MATHEMATICAL STUDIES OF COAL MEASURES SEDIMENTATION IN AYRSHIRE, SCOTLAND

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PREFACE

This thesis is concerned with the application of mathematical methods to the analysis of certain geological features of the Upper Carboniferous sedimentary rocks of the Ayrshire Coalfield. As such, it is a study in mathematical geology, a subject which has expanded rapidly in recent years, due in large measure to the increasing availability of computers.

Mathematical geology is a logical and very necessary development of a subject that seeks to decipher the bewildering complexity of the Earth's form and history. However, like many fields that straddle two disciplines, it is susceptible to certain weaknesses. Ideally, the best practitioners of the subject must be those who have a firm grounding in both mathematics and geology but, at the present state of the art, workers tend to be either primarily mathematicians or geologists. A mathematical approach will often yield elegant numerical formulae or models which are not rigorous tests of geological hypotheses, and are often interpreted in naive geological terms. On the other hand, geologists with poor mathematical backgrounds cheerfully apply mathematical methods to geological data whose form and interpretation abuses or strains the assumptions and strictures that underlie such methods. An exaggerated parody of the form that the results can take is provided in Mark Twain's "Life on the Mississippi," p.155:

"In the space of one hundred and seventy-six years the Lower Mississippi has shortened itself two hundred and forty-two miles. This is an average of a trifle over one mile and a third per year. Therefore, any calm person, who is not blind or idiotic, can see that in the Old Öolitic Silurian Period, just a million years ago next November, the Lower Mississippi River was upward of one million three hundred thousand miles long, and stuck out over the Gulf of Mexico like a fishing-rod. And by the same token any person can see that seven hundred and forty-two years from now the Lower Mississippi will only be a mile and three-quarters long, and Cairo and New Orleans will have joined their streets together and be plodding comfortably along under a single mayor and a mutual board of aldermen. There is something fascinating about science. One gets such wholesale returns of conjecture out of such a trifling investment of fact."

Another feature that also emerges from mathematical geology is the disturbing proliferation of jargon. While inevitably, new terms must be coined to define the vocabulary of a new, evolving subject, they should be restricted to useful expressions capable of geological meaning rather than being of pure mathematical significance or abstract 'buzzwords.'

The fears and philosophy expressed here underlie the approach used in this thesis. The assumptions and weaknesses of the mathematical methods employed have been examined on both theoretical and empirical grounds and allowance for potential abuse made in the geological interpretation of results derived from them. Hypotheses that have been tested have been primarily of simple geological character, with the advantage of specific results rather than the tenuous generalisations that follow sophisticated models that are not preceded by simple groundwork. However, interpretation beyond the range of these hypotheses has been made following the incorporation of additional qualitative geological data. At the same time, terminology has been restricted to vocabulary considered to have useful meaning in a geological context.

The study can be divided into three phases whose conclusions are inter-related:

(1) The examination of areal variation of sedimentary rock characters and structure at both regional and local scale using trend surface analysis (Chapters 2 and 3).

(2) The appraisal of long-term variation of sedimentary rock properties with time trend analysis (Chapter 4).

(3) The evaluation of short-term lithological variation in terms of potential ordering, cyclicity, facies relationships and controls, using Markov chain theory and Monte Carlo simulation models (Chapters 5, 6 and 7).

Chapter 1

INTRODUCTION AND GENERAL GEOLOGY OF THE AYRSHIRE COALFIELD

(1) Areal and Historical Setting

The Ayrshire Coalfield is situated in the south-west of the Midland Valley of Scotland and forms the area of study for this thesis.* The Coal Measures tract is bounded to the north and east by the Dusk Water Fault and the high ground of the Clyde Plateau lavas and to the south by faults of the Southern Upland Fault system. To the west, the outcrop extends under the Firth of Clyde, but appears to thin towards Arran where the Upper Carboniferous is extremely attenuated and barren of coals (Leitch, 1941).

Between these broad limits, the outcrop is divided into a number of structural basins defined to some extent by prominent faults of ENE orientation. A particularly interesting property of these faults is that their distribution can be related directly to areas of different sedimentation character within the Carboniferous, especially with regard to abrupt changes of thickness across their lines. This structural control is most noteworthy in the Carboniferous Limestone Series (and more particularly the Upper Limestone Group). Rapid increases in thickness across the Dusk Water and Inchgotrick faults were demonstrated by Anderson (1925) for the Limestone Coal and Upper Limestone groups, and the same relationship shown for the Kerse Loch Fault further south for these groups and the 'Millstone Grit' by Eyles and MacGregor (1925). More detailed examination of the stratigraphy of these units shows that subsidence on these fault lines was not continuous

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* see fig 1

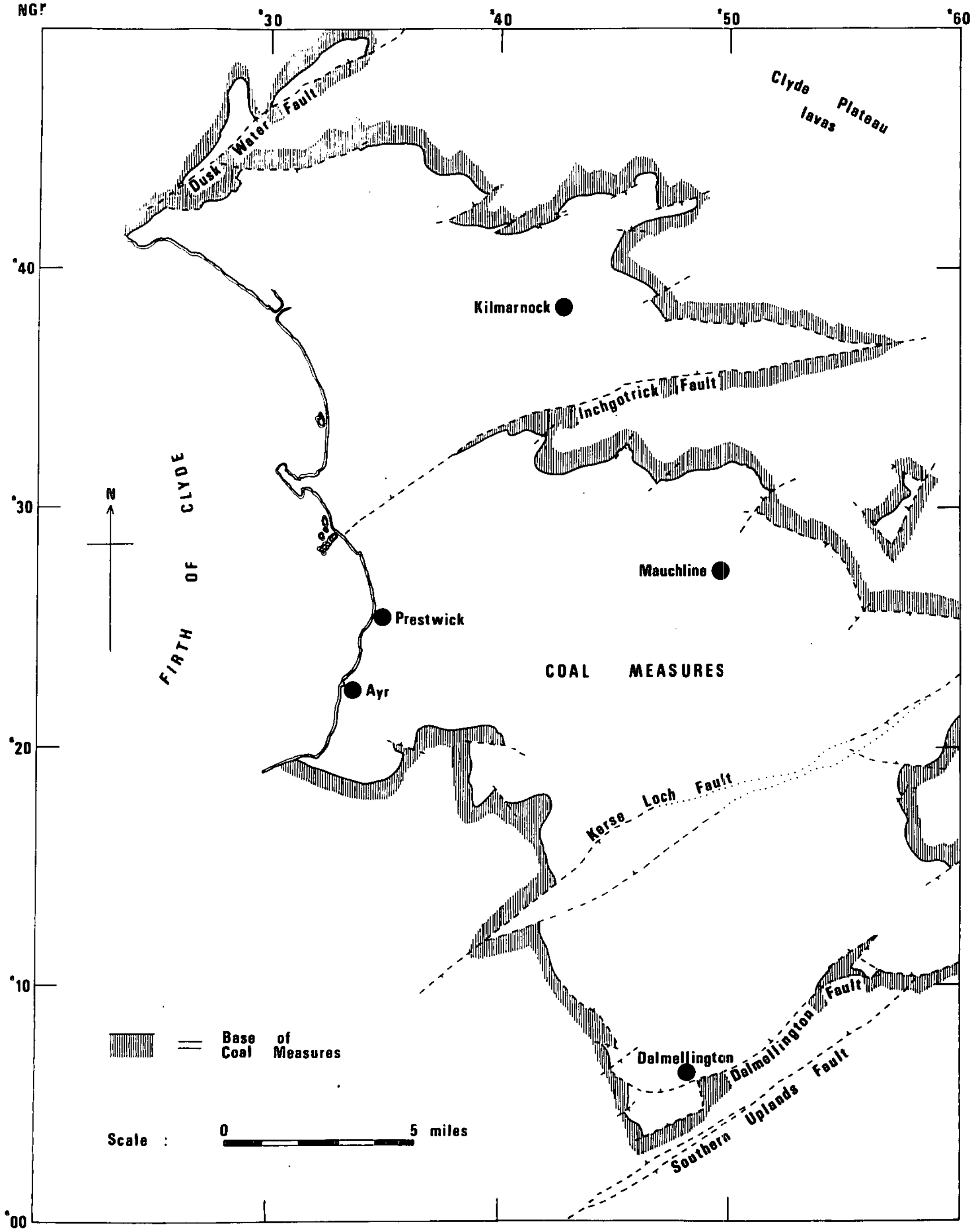
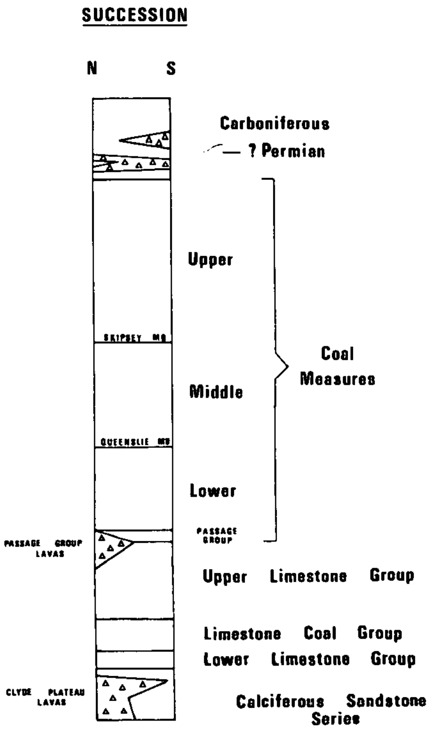


FIG. 1

OUTLINE MAP OF THE AYRSHIRE COALFIELD



but of somewhat episodic character. Fault control of sedimentation was suspected to extend upwards into the Coal Measures but with diminished effect, and this was confirmed by Mykura (1967).

