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Mathematical modelling of the coal instantaneous ash vs density curve

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ABSTRACT

The advancement of computer applications in the coal industry is focusing interest on the presentation of washability data by mathematical functions. The normal method of presenting washability data is in the form of five curves, usually fitted by eye or by cubic spline functions. It has been shown that coal washability can be characterised by two basic relations: the instantaneous ash vs relative density relationship and the instantaneous yield vs relative density relationship. In a new approach to the mathematical modelling of the instantaneous ash vs relative density relationship, the application of the algorithm to a data set from a mine in central Queensland was successful.

INTRODUCTION

Coal washability data is one of the fundamental inputs into coal quality assessment, mine planning and scheduling, preparation plant design and operation, and coal yield optimisation. These data are normally obtained from laboratory tests undertaken according to, for instance, Australian Standard AS 1661-1979. During these tests, coal is placed in a liquid of predetermined density. The float material which floats is dried, weighed and heat-treated under specific conditions to determine the percentage ash. This gives the percentage of material floating (incremental yield) and the ash content (incremental ash) for a series of densities. These results are then presented in the form of tables and curves.

Due to the advancement of computer applications in the coal industry, presentation of washability data by mathematical functions has been attracting increasing interest. Armstrong and Whitmore (1981) have shown that the washability data can be represented by the following two relationships:

a. the instantaneous ash vs relative density relationship, and
b. the instantaneous yield vs relative density relationship.

Their paper serves as a base for further examination of the relations. In particular, a new approach to mathematical modelling of the first relationship is presented here.

MATHEMATICAL MODELLING OF THE INSTANTANEOUS ASH VS DENSITY RELATIONSHIP

The proposed model for the instantaneous ash vs density relationship

Armstrong and Whitmore (1981) initiated the concept of mathematical modelling of the washability relations. To model the ash distribution, they present a linear equation relating instantaneous ash to the reciprocal of the relative density. Their equation can be put in the form

$$a(\rho) = \left[\frac{A_h\rho_a - A_l\rho_c}{\rho_a - \rho_c}\right] + \left[\frac{A_l - A_h}{\frac{1}{\rho_c} - \frac{1}{\rho_a}}\right] \times \frac{1}{\rho} \qquad (1)$$

where ρ is the density of an arbitrary particle (particles) in the sample, $a(\rho)$ is the ash fraction of the same particle (particles). The significance of the model parameters are as follows.

ρ_c - the density of pure coal.

A_l - the "Minimum Ash" parameter, is the ash fraction of pure coal.

ρ_a - the "Maximum Density" parameter, is the density of pure ash.

A_h - the "Maximum Ash" parameter, is the ash fraction of pure ash.

Float and sink analyses are undertaken over a range of densities, say, from 1.30 to 2.0. These analyses give an average ash content of particles with relative density lying in a certain range rather than at a specific density. This difficulty can be overcome by using the midpoint of the density range as an initial estimate of the relative density corresponding to the ash assay and later adjusting this value in order to improve the fit of the curve. Armstrong and Whitmore used a fitting procedure which is outlined below.

a. The midpoint of the density range is used as an initial estimate of the relative density corresponding to the ash assay.
b. Preset values of $A_l = 0.0$ and $A_h = 0.9$ are used to estimate ρ_c and ρ_a by fitting an ash assay vs density curve with the use of a least squares method and by extrapolating to $A(\rho) = 0.0$ and 0.9 respectively.
c. Adjustment of the relative density corresponding to the ash assay is undertaken to improve the fit of the curve.
d. The yield vs density relationship curve is fitted and A_l and ρ_c are adjusted to obtain the final model parameters.

Although successful, this fitting procedure can be cumbersome. Ilievski (1987) adopted and improved the Armstrong and Whitmore approach. The improvements were made mainly by using a different algorithm to estimate the model parameters.

Derivation of the fitting algorithm

Regardless of the final values taken by the coal washability parameters, equation 1 can be placed in the following form.

$$a(\rho) = k + m/\rho \qquad (2)$$

The introduction of a third parameter c greatly improves the quality of fitting in general and especially where the cumulative ash per cent is concerned. This is shown is equation 3.

$$a(\rho) = k + m/(\rho + c) \qquad (3)$$

Let the instantaneous yield function be $w(\rho)$. Then the incremental yield ($W(\rho_i)$) and the corresponding ash content ($A(\rho_i)$) at ith separating density are

$$W(\rho_i) = \int_{\rho_{i-1}}^{\rho_i} w(\rho)d\rho \qquad (4)$$

and

$$A(\rho_i) = \frac{\int_{\rho_{i-1}}^{\rho_i} a(\rho)w(\rho)d\rho}{\int_{\rho_{i-1}}^{\rho_i} w(\rho)d\rho} \qquad (5)$$

