CHAPTER SIX – LIBERATION MODELLING OF MINERALS AND MACERALS ASSOCIATED WITH TRACE ELEMENTS

The degree of liberation of minerals and macerals is significant as that indicates the expected processing efficiency achievable through the separation process in coal beneficiation. In contrast to conventional liberation testing of coal where the bulk properties of coal such as ash content are used, in this chapter the focus is on specific mineral and maceral liberation. In essence, the actual separation process takes place when minerals are separated from macerals rather than when low ash coal is separated from high ash coal. Through the generation of data for specific minerals and macerals and their associated microlithotypes, inputs can be generated for the simulation of real coal beneficiation processes and plants. In addition pollutants can be best quantified and correlated on this basis as was illustrated in Chapter 5, where actual minerals and macerals host specific pollutants. It is anticipated that an integrated model to predict beneficiation efficiency and subsequent utilisation efficiency could be derived from such liberation models.

The final section (Section 6.3.3) deals with the liberation indices of the specific mineral and macerals, where the expected separation efficiency due to the degree of liberation of the components are summarised. As described by King and Birtek (1990) it is difficult to specify the liberation of macerals or mineral matter in the conventional manner. Due to this constraint, use was made of a liberation index that reflects both the liberation characteristics and the potential for the clean separation of macerals from mineral matter (Kind and Birtek, 1990). On this basis all macerals and mineral matter are described. In Section 2.2 a description of the liberation modelling is given with reference to how the liberation index is derived. The raw data for the liberation modelling is contained in Appendix, Table X and XI.

6.1 General Liberation Modelling

The liberation and distribution of a coal constituent or component for example ash content, mineral matter, maceral and major or trace elements are given by (derived from King, 1990):

Equation 4: *The cumulative component liberation equation.*

$$f(x) = Ax^B e^{Cx} + Dx \quad (4)$$

Where f(x) = Cumulative component (ash, mineral, maceral, major element, trace element) per 100 units of feed.

The instantaneous component (ash, mineral, maceral, major element, trace element) content is given by the first order derivative of f(x):

Equation 5: *The derivative of the liberation equation giving the instantaneous concentration*

$$f'(x) = D + ABe^{Cx}x^{-1+B} + ACe^{Cx}x^B \quad (5)$$

The local minimum or maximum can be given by the second order derivative of f(x):

Equation 6: *The second derivative equation to determine the maximum or minimum concentration of the component*

$$f''(x) = AB(-1+B)e^{Cx}x^{-2+B} + ACBe^{Cx}x^{-1+B} + ABCe^{Cx}x^{-1+B} + ACCe^{Cx}x^B \quad (6)$$

The Liberation Index in its basic form is given by King *et al.*, (1998), given in Equation 7:

Equation 7: *Liberation Index equation (King et al., 1998) in its basic form*

$$LI = \frac{0.5f - \int_O^1 ZdQ}{0.5f - 0.5f^2} \quad (7)$$

Equation 8: *Simplified liberation Index equation, form (1)*

$$LI = \frac{f - 2AC^{B+1}\int_O^C t^B \exp(t)dt - D}{f - f^2} \quad (8)$$

Where Z is the ash content per 100 units of total feed, Q is the mass yield, and *A, B, C,* and *D,* are constants. The constants are not independent since the M-curve must satisfy the relationship Z = 1.0 at Q = 1.0, where 1 is the ash content of the feed sample. Based on the liberation function is this study the Liberation Index equation is given by:

Equation 9: *Simplified liberation Index equation, form (2)*

$$\mathrm{LI} = AC\exp(x^{1+B}) \quad (9)$$

This can also be given as:

Equation 10: *Simplified liberation Index equation, form (3)*

$$\mathrm{LI} = AC\exp(x).\exp(x)^{B} \quad (10)$$

And in natural logarithmic form:

Equation 11: *Simplified liberation Index equation, form (4)*

$$\ln(\mathrm{LI}) = \ln(x)(\mathrm{AC} + B) \quad (11)$$

In the case of the macerals and microlithotypes it was found that the King (1990) equation could not be applied. A new equation was derived to model macerals and microlithotypes.

The curve fitting exercise that resulted in the best suitable scenario gave the following equation:

Equation 12: *Simplified liberation Index equation for several macerals and microlithotypes*

$$f(x) = \frac{(x+A)}{(B+C(x+A)+D(x+A)^2)} \quad (12)$$

Witbank Coalfield No. 4 Seam

For the Witbank Coalfield No. 4 Seam it can be seen that the highest liberation is achieved in the fine fraction (minus 0.5 mm fraction) as expected, as illustrated in Figure 103. The liberation size fraction curves displayed in Figure 103 for the

Witbank Coalfield No. 4 Seam are for only three size fractions to replicate the traditional processing routes.

