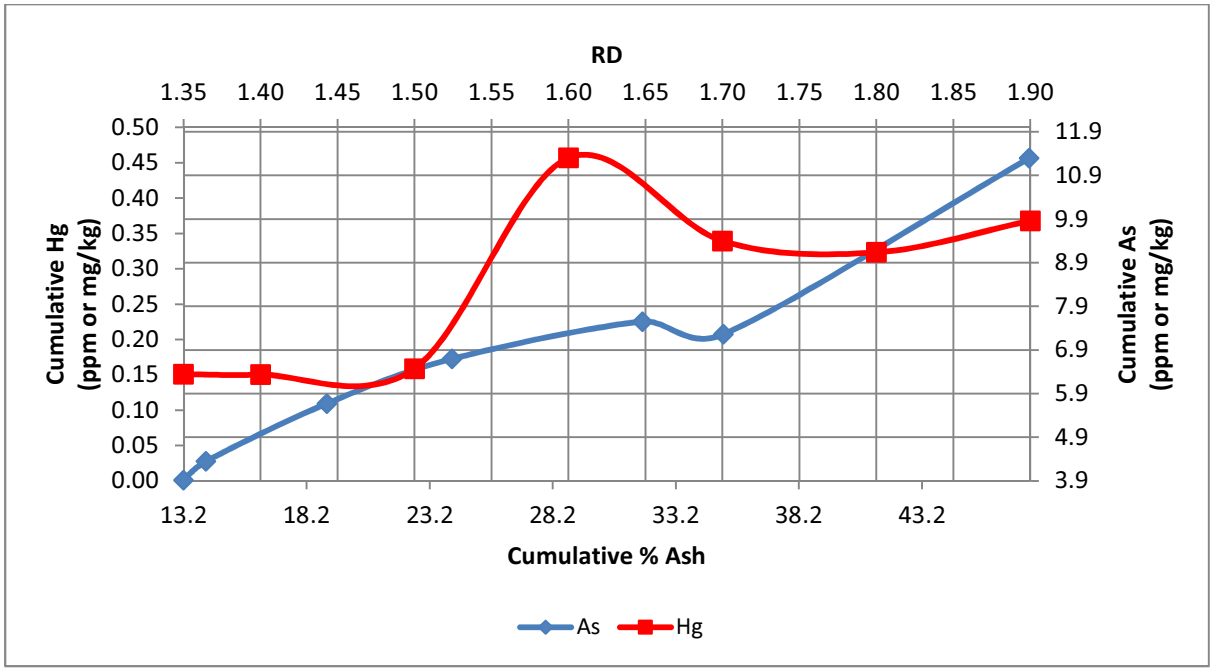

Figure 102: *Washability of Hg and As in Waterberg Upper Ecca*

Although it was found that a strong association exists between vitrinite, organic sulphur, Hg and As through the PCA analysis, it is shown in Figure 102 that As and Hg have a strong inorganic affinity in the Waterberg Upper Ecca and their respective concentrations increase with an increase in ash content. This could be explained by the occurrence of pyrite in both authigenic and syngenetic form throughout the 1.3 RD to 1.6 RD washability density fractions as illustrated in Section 4.5.

In summary, in Section 5 the Principle Component Analysis and correlation analysis indicated that there are distinct relationships between sulphur, Hazardous Air Pollutant trace elements and their host minerals for both the Witbank Coalfield No. 4 Seam and the Waterberg Upper Ecca.