Within the Midland Valley as a whole, the close similarity between the isopachyte map patterns of the Mid-Carboniferous and their structural contour trends led Goodlet (1959) p.225 to conclude, "that a close relationship may be reasonably assumed to exist between the present distribution and structure of these sediments and the pattern of subsidence at the time of their deposition." It therefore seems likely that Hercynian movements active elsewhere in Europe throughout the Carboniferous influenced sedimentation patterns in the Midland Valley, being particularly well marked in Mid-Carboniferous rock groups and, for Ayrshire at least, extending into the Coal Measures (see Mykura, 1967, pp.27 and 88).

A proved structural control for Coal Measure deposition can be usefully compared with other British Coalfields such as the East Pennine basin, where Duff and Walton (1964) were unable to relate thickness variation of sediments with tectonic structures in the <u>modiolaris</u> zone, though conceding the possibility of this relationship in higher zones as suggested by Wilcockson (1947) when proto-Hercynian movements presumably became more intense. (Owen (1964) also pointed out the relationship between contemporary tectonism and sedimentation in the South Wales coalfield).

The Ayrshire Coalfield is only one of a number of Coal Measure basins within the Midland Valley, so that its history is a function of the environment of the Midland Valley as a whole through Coal Measure times, but with important modifications of a local type peculiar to the Ayrshire basin.

Kennedy (1958) gave a useful summary of the tectonic development of the Midland Valley describing the change in its character from a stable shelf area in Lower Palaeozoic times to a depositional graben following the Caledonian orogeny. At various times in the Carboniferous there was extensive volcanic activity. The bulk of the material erupted in some phases was of an order to modify the geometry and hence depositional history of some local basins, so that, in the case of Ayrshire, the Clyde Plateau lavas (Calciferous Sandstone Series Age) and the Passage Group lavas show evidence of sub-aerial formation and there is a progressive overlap by younger sediments.

However, the main depositional framework of the Midland Valley as a whole was bounded to the north by a major land area of the Atlantean massif (Gilligan, 1920; Goodlet, 1959; Greensmith, 1966; and others) whose southern boundary was roughly described by the Highland Boundary Fault. This positive area appears to have supplied the bulk of detritus deposited in the Midland Valley throughout the Carboniferous, as indicated by cross-bedding directional studies (Walker, 1955; Robson, 1956; Greensmith, 1961; Shackleton, 1962; Mykura, 1967).

The southern limit of the Midland Valley basin complex was set by the area of the Southern Uplands, whose character seems to have changed progressively through the Carboniferous. At one time it formed a land mass supplying limited amounts of detritus, as is attested by the limited conglomeratic facies developed near the Dalmellington Fault in Limestone Coal Group times, but by Upper Limestone times, facies differences are negligible between this area and further north, while the presence of the Coal Measure outliers of Sanquhar and Thornhill within the Southern Uplands points to a progressive subsidence. Whether the Southern Uplands ever became completely submerged or survived as an island or isthmus is controversial (e.g. see George, 1960), but nevertheless it seems to have formed a neutral shoaling area in Coal Measure times.

The sedimentary facies of Middle and Upper Carboniferous age developed within the Midland Valley have generally been considered as products of a broadly deltaic environment modified by a marine influence (evidenced by marine sediments) of varying strength through time, so that within the Westphalian the marine contribution was rather weak and episodic (see e.g. Goodlet, 1959; Greensmith, 1966; Read, 1961).

Within Ayrshire itself, Mykura (1967) suggested that cross-bedding and slump-bedding directions in the thick sandstones of the Lower Coal Measures indicated derivation from the east or north-east, while the geometry of elongate sand bodies in the Middle Coal Measures was interpreted as showing a change of source direction to the west or north-west. The sporadic and limited surface outcrop of Coal Measure rocks in Ayrshire largely precludes a systematic statistical study of palaeocurrent configurations, but the map assembled of orientation data in the Dalmellington area in Fig.2 indicates that in the south, at least, the source direction appears to have lain to the north-east throughout both Lower and Middle Coal Measure times. However, the figure also emphasises the high variability of this pattern.

The Coal Measure sequence as a whole thickens in a south-east direction to the Dalmellington area, indicating an overall increase

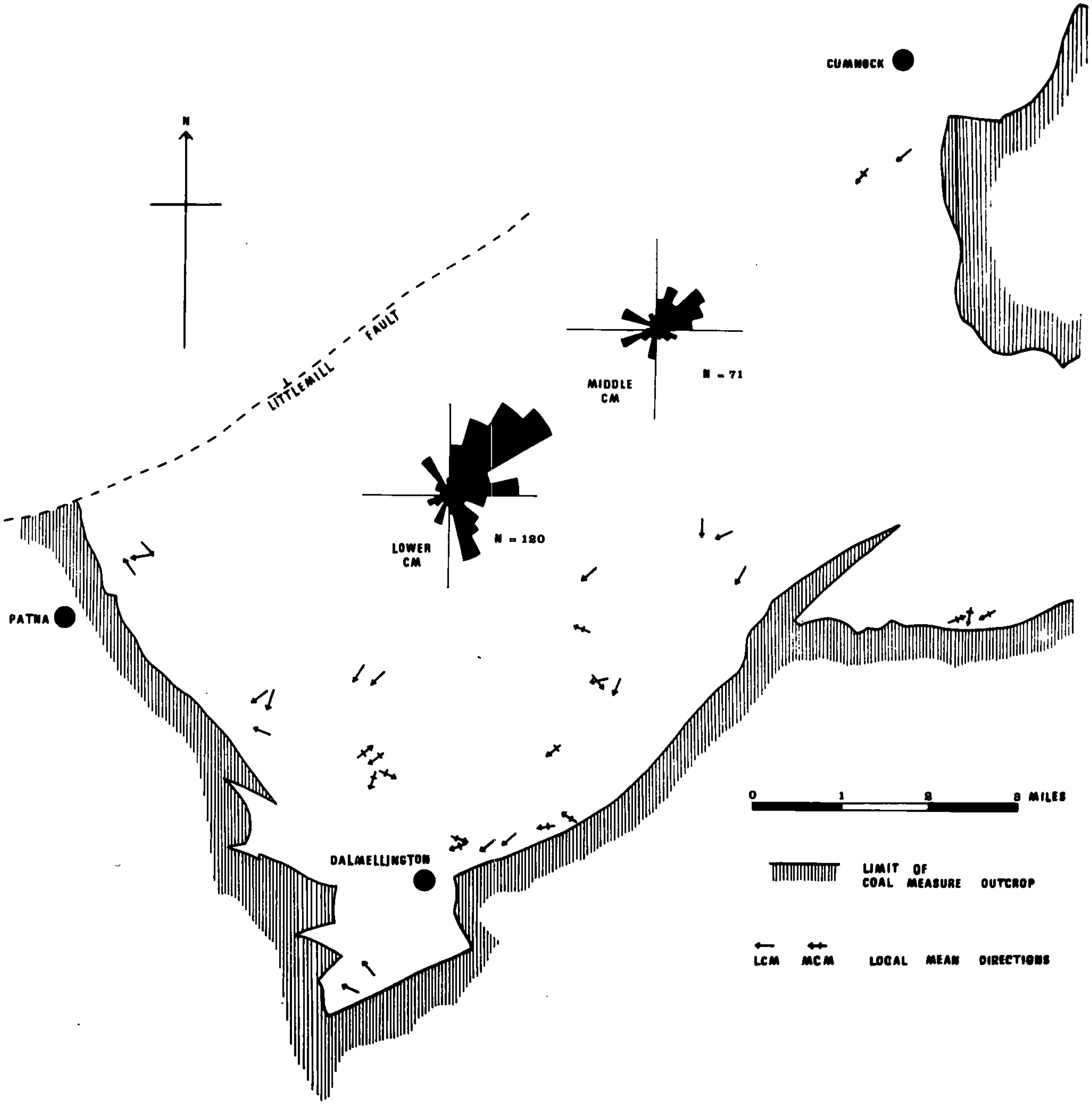


Fig. 2 South Ayrshire Coal Measure palaeocurrent directions indicated by cross bedding