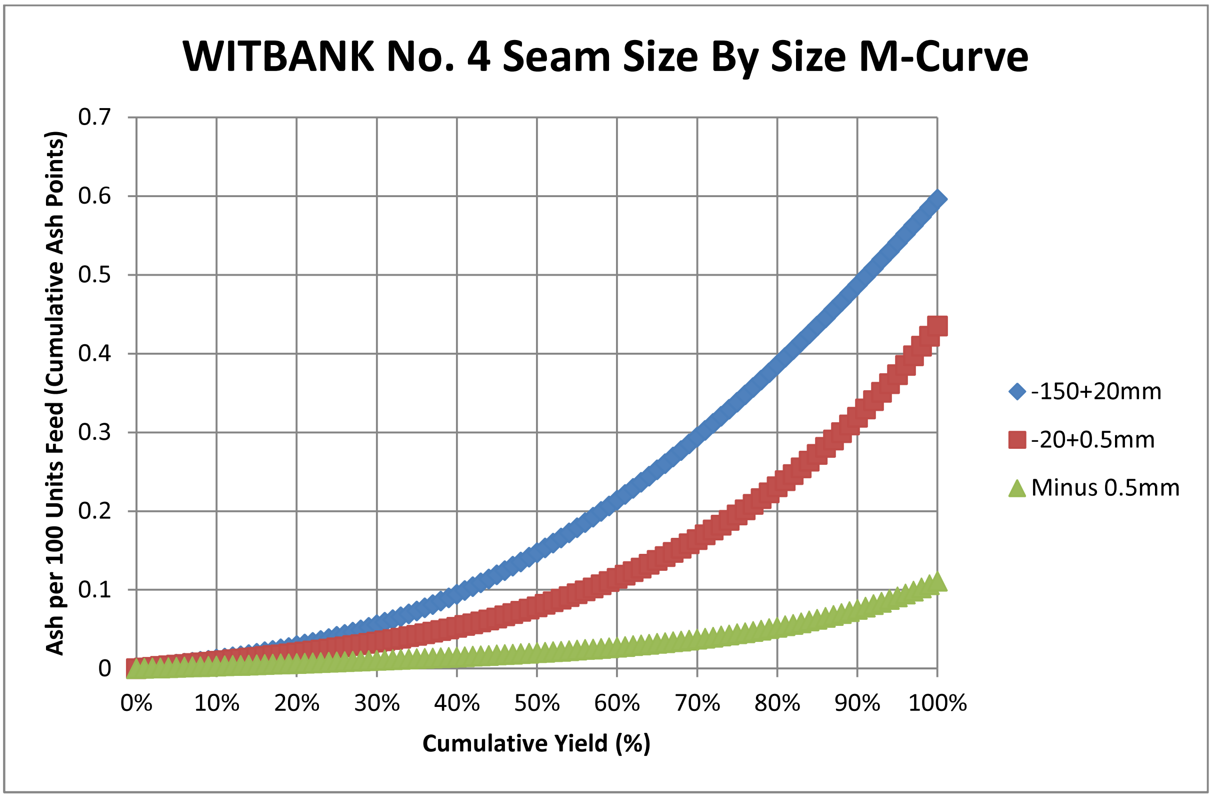

Figure 103: *Witbank Coalfield No. 4 Seam M-Curves at various liberation size fractions*

Waterberg Upper Ecca

From the Waterberg Upper Ecca M-Curves it can be seen that the improvement of the liberation coefficient with size is more complex than and not as predictable as the Witbank Coalfield No. 4 Seam. In the Waterberg Upper Ecca, multiple size fractions are considered due to the need to still establish the most suitable processing options. In addition the liberation is complex which lends itself to exploring multiple size fractions. From the results in Figure 104, the finer fraction remains more liberated than the coarser size fractions. The close to optimum liberation curve is represented by the -3+1 mm curve.

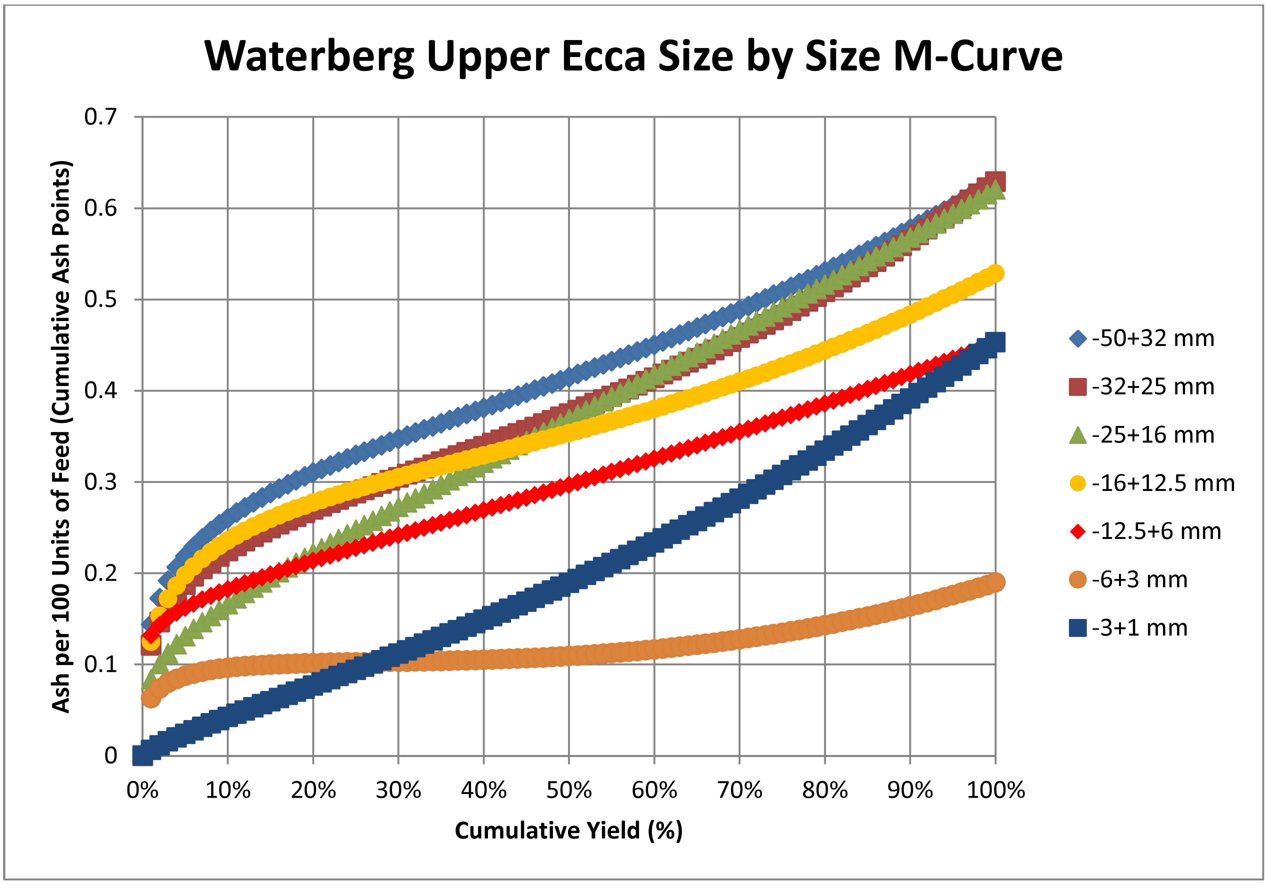

Figure 104: *Waterberg Upper Ecca M-Curves at various liberation size fractions*

6.2 Liberation Modelling of Mineral Matter

6.2.1 Mineral Liberation of Witbank Coalfield No. 4 Seam

In the curves described below, by plotting M-curves with the specific mineral data it can be seen that there is a good correlation between the plots and the liberation analysis with the QEMSEM analysis. A description of the methodology is given in Chapter 2.2.

(a) Pyrite

Based on the pyrite M-Curve it can be seen that the liberation of pyrite is poor and cannot be reduced readily with beneficiation in the lower cumulative yield section (corresponding RD 1.30-1.50). The R^2 of the fitted curve was 0.953.