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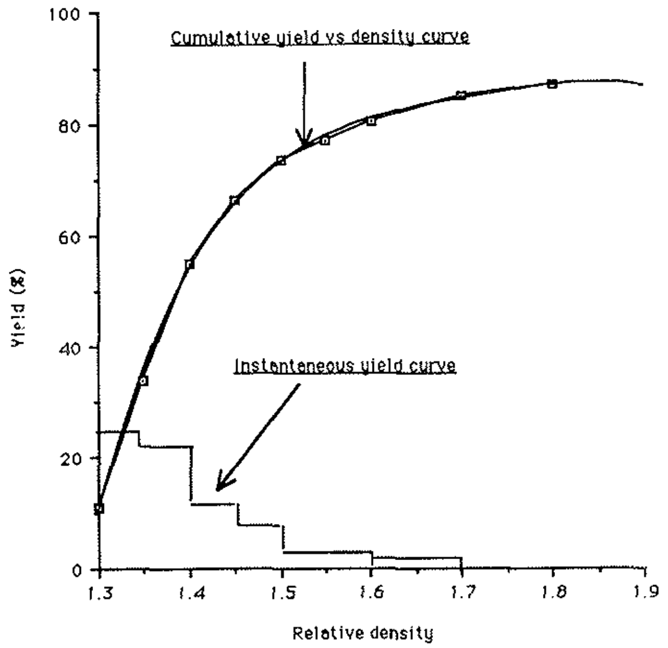


FIG 1 - Yield vs density relationship curves derived from data in AS 1661 - 1979 (*not in same scale*).

If the cumulative yield vs relative density curve is approximated by connecting the adjacent points using straight lines (see Figure 1),

$W(\rho) = k\rho + b \quad$ for $\rho i - 1 \leq \rho \leq \rho i \qquad (6)$

then

$w(\rho) = k\,(constant)$ for $\rho i - 1 \leq \rho \leq \rho i$

Substituting $w(\rho) = k$ into equation (5) gives

$$A(\rho_i) = \frac{\int_{\rho_{i-1}}^{\rho_i} a(\rho)d\rho}{\rho_{i-1} - \rho_i} \qquad (7)$$

Equation 7 indicates that under the straight line approximation, $A(\rho_i)$ is independent of $W(\rho_i)$. $A(\rho_i)$ can be viewed as the average instantaneous ash over the density i-1 to i for a coal sample. Since $A(\rho)$ can be known from the coal washability data, equation 7 can be used for the estimation of the instantaneous ash vs density function $a(\rho)$.

Suppose $a(\rho)$ has the form of equation 3. There are three parameters that need to be estimated. A popular way for the estimation is by the least squares method. With the parameter c in equation 3, equation 7 is no longer a linear model. This makes the least squares method complex to apply. Furthermore, there will be no systematic solution if general methods to deal with the non-linear model are used. To overcome these problems, the following procedure was used.

a. Set a value for c which allows equation 7 to become a linear model. It can be noted that when C = 0.0, equation 3 reduces to equation 2.

b. Use the general least squares method to fit this reduced linear model. The error model is

$$\min x^2 = \sum_{i=1}^{n}[A^*(\rho_i) - A(\rho_i)]^2 \qquad (8)$$

where i is the ith density, n is the number of separating densities used, $A^*(\rho_i)$ is the float and sink result of the incremental ash per cent from ρ_i - 1 to ρ_i. $A(\rho_i)$ is the counterpart of $A^*(\rho_i)$ calculated from equation 7. The unit weight was used for all the points.

c. Adjust the c value and proceed iteratively until a overall min x^2 is obtained.

This procedure still has cumbersome aspects. After some experimentation, it was found that the overall "optimum" value for c is always between 0.0 and 20. With this approach, a systematic version of the program was obtained.

One "imperfection" of the program is that ρ_0 is needed as ρi-1 is used when $i = 1$. ρ_0 ranges from 1.24 (the lightest particle of coal) to the first separating density in the float and sink test, normally 1.30. However, as soon as a best value in terms of minimising x^2 is found for a coal sample in a type of coal, this value can also be used for other samples for that coal seam without significantly affecting the optimum result.