of rate of subsidence in this direction. Marine bands also increase in number and thickness towards the south, and more particularly the south-west, so that the sea during Coal Measure time is inferred to lie somewhere to the south-west. Much of the succession is devoid of marine bands, the majority of these being limited to the *lenisulcata* and *similis-pulchra* zones. The areal extent of most bands is mainly restricted to irregular developments in the south part of the coalfield. With the notable exception of the Skipsey's Marine Band, the marine faunal character is rather feeble so that orthodox forms are rare, while *Lingula* is typical. These facts collectively suggest that marine influence was of a desultory character and relatively infrequent occurrence, and that Coal Measure sedimentation was largely of a fresh-water or brackish regime.

The imperfect correlations that exist between diagnostic horizons in the Scottish coalfields and 'standard' Coal Measure sections in England make it difficult to set precise time boundaries to the rocks studied in this thesis. Thus the lack of a Scottish equivalent of the *Gastrioceras subcrenatum* band (which defines the base of the Coal Measures in England) has necessitated the erection of basal boundaries of local significance in the Midland Valley coal basins. In the Ayrshire Coalfield, the base of the Coal Measures was originally set as the widely correlatable Lugar or Dalmellington Blackband Ironstone which is thought to be approximately at, or just below, the base of the *communis* zone. The intervening strata between this horizon and the top of the Upper Limestone Group has been termed 'Passage Group' by MacGregor (1960) and is comprised of beds of debatable age. In Ayrshire, this includes a significant development of lavas to the north and sediments with a fauna interpreted as belonging to the lenisulcata zone in the south. The most recent assessment of the lower boundary of the Coal Measures has hence been taken as the top of the uppermost limestone of the Upper Limestone Group in south Ayrshire (Mykura, 1967), though the demonstrable non-sequence that exists following the lavas further north, makes it difficult to assess whether these are of basal Coal Measures age.

The top of the Coal Measures in Ayrshire has been traditionally set at the base of a volcanic group designated on general grounds as 'Permian.' However, the discovery of plant remains of probable Upper Stephanian age in sediment intercalated between basal lava flows (Mykura, 1965; Wagner, 1966) indicates an unknown, slightly higher, level for the Coal Measure upper boundary.

A more detailed account of the geology of the area is to be found in the two Geological Survey regional memoirs (Richey, Anderson and MacGregor, 1930; Eyles, Simpson and MacGregor, 1949) and the four Economic Geology memoirs (Richey, Wilson and Anderson, 1925; Anderson, 1925; Eyles, Simpson and MacGregor, 1930; Simpson and MacGregor, 1932). A fine recent summary of the geology of the southern part of the area has been produced by Mykura (1967) that incorporates more modern data and includes studies of palaeogeography and structure, while, in the same paper, Calver and Wilson give the latest assessment of the palaeontological evidence.

(2) Lithological Characters of the Coal Measures

The Ayrshire Coal Measure succession can be broadly divided into the rock-types mudstone, siltstone, sandstone, seatearth and coal whose general attributes can be conveniently discussed under the following headings:

(i) Mudstones

These represent about 35% of all strata in the Coal Measures. Thickness ranges up to 70 ft. while the average thickness is 4.5 ft. Their colours are usually grey, sometimes black, and the mudstones often contain layers of sideritic ironstone nodules. They often have a feeble fissility so that many are more correctly termed 'shales.' Lamination is normally absent or vague except in the siltier varieties.

Mineralogically, they appear to be composed dominantly of illite (including mixed-lattice types) and chlorite together with subsidiary proportions of felspars, calcite and quartz (Appendix A). Geochemical analysis of a fresh borehole sample showed anomalously high Zinc and Titanium content which has no simple explanation. The analysis and a general interpretation are set out in Appendix B.

Non-marine lamellibranch-bearing mudstones are common, containing mainly the genera Anthracosia, Carbonicola, Anthraconaia, Anthracosphaerium and Naiadites. Fish scales, Spirorbis and ostracods are sometimes associated with these lamellibranchs. Marine mudstone faunas are mostly restricted to the lenisulcata and similis-pulchra zones and more commonly represented as Lingula bands, typically with a fauna of Lingula mytilloides and fish scales. Orthodox marine forms are less common and the areal distribution of marine/Lingula bands is generally limited (see Mykura, 1967).

(ii) Siltstones

Siltstones constitute about 29% of the Coal Measures succession. They average 4.0 ft. in thickness (with a maximum in the order of 40 ft.) and are commonly flaggy in bedding character and grey in colour (largely a measure of their mud content). As regards internal structures, they are most commonly massive, though this may be more apparent than real, as lamination when present is usually picked out by the alternation of finer (muddy) and coarser (sandy) fractions. These laminae are sometimes straight or form feeble cross laminations, and are commonly deformed, seemingly as a result of movement in waterlogged silt, or show small-scale load structures. Plant material is abundant, usually as comminuted carbonaceous fragments scattered on bedding surfaces, though well-preserved fronds of fern-like vegetation are common. Rootlet horizons (more frequently without overlying coal) are often found in thin siltstones with no development of fireclay characteristics.

Apart from fragmental and root vegetation, fossil remains are relatively uncommon, though non-marine lamellibranch faunas, limited in number, occur occasionally.

The lithology is characteristically found interbedded in a repetitive manner with sandstones or shales with which it commonly has gradational field relationships. It forms, essentially, a transition class in the spectrum of silty sandstone—sandy siltstone—siltstone—muddy siltstone—silty mudstone.

(iii) Sandstones

Sandstones represent 32% of the succession with an average thickness of 7.2 ft. while their thickest development is in the order of 90 ft.

Petrographically, they are orthoquartzites and sub-graywackes, generally with subrounded to subangular grain texture, except in the higher parts of the Upper Coal Measures where 'millet seed' grains, indicating the onset of aeolian conditions, make their appearance. Felspars form a minor constituent and include plagioclase, orthoclase and microcline. Muscovite mica is common, largely segregated on depositional laminae and is probably mostly diagenetic in origin.

Fossils are almost entirely absent, barring remainié material (almost invariably plant) that occurs in lag deposits, and the occasional occurrence of trace fossils (tracks and burrows).

The sandstones are most usefully considered by a broad subdivision into two classes that are roughly characterised by thick and thin sandstones. A more detailed analysis of the field characters of these two types is set out on p.102

(iv) Seatearths

Seatearth lithologies tend to be fine-grained and range from an inch to about ten feet in thickness, though this thickness appears to show no relationship with the thickness of the overlying coal. They are commonly grey in colour and often characterised by the occurrence of lozenge-shaped sideritic nodules. These appear to be associated with the carbonised stigmarian root traces that riddle this facies. Seatearths are primarily structureless in the upper parts, and the top, if fine-grained, often has a 'doughy' texture.

Mineralogically, the finer-grained varieties appear to be dominated by a kaolinite content with subsidiary proportions of illite, felspars and quartz (Appendix C).

Chapter 2

THEORY AND PRACTICE IN TREND SURFACE ANALYSIS

Introductory Theory

The study of areal variation of geological attributes is traditionally made by the method of hand-contoured maps produced by interpolation between observation-point data scattered over the area. Such maps are commonly complex in configuration, making generalisations difficult, and are also subject to the bias of the investigator. The method of trend surface analysis offers a simplification of the problems raised by these maps, in that it attempts to separate regional trends from the more local variation within the data and performs this operation in an objective manner. The regional trends are computed as gently-sloping surfaces which are conventionally described in terms of an integer power series using the geographic co-ordinates of the data as polynomials. (While this series is the most commonly used, there are a number of other possibilities such as the Fourier and Chebyshev series, e.g. Spitz, 1966; Harbaugh and Preston, 1965; Preston and Harbaugh, 1965). The use of this series leads to a hierarchy of possible surfaces of which the three simplest can be expressed as:

Degree of Surface	Surface Equation	Geometric Expression
Linear	$Z = A + Bu + Cv$	Plane
Quadratic	$Z = A + Bu + Cv + Du^2 + Euv + Fv^2$	Conic
Cubic	$Z = A + Bu + Cv + Du^2 + Euv + Fv^2 + Gu^3 + Hu^2v + Iuv^2 + Jv^3$	Complex

Where Z = computed value of surface at (u,v);

u,v = co-ordinates (e.g. geographic) of data points;

A - J = computed polynomial coefficients.