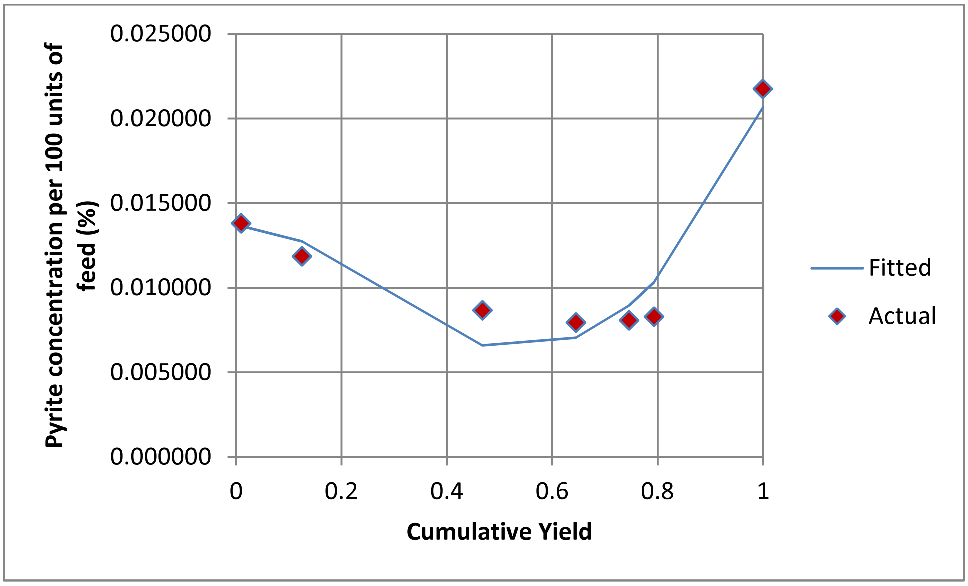

Figure 105: *Witbank Coalfield No. 4 Seam Pyrite M-Curve*

(b) Kaolinite

In the kaolinite curve it can be seen that the distribution is close to the feed line (see Chapter 2.2). This would indicate that the concentration of the kaolinite is linearly reduced with beneficiation. The R^2 of the fitted curve was 0.999.

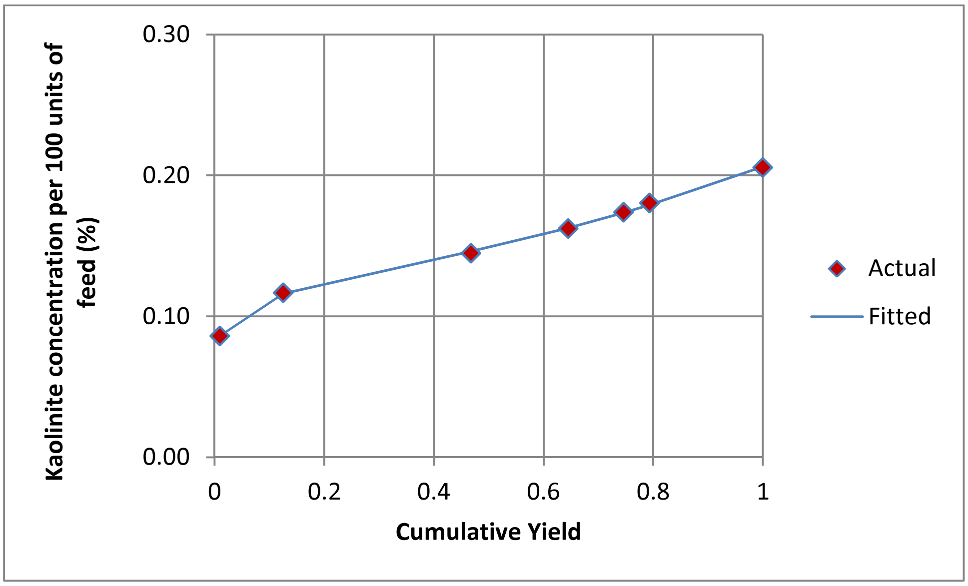

Figure 106: *Witbank Coalfield No. 4 Seam Kaolinite M-Curve*

(c) Calcite

The liberation of calcite as seen in the QEMSEM analysis is poor especially above the 1.60-1.70 RD fractions. The liberation index of calcite is very low. It should be noted that with XRD, it is difficult to distinguish the calcite and dolomite mineral phases. The R^2 obtained through curve fitting for calcite was 0.915.

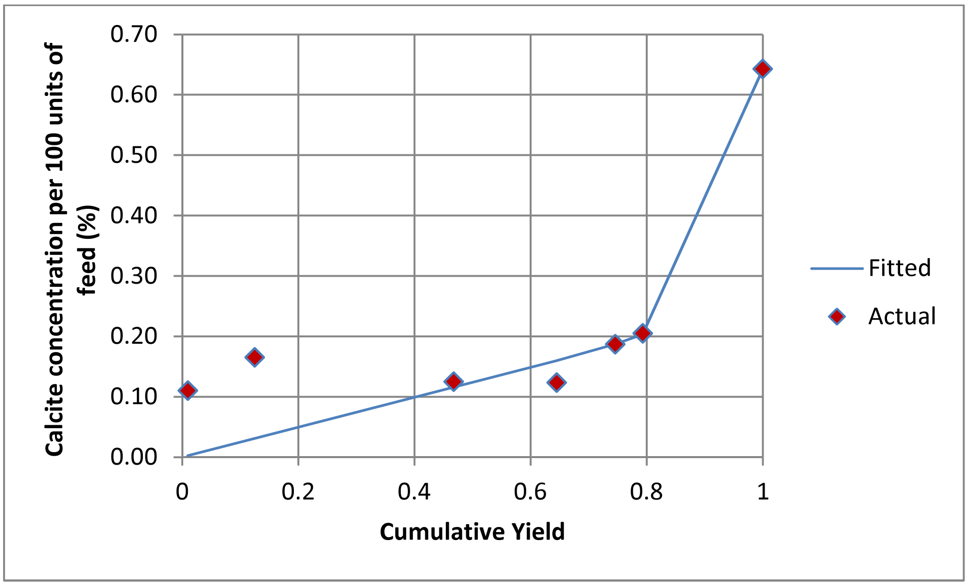

Figure 107: *Witbank Coalfield No. 4 Seam Calcite M-Curve*

6.2.2 Mineral Liberation of Waterberg Upper Ecca

(a) Pyrite

Based on the pyrite M-Curve it can be seen that the liberation of pyrite is higher compared to the Witbank Coalfield No. 4 Seam. The R^2 of the fitted curve was 0.999.