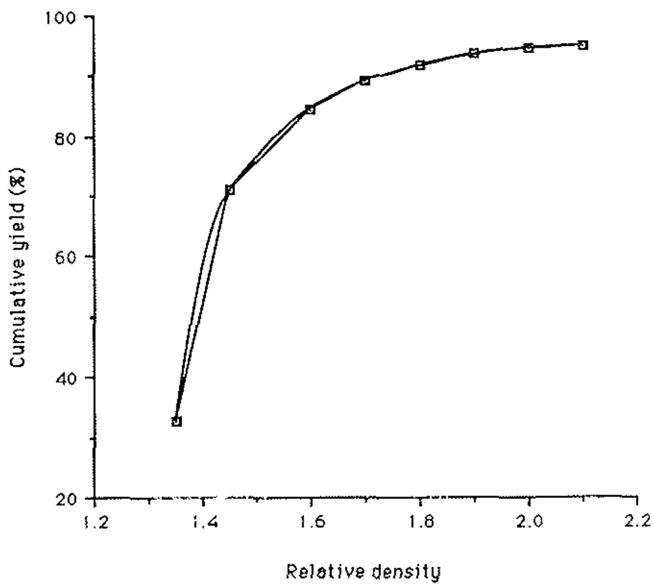


FIG 2 - Cumulative yield vs density relationship (average coal quality from two pits).

Discussion on the straight line approximation

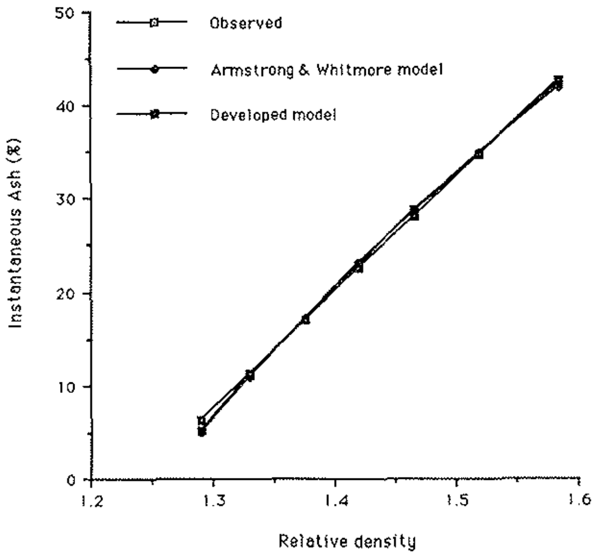
In the derivations above, the cumulative yield vs relative density curve is approximated by connecting the adjacent points using straight lines. This approximation is referenced in this work as the straight line approximation. The justification for using a straight line approximation in developing the algorithm is outlined below.

a. This approximation is common industry practice in most applications when coal washability tables are employed.

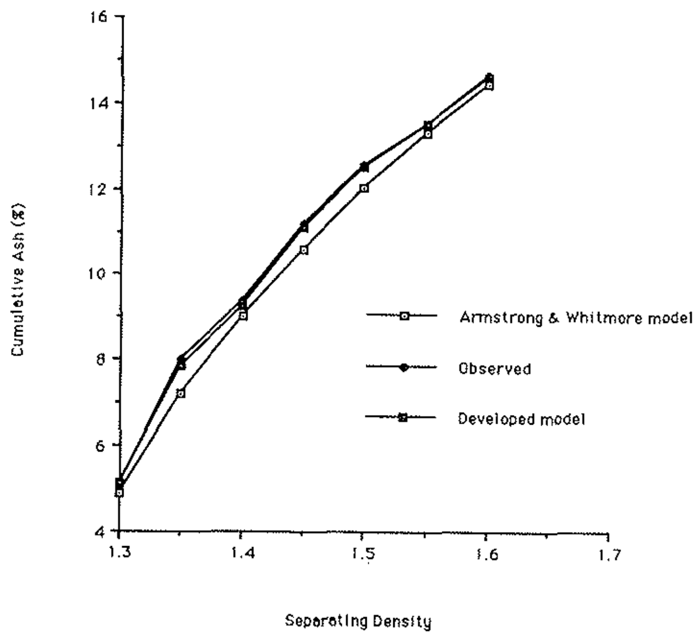
b. Where coal has been analysed according to, say, AS 1661-1979, it can be seen that for most density intervals, this approximation is very close to the underlying "true" curves. This is illustrated in Figures 1 and 2.

c. In the case where certain sections of the cumulative yield vs density curves (such as the first part in Figure 2) are not well approximated by straight lines, the optimum results are only distorted over the deviating fractions of the curves (equation 8).

Previous work (Clarkson and Leach, 1981; Ilievski, 1987) indicated that the relationship between instantaneous ash and relative density is almost constant over a certain area. This was also verified by intensive data (213 bore cores from each of the two plies in a mined out area) obtained from a central Queensland mine in this project. This suggests that the straight line approximation may be only used in deriving the algorithm above. The mathematical modelling of the instantaneous yield vs density relationship can be carried out independently. It will also be shown later that the algorithm developed above is not sensitive to the number of densities over which the coal sample has been analysed.