The surfaces become more complex by the inclusion of progressively higher powered terms so that the linear surface is expressed by 'linear terms,' the second by the addition of 'pure quadratic terms,' and the third by further addition of 'pure cubic terms.' Each surface is computed by the least-squares criterion so that, in passing through the total cluster of points, expressed in three-dimensional space by the attribute values and their geographic co-ordinates, the sum of the squares of the deviations of these points from the surface is made the minimum possible. (Computational details are given in such texts as Krumbein and Graybill, 1965; Harbaugh and Merriam, 1968). The resulting surface is one of 'best-fit.' The deviations of raw data point values from a computed surface are known as 'residuals,' which have a positive or negative sense.

The separation of the original data values into the two complementary parts of trend component and residual fraction correspondingly splits the areal variation into a broad 'regional'(relative to the map area) trend represented by the trend surface and a pattern of more local significance produced by contouring the residual values.

The Significance of Trend Surfaces

The existence of trend surfaces to express the broad geographic variation of 'data' does not, in itself, prove systematic large scale effects of potential geological meaning, as the method can calculate such surfaces for totally random data. While such random 'trends' may have some abstract philosophical significance, the nature of their basic data precludes any possibility of their interpretation as the products of systematic areal processes as one would hope to find in geological data. Tests must therefore be devised to assess the significance of any computed trends. To a certain extent, an essentially random areal pattern of data variation can be suspected when the reduction in the sums of squares of deviations of the original data by surfaces is low. Howarth (1967) computed trend surfaces for sixty sets of random data and demonstrated that the proportion of squares of the original data accounted for by these surfaces (known as the 'coefficient of determination') were low and of the order:

Surface	Mean Coefficient of Determination
Linear	1.7%
Quadratic	6.8%
Cubic	15.7%

However, these figures cannot be used as the supreme arbiter to gauge the significance of surfaces calculated in geological research as Howarth's data points were randomly distributed across the map area, a condition which frequently cannot be reproduced in a geological context, such as where observations are made on elongate outcrops. Further, while low-fit values can be interpreted to indicate an essentially random large-scale areal pattern, certain surfaces with values close to the orders given by Howarth can be shown on other grounds to have geological significance (e.g. Tinkler, 1969).

Other methods that have been used to test the significance of trend surfaces are:

1. Confidence limits.
2. Analysis of variance.
3. Comparison between real surfaces and surfaces produced by randomising data values between data points by
   - (i) contrasting the sums of squares of the raw data accounted for by real and random surfaces,
   - and (ii) visual comparison of the real and random surface maps.

1. Confidence Limits

Envelopes of surfaces for appropriate confidence levels (e.g. 95%) have been computed to enclose trend surfaces as a three-dimensional expression of confidence lines that are commonly fitted to best-fit lines (e.g. Allen and Krumbein, 1962). In using this method, certain statistical assumptions are either unsatisfied or only approximately met (these include the requirement of a frequency distribution of values of the dependent variable and a lack of mutual correlation in the deviations). Such confidence surfaces are very difficult to calculate when the number of data points is large or the surface is higher than linear in degree.

2. Analysis of Variance

The most widely used measure of the validity of a trend surface is the sums of squares F test used by Allen and Krumbein (1962), Dawson and Whitten (1962), Harbaugh (1964), Tinkler (1969) and others. In this technique, successively higher order pure terms underlying the computed surfaces are tested against the residuals representative of higher terms in a ratio of mean sums of squares against the hypothesis of no regression. The appropriate significance level is obtained from standard tables of F. Krumbein and Graybill (1965) p.337, point out that "the assumptions necessary to interpret the F values ..... may not be satisfied, in that the residuals may contain systematic effects," so that the method is best used to decide when to stop fitting higher order surfaces, when the significant lower orders contain the broad regional variation.

3. Comparison between real and random surfaces

Tinkler (1969) suggested randomising observed values between real data points as a method for producing surfaces that have no significant trends, with which the real surfaces can be directly compared. The proportion of the sums of squares of the raw data accounted for by these random surfaces serves as an estimate of the limit that should be exceeded by real data surfaces, if these have real significance.

Tinkler also considered that trend surface maps produced from real and randomised data can be usefully compared visually to assess whether the real data has systematic trend characters. The criteria (p.120) are that, "on the actual data .... the trends observed make sense all over the map, as they should do since they are essentially generalisations of it. For the random surfaces it is possible to make 'sense' of parts of the pattern in terms of the problem but then the interpretation is confounded by a lack of 'sense' over other sections of the map." In other words, the geological interpretation is used to test the reality of the map, which if successfully 'real' is then used for geological interpretation (or 'which came first - the chicken or the egg?'). The use of this technique is common in the literature, though usually in a disguised form.

The variety of possible methods that exist to establish the significance of trend surfaces as 'valid' indicators of real regional trends highlights the failure of any one method to emerge as pre-eminently suitable. The most popular technique is that of analysis of variance but, as already indicated, this makes certain statistical assumptions regarding the data that may or may not be satisfied. The commonest form that the test takes is the computation of the ratio:

$$F = \left(\frac{SS_x - SS_{x-1}}{SS_{ToT} - SS_x}\right) \left(\frac{N - (x + 1)(x + 2)/2}{(x + 1)}\right)$$

for which significance levels are taken from tables of F for appropriate numbers of degrees of freedom ($x + 1$ and $N - (x + 1)(x + 2)/2$) for successively higher order surfaces where,

SS_R = sums of squares accounted for by R^{th} surface;

SS_{ToT} = total sums of squares of data;

N = number of data points;

x = order of surface tested.

How efficient this method is in practice is difficult to say, particularly when bearing in mind that surfaces from one of Tinkler's sets of randomised data tested in this fashion (p.117)proved to be significant at linear, quadratic and cubic levels. Some workers question the value of a variance ratio that uses successively higher order residual mean sums of squares as denominator and suggest that trends should be contrasted with total map variability as an F ratio (e.g. Chayes and Suzuki, 1963). Goodell (1967) used this latter form of the test, but the approach would appear to have greater chance of violating statistical assumptions than the more conventional form of the test.

Data-Point Distribution

Trend surface analysis is best performed with gridded (orthogonal) data points, but such an ideal situation is rarely possible in the study of rock attribute variation, as the siting of observations is usually dictated by the vagaries of outcrop patterns or borehole locations. When plotted on a map, the total population of observations commonly show high concentrations in some areas, while being sparse or absent in others. Ideally, points should be distributed roughly equally about the map so that the computed trend surfaces are fair representations of the whole map area. In the event of a pronounced 'clustering' of points in certain parts of the area, a weighted emphasis is made of their contribution to the trend surface configuration so that the surface will tend to fit a cluster of points in preference to an isolated point. Therefore, in preparing data for trend surface analysis, a weeding out of available data points should be made (preferably by an impartial method based on random numbers to avoid personal bias in selection) to ensure a broadly homogeneous distribution.

Even with precautions of this kind, the shapes of the areas for which information is available within the mapped region may introduce problems in the production of meaningful trend surfaces. In the case of long narrow outcrop or extended sub-surface patterns, elongate distributions of points are inevitable and produce strong distortions of the trend surfaces. This is shown in a gross parallelism or sub-parallelism of the surface contours with the sense of elongation of the data-point distribution. Examples of such strongly aligned arrangements of data points are common in the literature (e.g. Chorley, 1964; Goodell, 1967; Vistelius, 1967; Tinkler, 1969), though the problems this raises are rarely mentioned. Tinkler however, stated that (p.118) "it would seem that orientated data locations cannot affect the form of the surface," an extraordinary observation when it can be clearly seen that the contours of all his cubic surfaces for both real and random data, roughly parallel his data point distribution. The degree of elongation of the point population is related to the UV (geographic co-ordinates) correlation coefficient so that, if the latter is high, appreciable distortion can be expected, while if close to zero, the data point distribution is either gridded or random, the optimum condition for 'true' surfaces.

Emphasis has been placed on the difficulties raised by this aspect of data point arrangements because the areal pattern of the basins within the Ayrshire Coalfield results in a Coal Measure tract whose long axis is orientated roughly NW-SE. It follows that however well data points are selected within this belt, some degree of UV correlation is inevitable. The possible effect that this external factor exerts on surfaces of intended geological significance is considered in the following section.