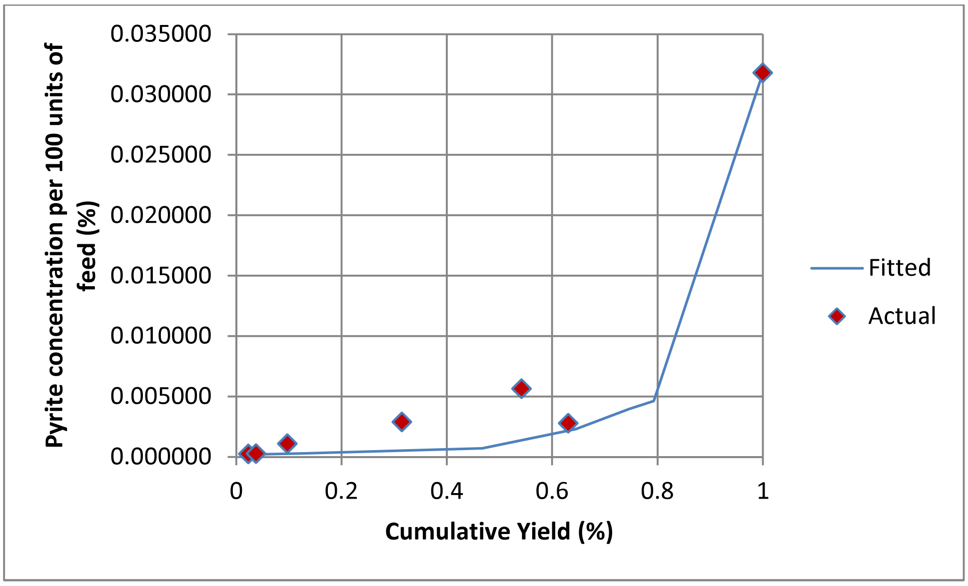

Figure 108: *Waterberg Upper Ecca Pyrite M-Curve*

(b) Kaolinite

Kaolinite, according to the M-Curve illustrates improved liberation and a higher LI. The R^2 of the fitted curve was 0.999. Figure 109 shows the increased liberation curve with a linear uniform reduction in kaolinite content through beneficiation.

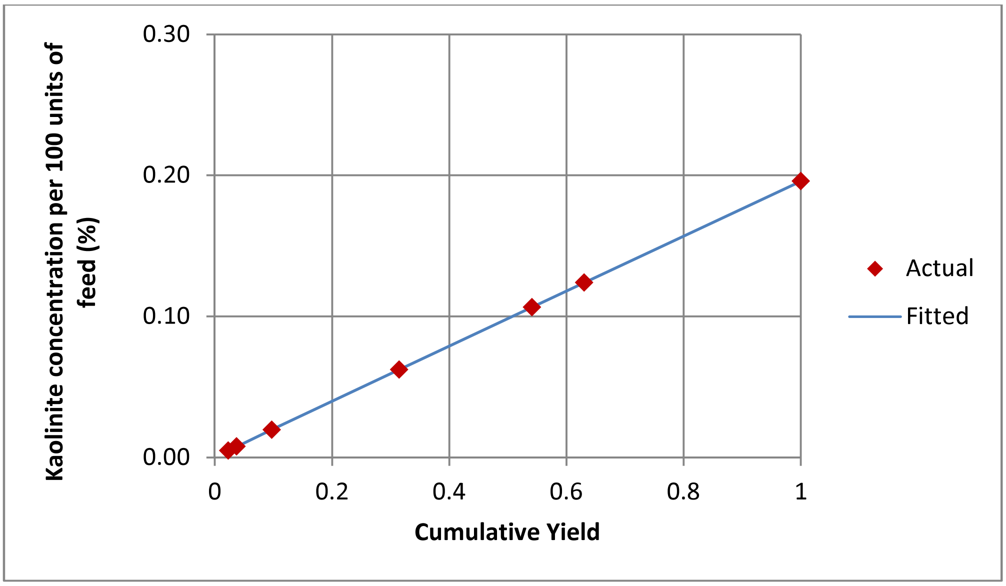

Figure 109: *Waterberg Upper Ecca Kaolinite M-Curve*

(c) Calcite

Calcite similar to the Witbank Coalfield No. 4 Seam indicates that it will be poorly liberated and will not be readily reduced. As previously mentioned with XRD, calcite and dolomite mineral phases cannot always be readily distinguished using XRD analysis and might have similar peaks. The R^2 obtained through curve fitting for calcite was 0.799.

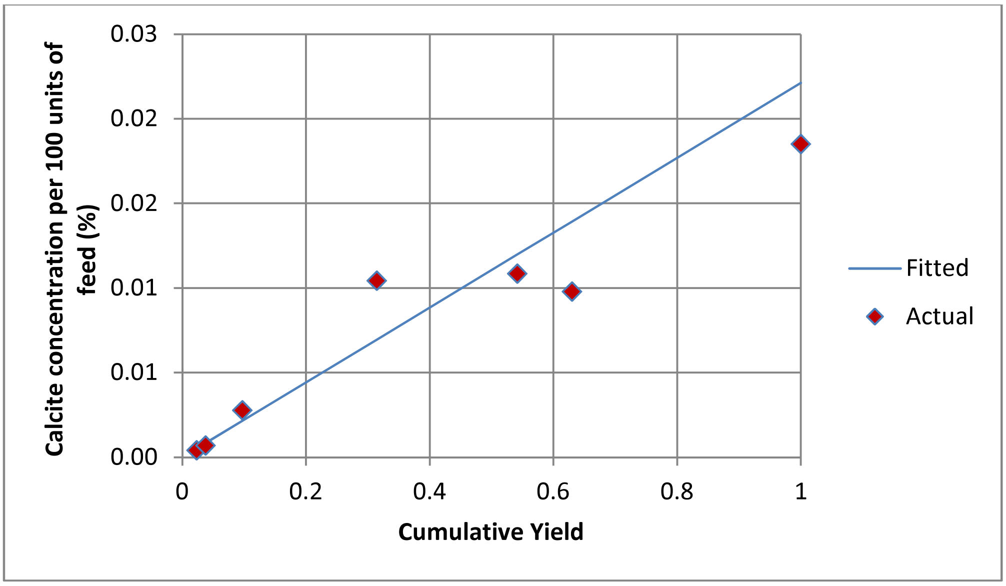

Figure 110: *Waterberg Upper Ecca Calcite M-Curve*

6.3 Liberation Modelling of Macerals

6.3.1 Maceral & Microlithotype Liberation of Witbank Coalfield No. 4 Seam

The liberation models (M-Curves) of the Witbank Coalfield No. 4 Seam macerals are given below.

Macerals:

(1) Vitrinite

Vitrinite proves to be relatively poorly liberated in the Witbank Coalfield No. 4 Seam, as was identified in the QEMSEM and petrographic analysis. The R^2 obtained through curve fitting for vitrinite was 0.999.