(3a) Instantaneous ash per cent vs density relationship.



3(b) Cumulative ash per cents separating densities relationship.

FIG 3 - Comparisons with the model of Armstrong and Whitmore (1981).

COMPARISON WITH THE OTHER FITTING METHODS

Comparisons undertaken

It was difficult to make a complete comparison between this method and others (Armstrong and Whitmore, 1981; Ilievski, 1987) since the computer programs for the other methods were not available. However, the following was done for the comparison.

a. Fitting the model using the algorithm above to the example given by Armstrong and Whitmore (1981) and analysing the results.
b. Fitting the model using the algorithm above to the fitting results given by Ilievski (1987) and analysing the results.
c. Fitting the model using the algorithm above and comparing it with the model fitted by the same algorithm but with $c = 0.0$.

Armstrong and Whitmore's results

The fitting example, coal No 3 (Armstrong and Whitmore, 1981) was also fitted by the algorithm developed. The model for the instantaneous ash vs relative density curve fitted by Armstrong and Whitmore's "COALFIT 1" program is

$$a(\rho) = 203.43 - \frac{256.15}{\rho} \qquad (9)$$

The model obtained from the algorithm developed is

$$a(\rho) = 1787.6 - \frac{25276.8}{(\rho + 12.9)} \qquad (10)$$

The graphic presentation of these formulae together with the observed values corresponding to the adjusted densities by Armstrong and Whitmore is shown in Figure 3. From this figure, it can be seen that the models are very close except the first point which is at the extremity for practical curve use.

The results for incremental ash per cents at relative density intervals are listed in Table 1. The results for cumulative ash per cents are listed in Table 2 and Figure 6. Table 1 shows little difference for the two methods. However, Table 2 and Figure 3 show that the method developed performs much better than the other method in terms of cumulative ash per cents.

It should be mentioned that the parameters in the model obtained from the algorithm developed for the instantaneous ash vs relative density relationship do not have any physical meaning as in the other models.

TABLE 1

Comparison of incremental ash per cents at density intervals with the model of Armstrong and Whitmore (1981).

Relative density intervals	Observed Ash(%)	Arm. & Whit. model Ash(%)	Developed model Ash(%)
F 1.3	5.1	4.90	5.12
1.3 - 1.35	11.0	10.87	10.69
1.35 - 1.4	16.9	17.17	16.90
1.4 - 1.45	22.8	23.07	23.06
1.45 - 1.5	28.8	28.61	29.19
1.5 - 1.55	34.6	34.93	35.31
1.55 - 1.6	42.2	41.84	41.38

TABLE 2

Comparison of cumulative ash per cents with the model of Armstrong and Whitmore (1981)

Relative density	Observed Ash(%)	Arm. & Whit. model Ash(%)	Developed model Ash(%)
1.3	5.10	4.90	5.12
1.35	8.00	7.21	7.86
1.4	9.37	9.03	9.25
1.45	11.19	10.60	11.12
1.5	12.54	12.01	12.51
1.55	13.53	13.32	13.52
1.6	14.62	14.45	14.59

Ilievski's results

Two typical fittings for the bulk samples from Ilievski (1987) are listed in Tables 3, 4, 5 and 6. Figures 4 and 5 are the graphic presentations of Tables 4 and 6. The curve fit from the algorithm developed is obviously good especially where the cumulative ash per cent vs density curve is concerned.

TABLE 3

Comparison of incremental ash per cents at density intervals with the model of Ilievski (1987) (BBC bulk sample -0.25 + 0.125 mm).

Relative density intervals	Observed Ash(%)	Ilievski's model Ash(%)	Developed model Ash(%)
F 1.3	5.2	1.1	3.4
1.3 - 1.35	6.6	5.3	6.1
1.35 - 1.4	10.0	11.2	10.5
1.4 - 1.45	14.3	16.5	14.8
1.45 - 1.5	17.4	21.4	19.2
1.5 - 1.55	22.6	25.9	23.5
1.55 - 1.6	28.1	30.2	27.8
1.6 - 1.7	34.0	36.0	34.1
1.7 - 1.8	42.8	43.1	42.5
1.8 - 1.9	51.9	49.5	50.7
1.9 - 2.0	58.4	55.2	58.8

TABLE 4

Comparison of cumulative ash per cents with the model of Ilievski (1987). (BBC bulk sample -0.25 + 0.125 mm.)