Trend Surface Analysis of Artificial Models

A surprising feature in the application of trend surface analysis and other mathematical techniques to geology is the reluctance of investigators to test the method on material whose parameters are precisely known. In other lines of research, such as the estimation of heavy mineral contents or geochemical analysis, it is customary to preface the study with preliminary work on standard samples designed to test the efficiency of the method and its tolerance of varying conditions. The previous sections have indicated that the geometry, and hence validity, of computed trend surfaces is sensitive to the nature of the data point distribution, which frequently cannot be optimised in geological situations. The inherent weaknesses of methods used to test the significance of these surfaces has also been touched upon. These factors are widely appreciated in the literature, but allowance for them is conventionally made within the geological interpretation of computed surfaces on somewhat arbitrary grounds. There is therefore a need to disentangle geological variation from external effects and these are best isolated by considering trend surfaces describing data whose areal variation has already been set.

Following this philosophy, artificial models were constructed for the Ayrshire Coalfield to assess:

(i) the distortion effect of data point distributions typical of Coal Measure data on computed trend surfaces;

and (ii) the best criteria by which to judge the significance of such surfaces.

The two varieties of model that can be used for this purpose are:

(a) Random data models

Models of this type were used by both Howarth (1967) and Tinkler (1969) with the aim of producing estimates of the proportion of sums of squares accounted for by such 'random surfaces' as lower limit figures for meaningful surfaces encountered in geological studies. With a relatively small population of observations, it is possible to have a spectrum of computed surfaces, each representative of a different set of random numbers, though their characteristics will tend to cluster about a mean. A drawback of such surfaces is that it is difficult to interpret distortion produced by a poor data point distribution as opposed to random fluctuations within the data.

(b) Deterministic models

The choice of a deterministic geometric model is attractive, in that artificial trends and residual patterns can be set within the area and the power of trend surface analysis to describe these is then readily ascertained, both with regard to the nature of the computed map surface and the potential tests of significance. The sense of distortion introduced by poor data point configurations is immediately apparent when contrasting computed surface maps against their ideals for these models.

A problem arises in the selection of standard geometrical shapes for this exercise. On the one hand, a body whose form is broadly similar to a possible geological variation surface is preferable, so that generalisations can be meaningfully extended to the geological context. On the other hand, the artificial model should be geometrically simple so that trends of undoubted regional significance can be incorporated within it while distortions of computed surfaces are readily apparent.

Artificial Cone Models

The basic model chosen for studies related to Ayrshire took the form of an inverted cone-shaped surface with its apex at the centre of the area. The radial symmetry of this model ensures that any distortion of trend surfaces is easily measurable (in much the same sense that originally spherical bodies are the ideal shape for the measurement of strain in rock deformation studies). This model also has some parity with potential variation of geological variables in the Ayrshire Coal Measures. Examination of the trend surfaces of the structural contour configuration of the Main Coal (Fig.9) shows that, in structural terms at least, the regional pattern is one of an elongate basin whose centre is a short distance north-east of the centre of the map. Therefore, an inverted cone presents some sort of approximation to geological variation, and lessons learned from this artificial model will have some generalised applications.

The data point distribution used throughout this exercise was deliberately chosen as the worst set (from the point of view of gross geographic orientation) used in the generation of trend surfaces of geological variables. This set was that used in the estimation of clastic variation within the interval bounded by the Ell and Main coals, and has a negative UV correlation ("easting' v. 'northing') of 41%. The basic cone model was modified into three types of surface designed to simulate possibilities arising in geological attribute variation.

1. Model A (Simple Cone)

A simple cone surface is described for the most part by a quadratic function, though a linear surface will account for a significant proportion of total map variability if the apex angle is large. The model therefore has significant linear and quadratic regional trends and a very minor residual component.

A cone with apex angle 168° 37' (the sides have a dip slope of one in horizontal ten) was drawn for the area as the simplest model as shown in Fig.3A.

2. Model B (Cone with steeply sloping sine-wave sides)

The simulation of residual patterns of systematic local character was made by transforming the cone surface into one of concentric sine-wave form in which distances along the simple cone surface (used as a datum plane) were scaled as radian measurements (10 KM. = 2π), so that the wavelength of the computed surface was 10 km. with amplitude of 1 km. The source of these waves was set at the centre of the map so that the complete surface is one of a conical basin with concentric corrugations. While geological analogies for such a component would be difficult to find, this modification preserves the radial symmetry of these models. The expansion of the sine-wave function yields a power series, so that the component that this provides is described by complex terms in the trend surface polynomial series. The slope of the cone that defines the datum of the sine-wave configuration was set as 16° 42' (a slope of three in horizontal ten) with the result that while the sine-wave surface provides significant local variation, the total variation is dominated by the relatively simple trend of the underlying conical datum plane. (This can be appreciated by reference to the profile of this model in Fig.3B).

3, Model C (Cone with gently sloping sine-wave sides)

The third model was prepared by a reiteration of the process described for the second model, maintaining the wavelength and amplitude dimensions of the sine-wave surface, but setting the slope of the cone datum plane at 5° 43' (a slope of one in horizontal ten), so that a more significant proportion of the total map

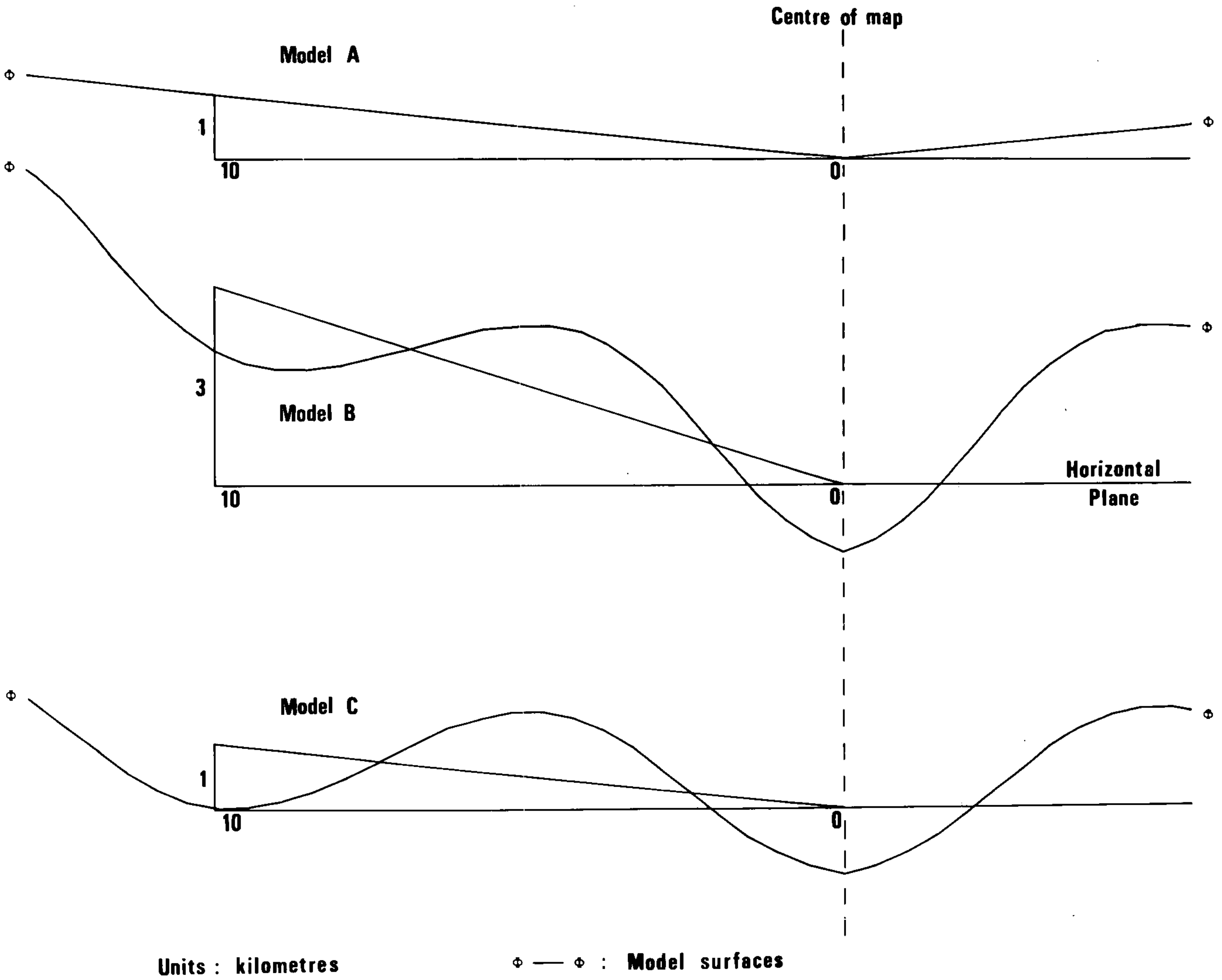


Fig. 3 Artificial Cone Model Profiles

variation is contained in the complex surface while the strength of the simple trend of the conical datum is dampened. (For profile, see Fig.3C).