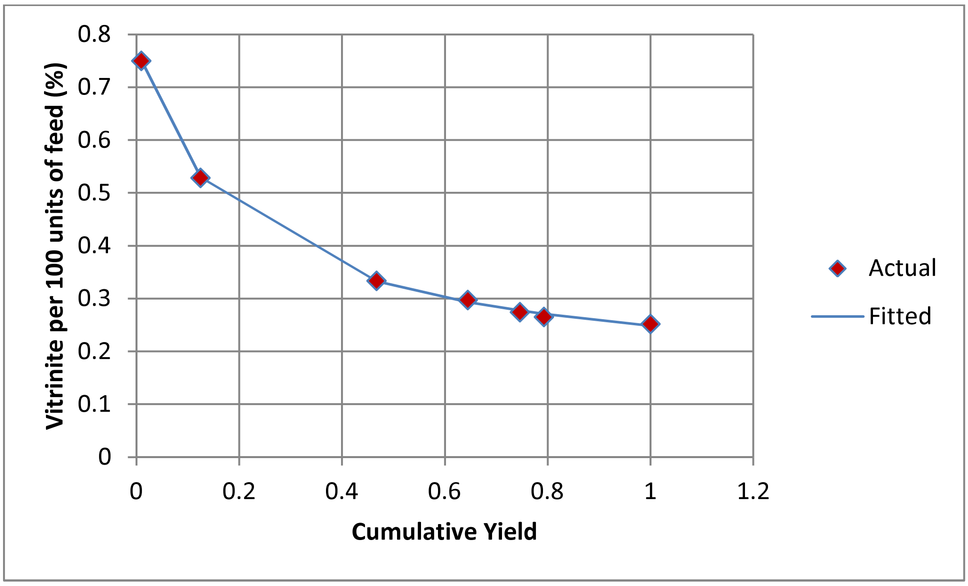

Figure 111: *Witbank Coalfield No. 4 Seam Vitrinite M-Curve*

(2) Liptinite

The density of liptinite is low at approximately 1.1, but it remains poorly liberated in all density fractions. The liptinite concentrations in the composite and the various washability density fractions were low compared to Northern Hemisphere coals. The R^2 obtained through curve fitting for liptinite was 0.992.

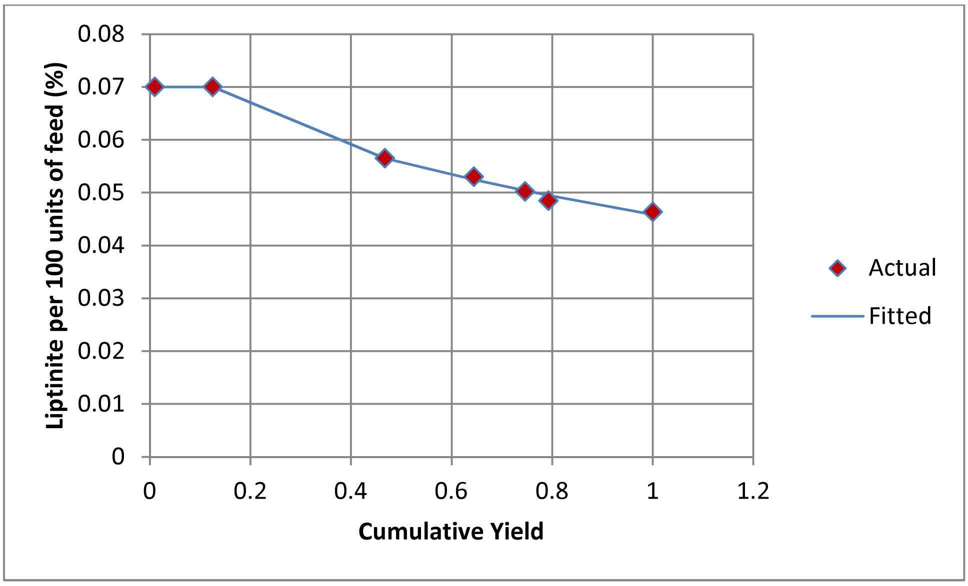

Figure 112: *Witbank Coalfield No. 4 Seam Liptinite M-Curve*

(3) Reactive Inertinite

It was found that a large portion of the inertinite was in fact reactive inertinite. The data as per Appendix F does show that a large portion of the inertinite was in fact reactive inertinite in excess of 29 %. A statistically good fit to Equation 12 was obtained. The R^2 obtained through curve fitting for reactive inertinite was 0.999.

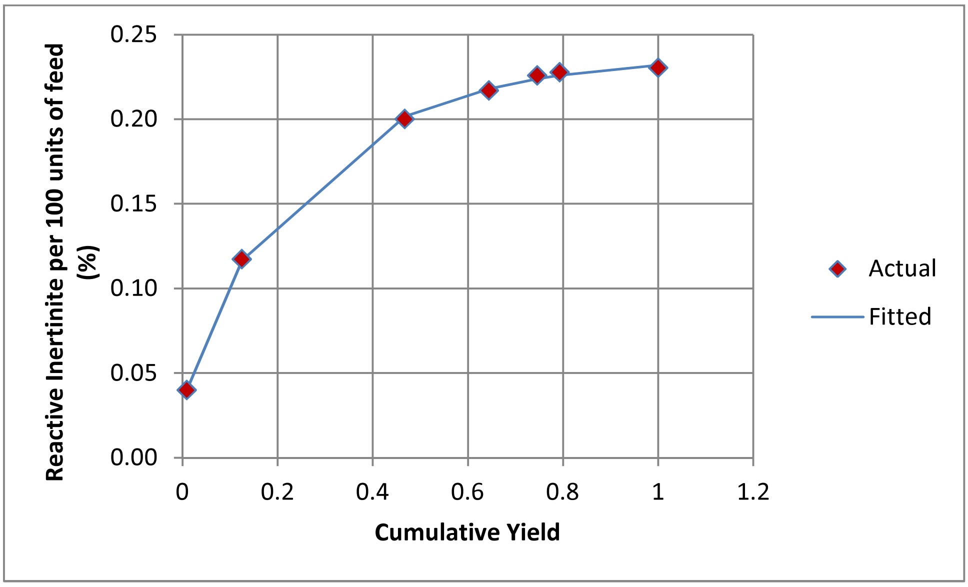

Figure 113: *Witbank Coalfield No. 4 Seam Reactive Inertinite M-Curve*

(4) Inertinite

The inertinite with a higher comparative density than other macerals can be reduced through beneficiation. The R^2 obtained through curve fitting for reactive inertinite was 0.997.

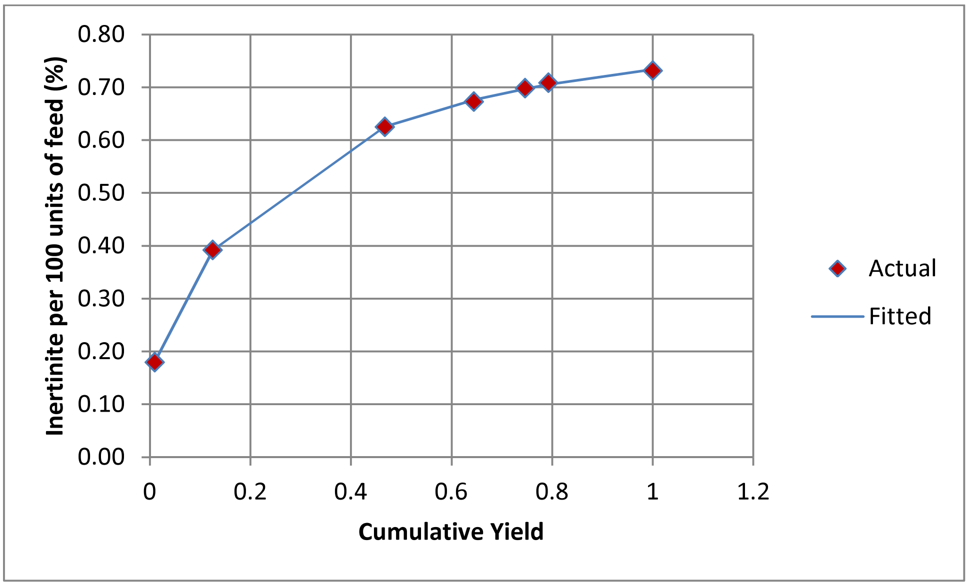

Figure 114: *Witbank Coalfield No. 4 Seam Inertinite M-Curve*

Microlithotypes

(1) Inertite

The R^2 obtained through curve fitting for inertite was 0.999.