Relative density	Observed Ash(%)	Ilievski's model Ash(%)	Developed model Ash(%)
1.3	5.2	1.1	3.4
1.35	5.67	2.69	4.28
1.4	6.24	3.97	5.11
1.45	7.39	5.05	6.50
1.5	8.16	6.02	7.48
1.55	8.75	6.89	8.13
1.6	9.45	7.69	8.85
1.7	10.72	9.07	10.15
1.8	11.48	10.33	10.92
1.9	12.64	11.36	12.06
2.0	13.54	12.37	13.00

TABLE 5

Comparison of incremental ash per cents at density intervals with the model of Ilievski (1987). (BBC bulk sample - 12.7 + 6.35 mm.)

Relative density intervals	Observed Ash(%)	Ilievski's model Ash(%)	Developed model Ash(%)
F 1.3	3.3	4.5	3.3
1.3 - 1.35	7.6	8.8	6.9
1.35 - 1.4	12.3	14.3	12.6
1.4 - 1.45	17.3	19.3	17.9
1.45 - 1.5	22.4	23.8	23.0
1.5 - 1.55	27.4	28.1	27.7
1.55 - 1.6	32.5	32.1	32.2
1.6 - 1.7	39.6	37.3	38.4
1.7 - 1.8	46.3	43.9	46.0
1.8 - 1.9	52.3	49.8	52.9
1.9 - 2.0	59.1	55.1	59.1

TABLE 6

Comparison of cumulative ash per cents with the model of Ilievski (1987). (BBC bulk sample - 12.7 + 6.35 mm.)

Relative density	Observed Ash(%)	Ilievski's model Ash(%)	Developed model Ash(%)
1.3	3.3	4.5	3.3
1.35	4.30	5.47	4.11
1.4	4.89	6.07	4.74
1.45	5.36	6.48	5.24
1.5	5.63	6.78	5.52
1.55	5.80	7.00	5.69
1.6	5.92	7.20	5.81
1.7	6.07	7.43	5.96
1.8	6.20	7.59	6.09
1.9	6.35	7.73	6.25
2.0	6.52	7.78	6.42

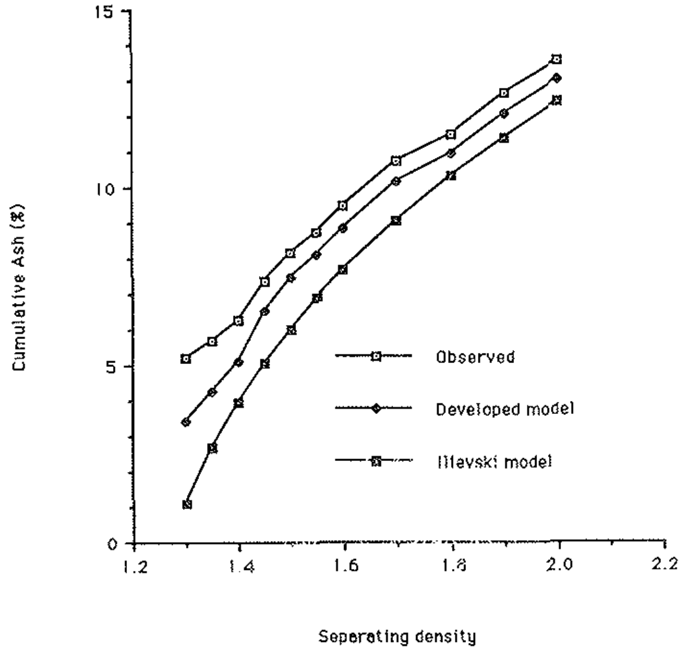


FIG 4 - Cumulative ash per cent comparisons with the model of Ilievski (1987) (-0.25 + 0.125 mm size).

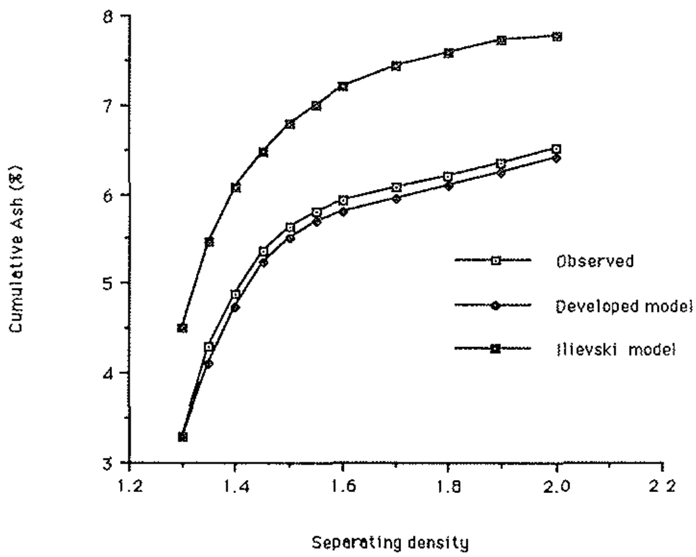


FIG 5 - Cumulative ash per cent comparisons with the model of Ilievski (1987) (-12.7 + 6.35 mm size).