The three models provide a broad spectrum of possibilities ranging from Model A, where regional variation is almost entirely ascribed to simple trend surfaces, through Model B, where such simple regional trends remain dominant, but a significant contribution is made by a relatively local component of complex character, to Model C, where there is an interplay between the weakened simple regional trends represented by the cone datum and the complex component provided by the sine-wave function.

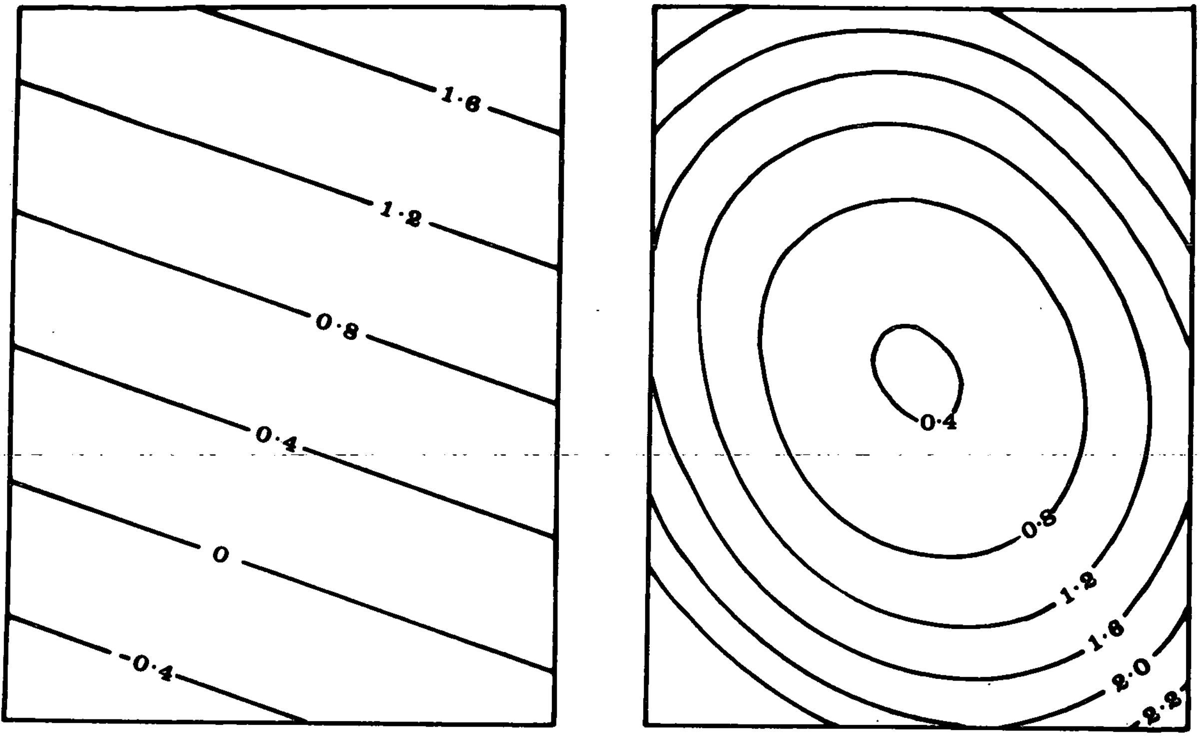
For each model surface, values of height above a horizontal datum plane were calculated for the locations represented by the data points in the Ell-Main clastics studies. Trend surfaces were computed to cubic level and are shown in Figs. 4, 5 and 6. The trend surface programme used was written by M.R. Osborne of the ERCC, in Atlas Autocode and incorporates subsequent modifications by A.J. Parsley.

Assessment of Artificial Model Trend Surfaces

1. Distortion introduced by an inhomogeneous data point distribution

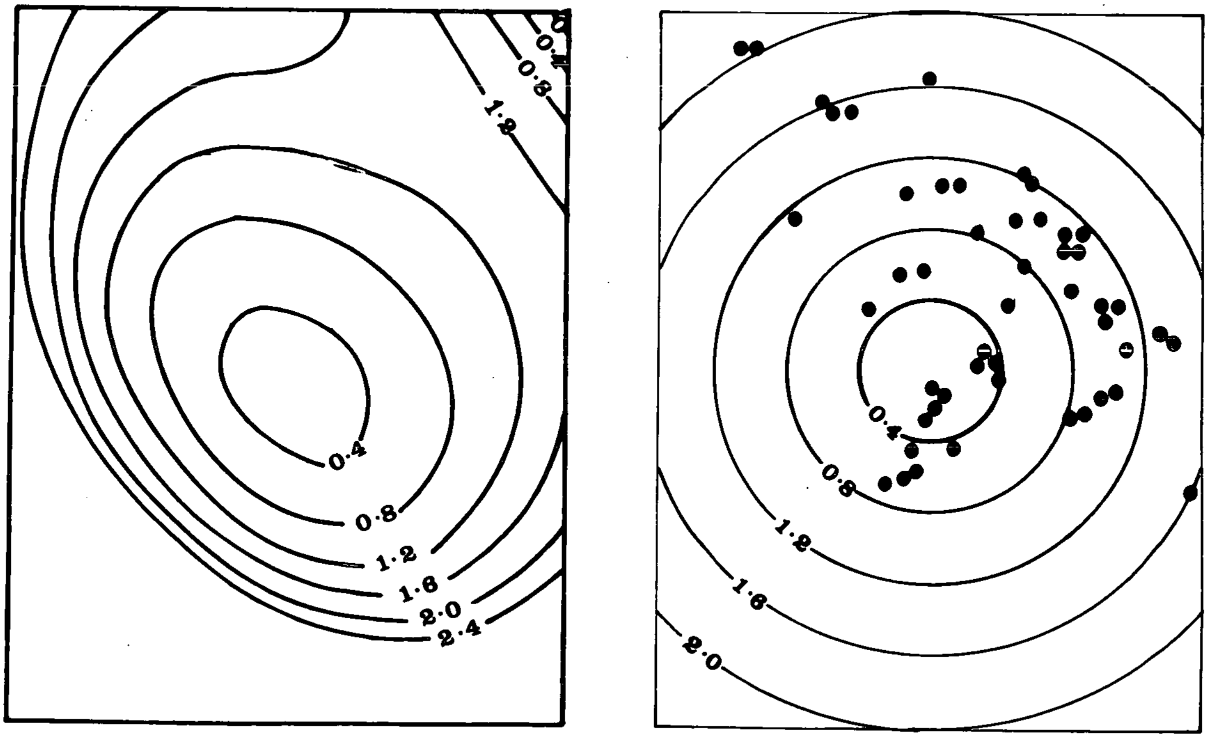
(i) Gross orientation of data points

It will be observed that all three models register the essentially quadratic sides of their definitive cones in the quadratic surfaces of Figs. 4, 5 and 6, which are expressed as 'bulls-eye' contour patterns. The radial symmetry of these models demands that if the quadratic surfaces are to be faithful representations, they