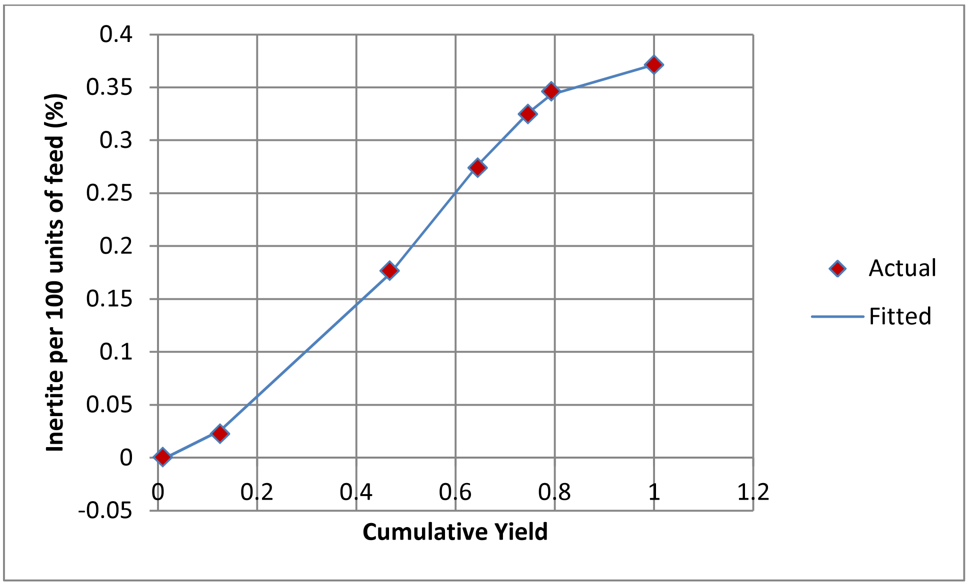

Figure 115: *Witbank Coalfield No. 4 Seam Inertite M-Curve*

(2) Minerite

The R^2 obtained through curve fitting for minerite was 0.999.

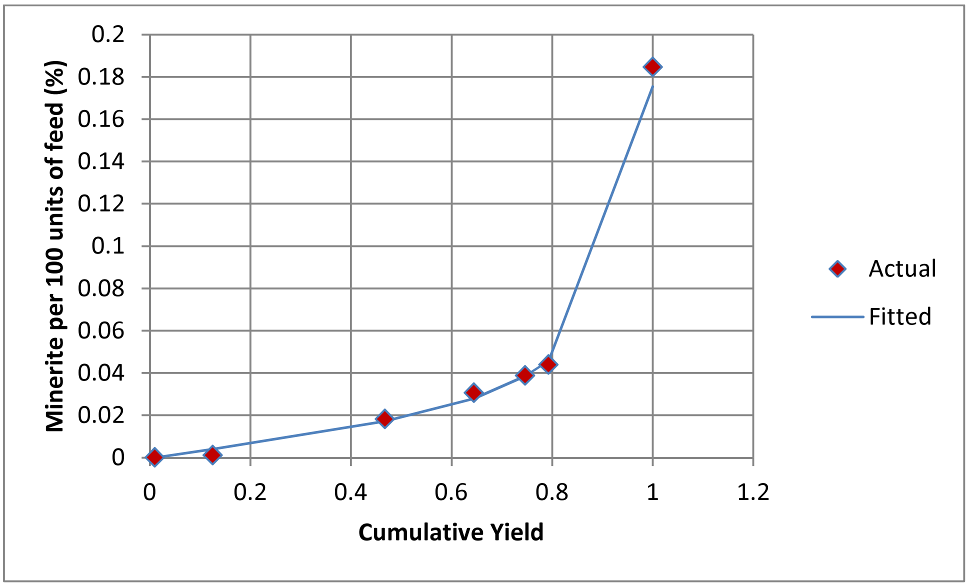

Figure 116: *Witbank Coalfield No. 4 Seam Minerite M-Curve*

6.3.2 Maceral & Microlithotype Liberation of Waterberg Upper Ecca

The liberation models (M-Curves) of the Waterberg Upper Ecca macerals are given below.

Macerals

(1) Vitrinite

The R^2 obtained through curve fitting for vitrinite was 0.999. A similar distribution to that of the Witbank Coalfield No. 4 Seam was found. The form of the Waterberg Upper Ecca vitrinite curve was however more linear.

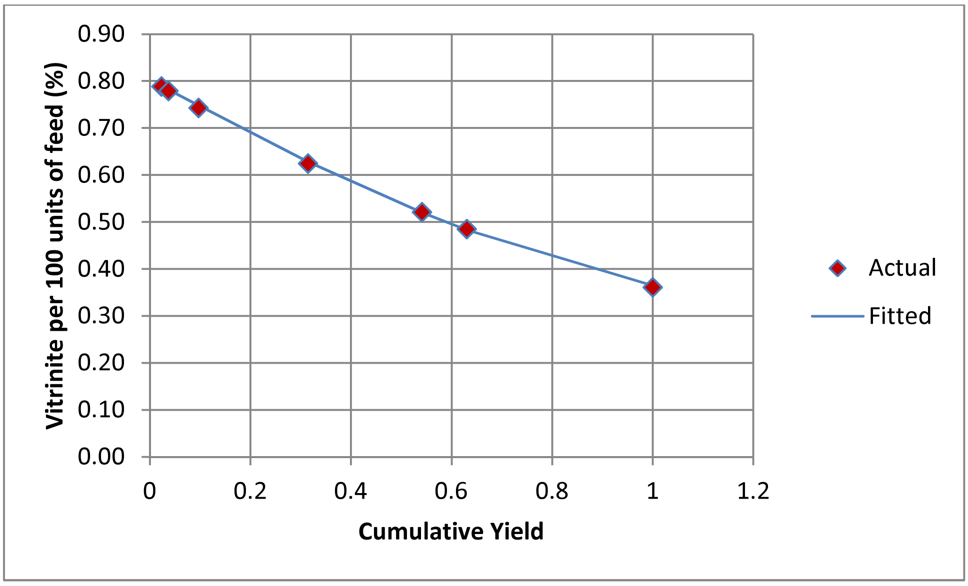

Figure 117: *Waterberg Upper Ecca Vitrinite M-Curve*

(2) Liptinite

The R^2 obtained through curve fitting for liptinite was 0.992. A different distribution to that of the Witbank Coalfield No. 4 Seam was found.