Results when $c = 0.0$

A typical drill hole in the data of the mine is presented to illustrate the comparison. For $c = 0.0$, the model for the instantaneous ash vs relative density is

$$a(\rho) = 167.50 - \frac{218.52}{\rho} \tag{11}$$

The optimum model obtained after introducing parameter c is

$$a(\rho) = 715.63 - \frac{5769.86}{(\rho + 6.8)} \tag{12}$$

The prediction results are listed in Tables 7 and 8 and Figure 6. The improvements can easily be observed.

TABLE 7
Comparison of incremental ash per cents at density intervals with the case of c = 0.0 for a typical bore.

Relative density intervals	Observed Ash(%)	Developed model (C=0.0) Ash(%)	Developed model Ash(%)
F 1.35	7.50	5.03	7.21
1.35 - 1.45	12.39	11.35	11.98
1.45 - 1.6	21.28	24.09	22.53
1.6 - 1.7	32.35	35.02	32.80
1.7 - 1.8	40.69	42.60	40.78
1.8 - 1.9	50.07	49.35	48.59
1.9 - 2.0	57.22	55.42	56.21
2.0 - 2.1	62.25	60.89	63.66

TABLE 8
Comparison of cumulative ash per cents with the case of c = 0.0 for the typical bore core.

Relative density	Observed Ash(%)	Developed model (C=0.0) Ash(%)	Developed model Ash(%)
1.35	7.50	5.03	7.21
1.45	10.64	9.09	10.27
1.6	12.31	11.41	12.20
1.7	13.22	12.51	13.13
1.8	13.77	13.11	13.69
1.9	14.56	13.90	14.45
2.0	15.29	14.61	15.16
2.1	15.49	14.81	15.37

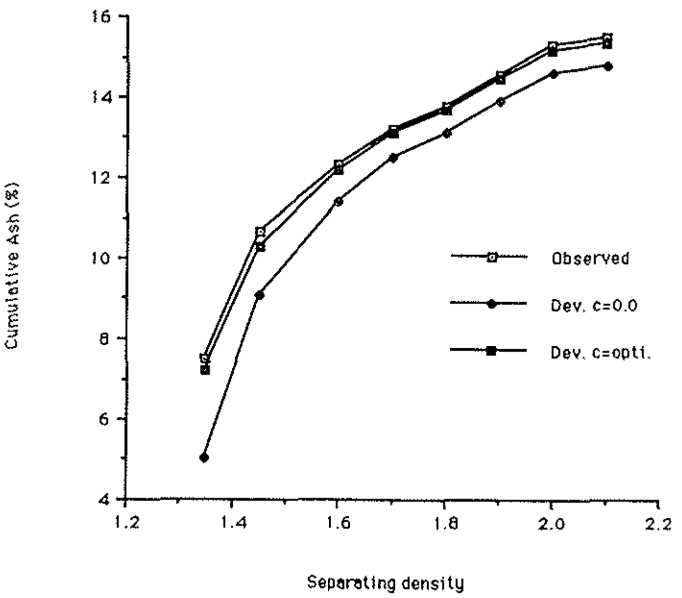


FIG 6 - Comparison of cumulative ash per cents between the case of c = 0.0 and optimum c value.

Sensitivity to the number of points analysed for a coal sample

The developed algorithm is not sensitive to the number of separating densities used for the float and sink test on the sample. This is the result of the following.

a. In general, the curves generated by the model as expressed in equation 3 take the shape of the instantaneous ash vs relative density curve and moreover it is of "smooth shape" (see Figure 3).
b. Most parts of the cumulative yield vs relative density curve can be approximated by straight lines and in the parts that this is difficult, there is only partial influence on the general results in the developed algorithm.

The results listed in Tables 9 and 10 were obtained by assuming that the bore core presented above (Tables 7 and 8) was only analysed for five densities. It can be seen that the disturbance is small. It should be noted that this is only an illustration. These specific results should not be generalised.

TABLE 9
Results of incremental ash per cents at density intervals for the reduced sample.