linear

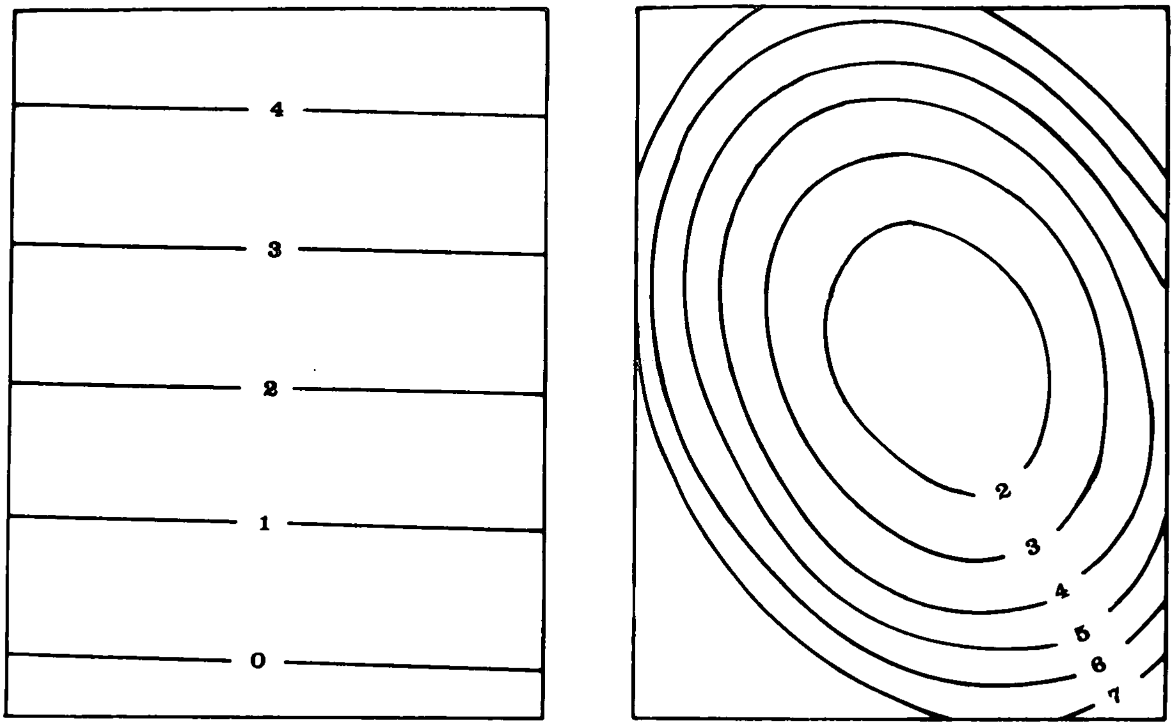
quadratic



cubic

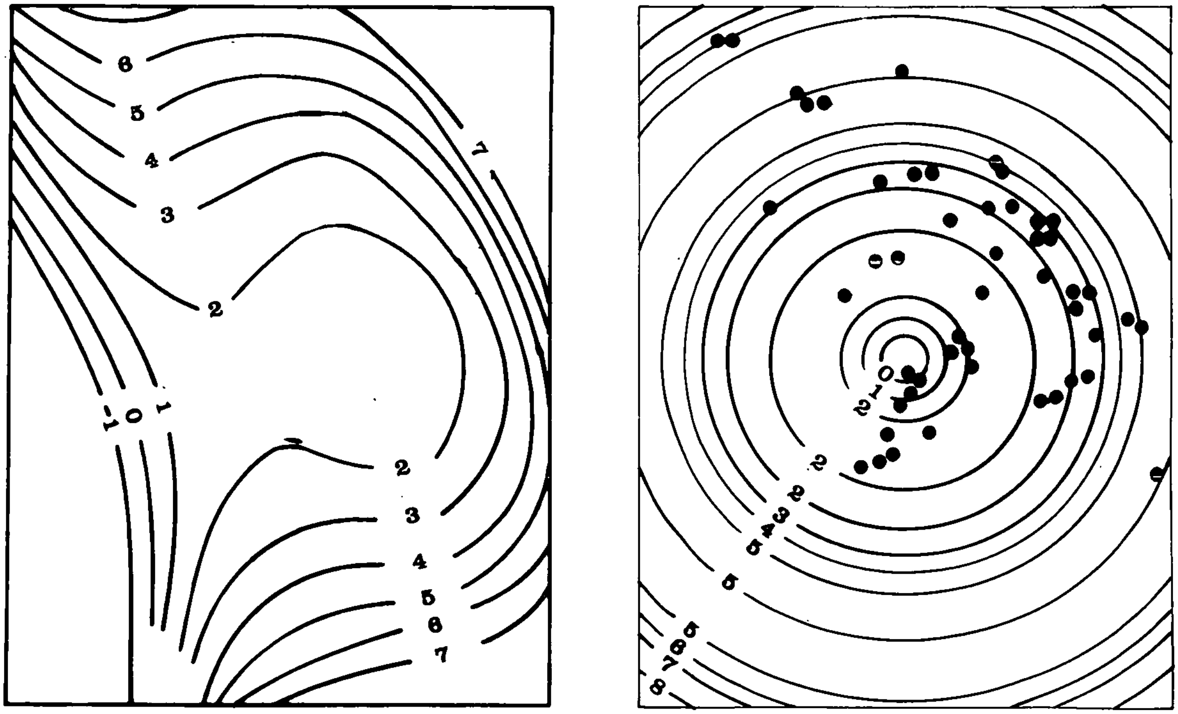
MODEL CONTOURS
& DATA POINTS

FIG. 4 TREND SURFACES OF MODEL A



linear

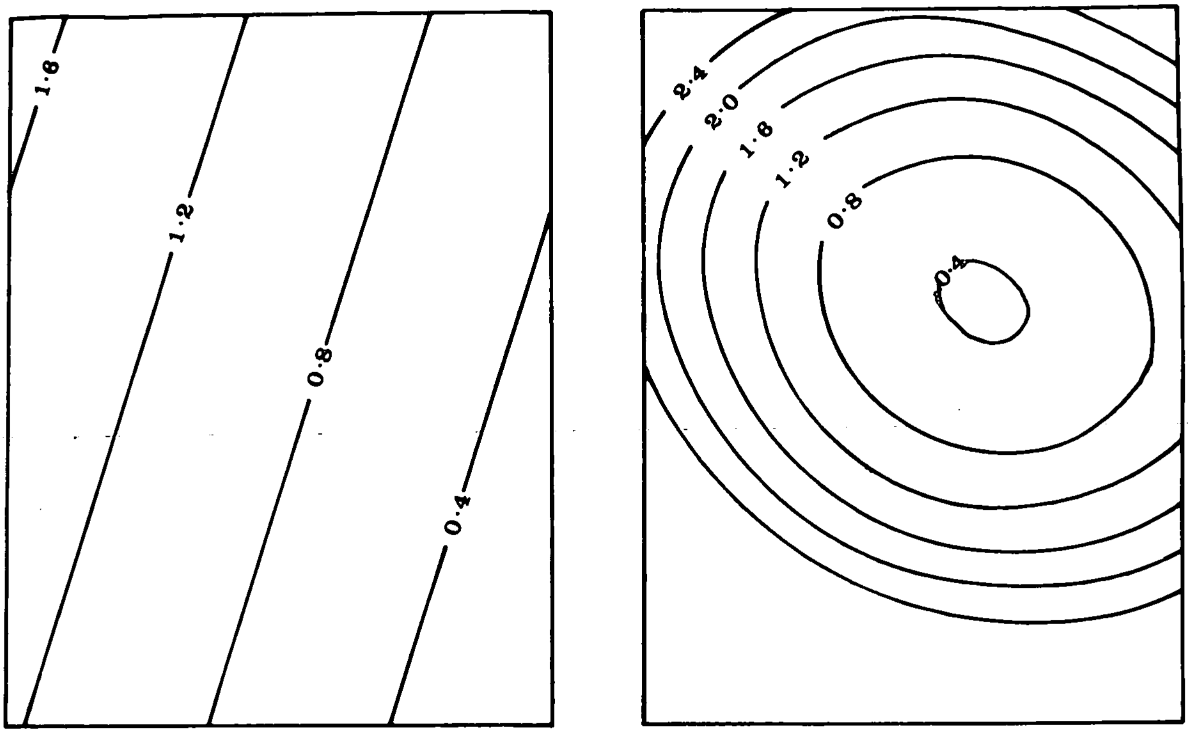
quadratic



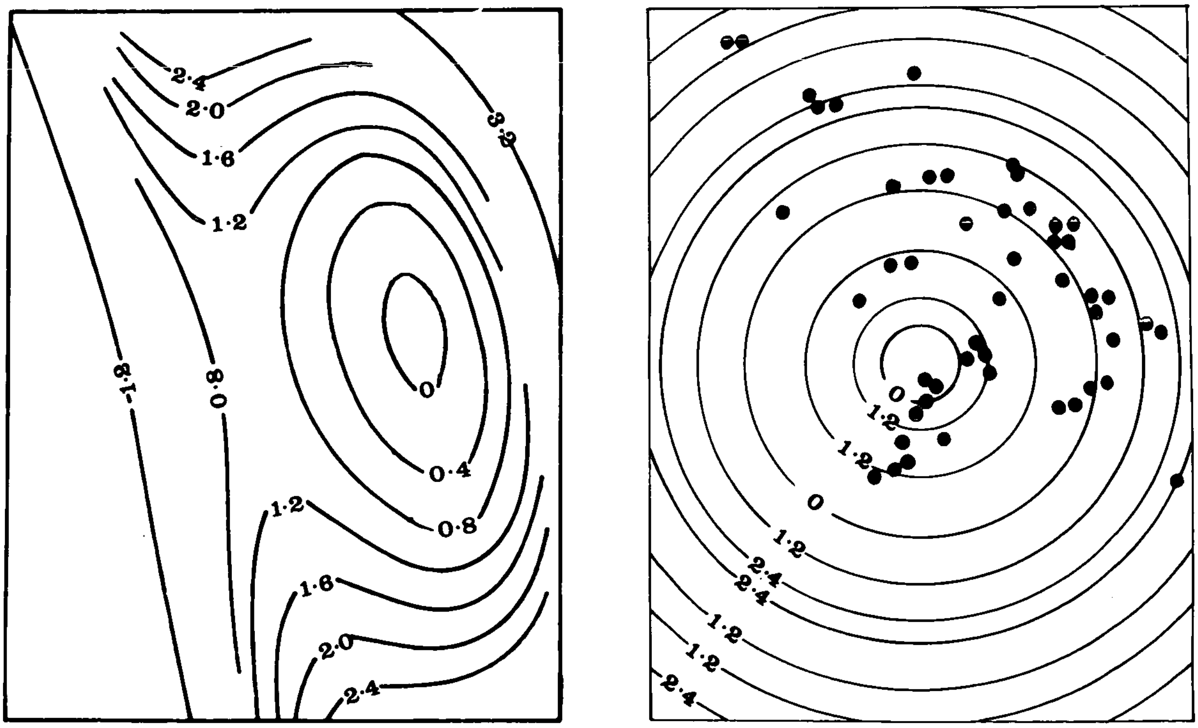
cubic

MODEL CONTOURS
& DATA POINTS

FIG.5 TREND SURFACES OF MODEL B



linear quadratic



cubic

MODEL CONTOURS
& DATA POINTS

FIG.6 TREND SURFACES OF MODEL C

too should be radially symmetrical about the centre of the map. This stipulation was checked by the construction of Fig.7, where the trace of an arbitrary contour on the ideal cone (dotted circle) is compared with its quadratic surface configuration on the three models. Examination of this diagram shows distortion both in terms of elongation and displacement.

(a) Elongation

The degree of elongation can be expressed as follows:

Model A : Long axis/Short axis = 1.2
" B : " = 1.4
" C : " = 1.2
Ideally : " = 1.0

The conical datum surfaces describing Models A and C have slopes of one in horizontal ten, while that of B is of three in ten. This indicates that the magnitude of elongation is a function of the steepness of the underlying regional pattern. The orientation of the induced long axis is clearly related to the sense of elongation of the data point distribution (expressed by the best fit line [reduced major axis]), this being shown more clearly by Model A, where there are no secondary effects from sine-wave modifications.

(b) Displacement

While the contour of the quadratic surface of Model A is centred roughly at the centre of the map, there is a progressive displacement to the north-east through the model-series as the contribution of the local (at this level) sine-wave component increases in magnitude, so that, in Model C, the centre is approximately sited at the mean co-ordinate position of the data point population. This shows that in surfaces that account for a relatively low

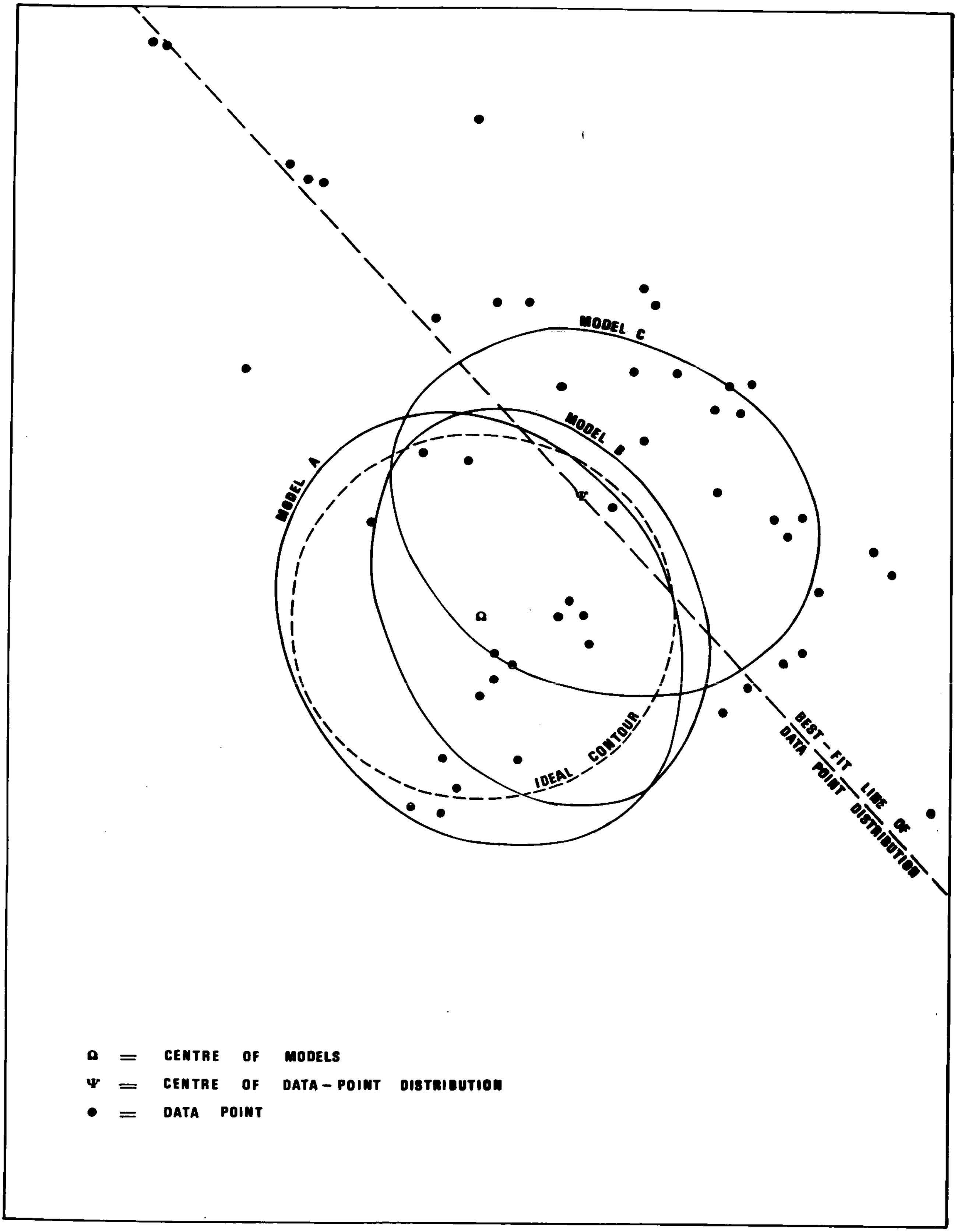