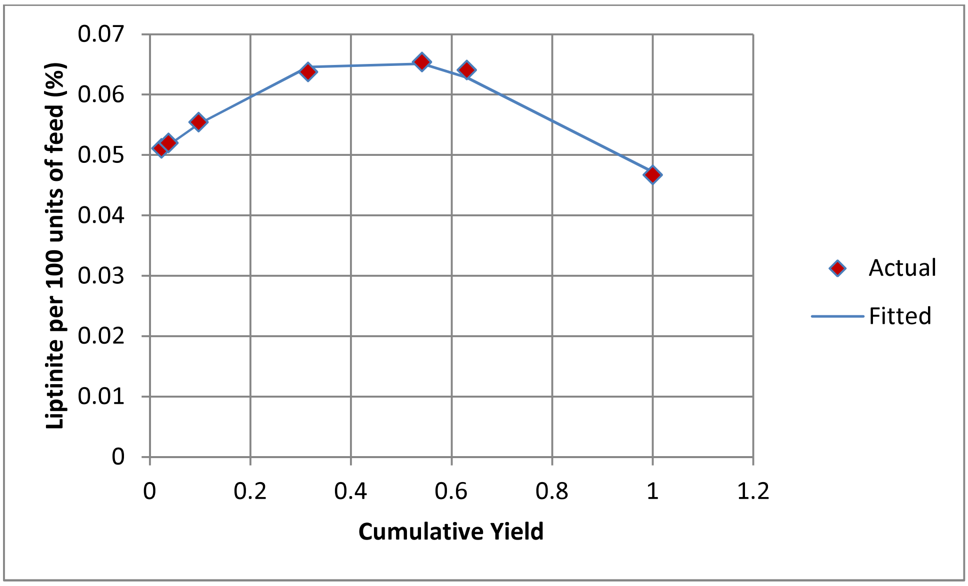

Figure 118: *Waterberg Upper Ecca Liptinite M-Curve*

(3) Reactive Inertinite

The R^2 obtained through curve fitting for reactive inertinite was 0.999. A similar distribution to that of the Witbank Coalfield No. 4 Seam was found. A similar concentration of composite reactive inertinite was also found.

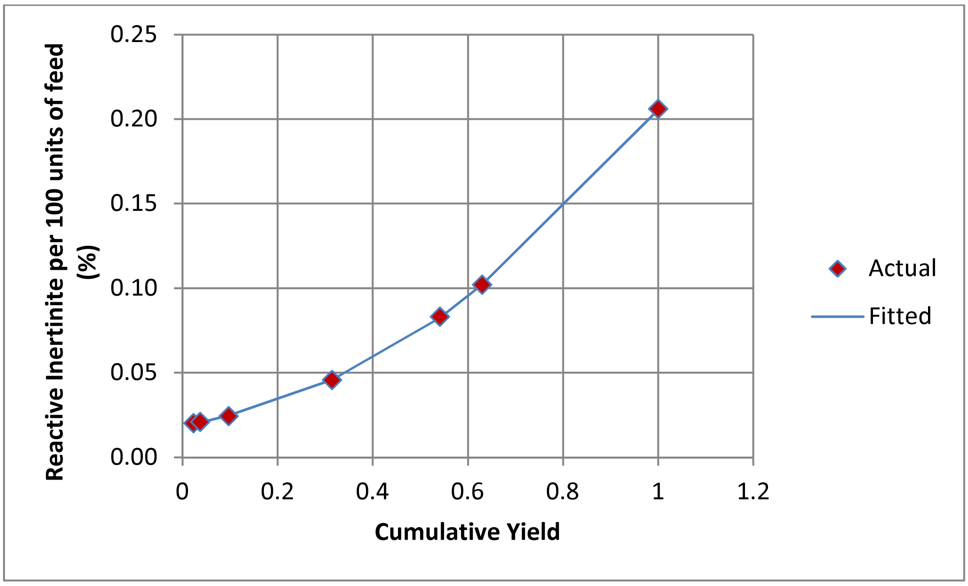

Figure 119: *Waterberg Upper Ecca Reactive Inertinite M-Curve*

(4) Inertinite

The R^2 obtained through curve fitting for inertinite was 0.999. A different distribution to that of the Witbank Coalfield No. 4 Seam was found. The concentration of inertinite in the Waterberg Upper Ecca was in fact lower than in the Witbank Coalfield No. 4 Seam.

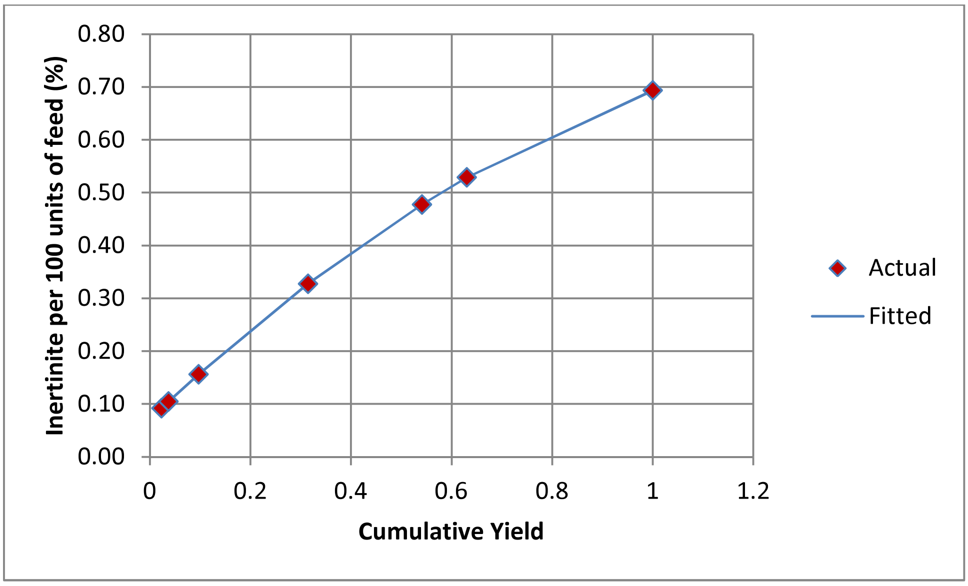

Figure 120: *Waterberg Upper Ecca Inertinite M-Curve*

Microlithotypes

(1) Inertite

The R^2 obtained through curve fitting for inertite was 0.998. In Figure 115 a different distribution to that of the Witbank Coalfield No. 4 Seam was can be observed.