Relative density intervals	Observed Ash(%)	Developed model Ash(%)
F 1.35	7.50	7.26
1.35 - 1.45	12.39	11.78
1.45 - 1.7	23.85	26.00
1.7 - 1.9	45.63	43.70
1.9 - 2.1	58.23	58.86

TABLE 10
Results of cumulative ash per cents for the reduced sample.

Relative density	Observed Ash(%)	Developed model Ash(%)
1.35	7.50	7.26
1.45	10.64	10.16
1.7	13.22	13.26
1.9	14.56	14.51
2.1	15.49	15.46

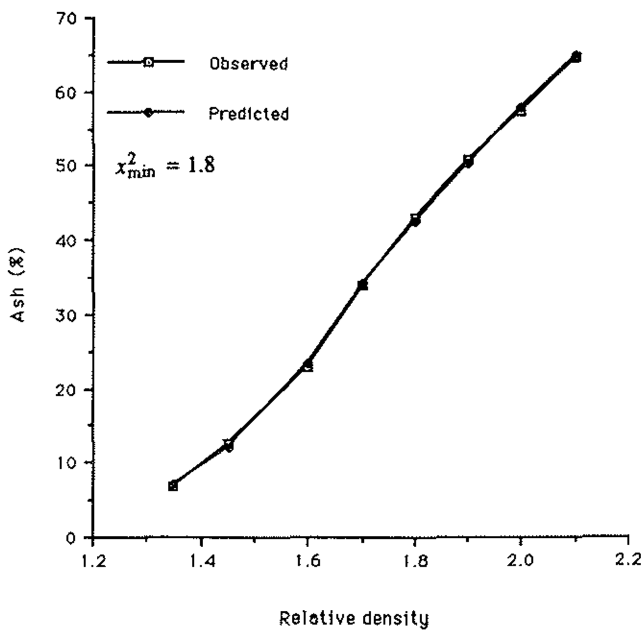


FIG 7 - An example from the group where x^2_{min} <10.0 .

Fitting results for the borecores in the area of two mining pits

A total of 78 bore cores in an area were fitted using the algorithm. Fifty-four (69.2 per cent) of the bore cores were fitted with the value of x^2_{min} less than 10.0. Nineteen (24.4 per cent) of the bore cores were fitted with x^2_{min} values ranging from 10.0 to 30.0. Only five (6.4 per cent) bore cores were fitted with x^2_{min} values greater than 30.0. In these cases, the original test data were certainly doubtful. Figure 7 to Figure 9 show some typical prediction results in each group. In these figures the incremental ash values were

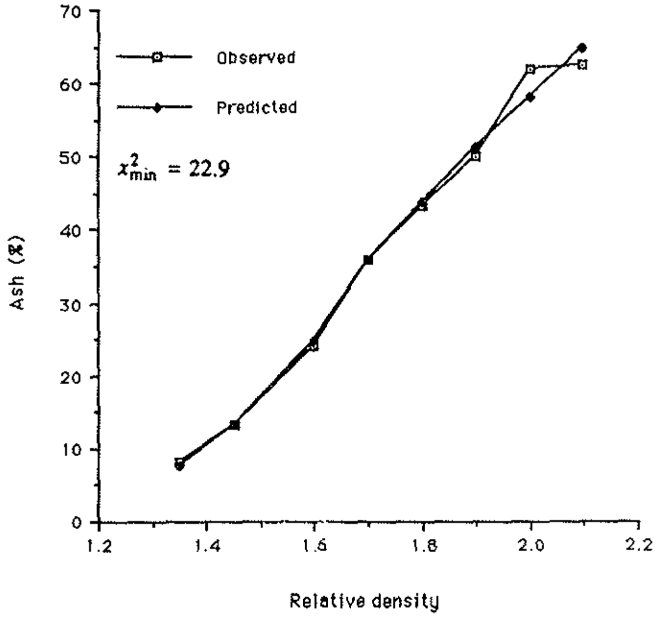


FIG 8 - An example from the group where $10.0 < \chi^2_{min} < 30.0$.

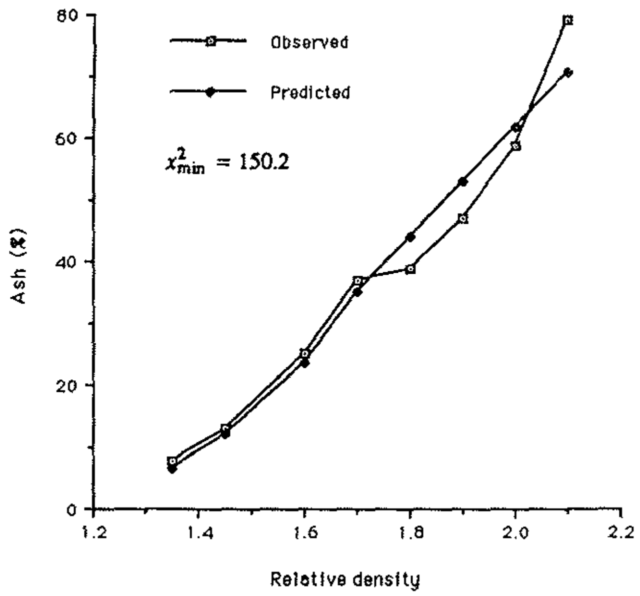


FIG 9 - An example from the group where $\chi^2_{min} > 30.0$.

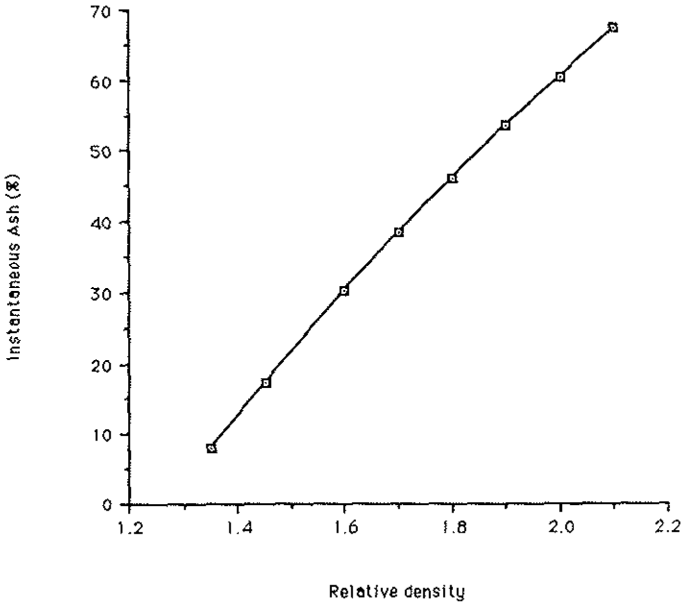


FIG 10 - An example of the instantaneous ash vs relative density curve.

TABLE 11

Fitting results for the average coal quality of an selected area.

Observed	Fredicted	Residual	Relative err.
7.656	7.706	-0.049	-0.641
12.992	12.741	0.251	1.935
22.968	23.751	-0.783	-3.408
34.549	34.207	0.342	0.990
42.708	42.161	0.547	1.282
49.888	49.788	0.100	0.200
56.800	57.105	-0.305	-0.537
64.032	64.133	-0.101	-0.158
a(p)=411.9987-1756.663/(p+3.0)			c=3.00
X**2=1.208			
Cumu. comparison			
7.656	7.706	-0.049	-0.641
10.542	10.429	0.113	1.076
12.556	12.588	-0.032	-0.254
13.708	13.721	-0.012	-0.089
14.512	14.508	0.003	0.022
15.242	15.237	0.005	0.034
15.668	15.666	0.002	0.013
15.949	15.948	0.001	0.009

drawn against the corresponding separating densities (they are not the instantaneous ash vs density curves). Figure 10 shows the instantaneous ash vs relative density curve for one of the bore cores.

For the cumulative yield per cents at different separating densities, the predicted values are very close to the observed ones. Among the 78 fitted bore cores, 52 (66.7 per cent) of them have absolute prediction errors less than 0.1 per cent, 18 (23 per cent) of them have absolute prediction errors between 0.1 to 0.2 per cent and only eight (10.2 per cent) of them have absolute errors more than 0.2 per cent for separating densities greater than 1.45. The cumulative ash per cents at separating densities less than 1.45 are in any case not important for this type of coal. These results also indicate that using incremental ash per cents alone to estimate the instantaneous ash vs relative density relationship model is correct and effective. The printed fitting results for the average values of the area studied are listed in Table 11.

CONCLUSION

An algorithm for fitting the instantaneous ash vs relative density relations has been presented. Based on this algorithm, a systematic program was written. The performance of this algorithm was compared with the other predictive models. In all the cases, the predictions for cumulative ash per cents were better than those calculated using the other approaches.

Considering the constant nature of instantaneous ash vs density relationships over a certain area, the instantaneous yield vs density relationship may be fitted independently of the instantaneous ash vs relative density relationship even though a 'straight line approximation' was used in the algorithm development for the latter. In fact, the successful application of the algorithm strongly indicates that the two relationships above can be modelled independently without considering the relative constantness of the instantaneous ash vs relative density relationship.

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