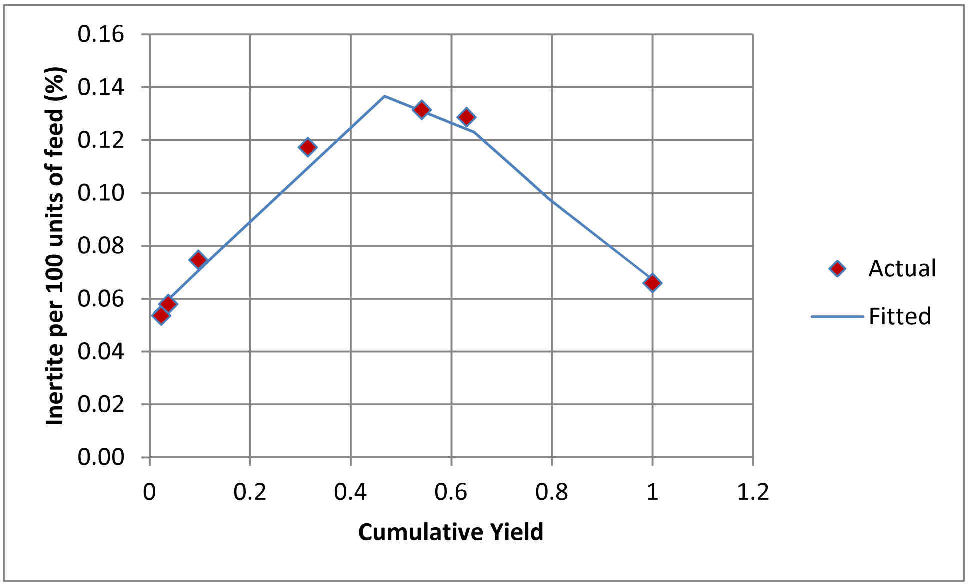

Figure 121: *Waterberg Upper Ecca Inertite M-Curve*

(2) Minerite

The R^2 obtained through curve fitting for liptinite was 0.999. A similar distribution to that of the Witbank Coalfield No. 4 Seam was found.

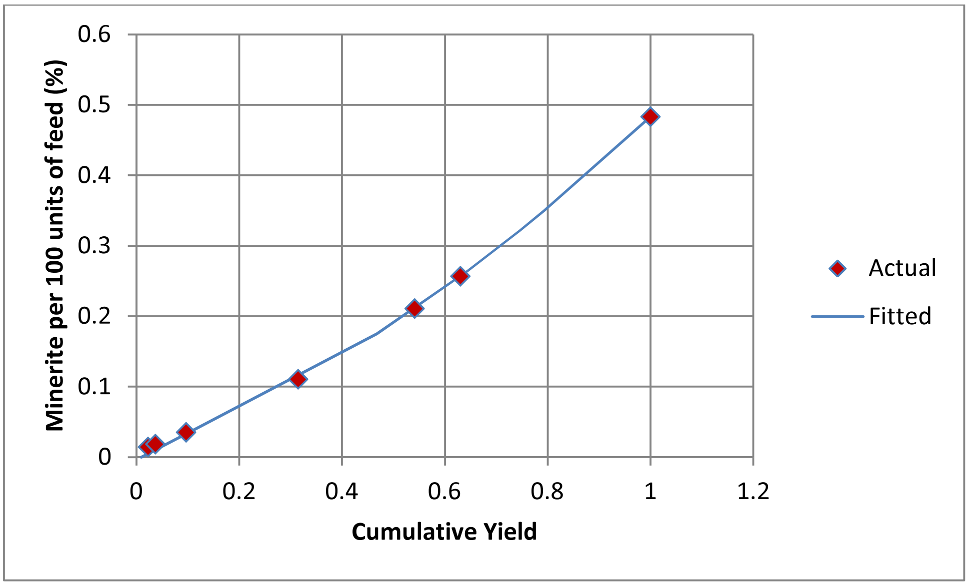

Figure 122: *Waterberg Upper Ecca Minerite M-Curve*

6.3.3 Summary Liberation of Witbank No. 4 Seam and Waterberg Upper Ecca

The Liberation Indices (LI) in Table 20 range from 0 to 100. The Liberation Index (LI) number varies depending on the degree of liberation or separation of the macerals from the mineral matter. Clean coal would theoretically have a liberation index close to I00 when it is well liberated from the mineral matter. In such an event a low ash coal could be produced. The opposite would be true for a high ash, low grade coal. When the mineral associated with an undesirable pollutant has a low LI (difficult to liberate), a challenge could exist during separation. In this research, the relationships of liberation indices of specific macerals and mineral matter and the production of high ash low grade export coal are explored in Section 7.

Table 20: *Liberation parameters for specific mineral matter and macerals*

			Parameters				Liberation Index
			A	B	C	D	LI
Witbank Coalfield No. 4 Seam	Mineral Matter	Calcite	0.154200	16.900000	0.940500	0.247700	13
		Dolomite	98.100000	8.420000	-7.587000	0.004220	14
		Kaolinite	0.149300	0.117900	0.683100	-0.089370	25
		Pyrite	0.022400	0.098870	1.424000	-0.072390	16
		Quartz	0.019550	1.284000	1.478000	0.018340	84
		Hydroxyapatite	0.069620	2.255000	-5.409000	0.001312	18
		Siderite	0.035592	6.542000	-0.823700	0.001478	76
	Macerals/Microlithotype	Vitrinite	0.839000	-3.627000	5.270000	0.395000	32
		Liptinite	-0.114200	-0.008905	15.010000	7.692000	13
		Inertinite	0.045660	0.245300	1.113000	0.014810	75
		Reactive Inertinite	0.029020	0.843600	3.042000	0.437200	63
		Inertite	-0.017660	4.935000	-7.653000	5.417000	62
		Minerite	-0.031580	20.690000	32.790000	-50.033000	89
Waterberg Upper Ecca	Mineral Matter	Calcite	0.000000	4.165000	-0.108400	0.000221	51
		Dolomite	0.000999	1.086000	-0.002348	-0.000926	52
		Kaolinite	0.000037	0.597400	0.048210	0.001919	73
		Muscovite	0.000001	-0.291400	0.108500	0.000408	65
		Pyrite	0.000000	-0.713300	0.149900	0.000094	78
		Quartz	0.000044	0.694200	0.043260	0.001255	96
		Rutile	0.000052	0.569600	0.018520	0.000000	53
		Siderite	0.000006	2.237000	-0.025850	0.000108	54
	Macerals/Microlithotype	Vitrinite	2.446000	13.550000	-11.890000	3.106000	65
		Liptinite	2.569000	621.700000	-398.300000	68.730000	16
		Inertinite	0.078900	1.081000	0.229300	0.195800	76
		Reactive Inertinite	0.526500	53.900000	-56.730000	17.220000	67
		Inertite	1.502000	287.100000	-281.100000	72.430000	78
		Minerite	0.029810	3.916000	-2.567000	0.810400	90