Fig. 7 Distortion of model Quadratic trend surfaces

proportion of the total map variability, there is a sense of displacement of the 'true' surface towards a location representing the mean of the data point distribution.

(ii) Clustering effects

The geometrical effects produced by local clusters of points are shown in the cubic surfaces which by virtue of their complexity are sensitive to the local distortions of this order. On the cubic surface of Model A (Fig.4), the prominent saddle development in the north-east of the area can be attributed to the relatively high concentration of data points of similar value in this direction. The distortions shown on the cubic surfaces of the more complex models B and C (Figs. 5 and 6) reflect the varying degrees of information regarding the sine-wave component provided by a patchy point distribution. The sensitivity of the cubic (and higher) surface to clustering indicates that where clustering is likely, only limited analysis of cubic surface map configurations is possible.

2. Measures of significance applied to artificial models

The methods currently available have already been reviewed (pp.16-19) and it was pointed out that analysis of variance was probably the best approach, though there is a danger of violating statistical assumptions in its geological interpretation. *F* tests were conducted in the form used by Allen and Krumbein (1962) and others, in which the contribution of successively complex terms were set against higher residuals as a mean sums of squares ratio with appropriate degrees of freedom, whose level of significance was found from standard tables of *F*. The computational parts and results are set out in Table 1.

It can be seen immediately that pure linear, quadratic and

Table 1

ANALYSIS OF VARIANCE F TESTS OF ARTIFICIAL MODELS TREND SURFACE DATA

(SSQ = Sum of Squares ; DF = Number of degrees of freedom ;
MSQ = mean square ; F = F ratio ; SIGNIF.L = o/o Significance level ;
SSQ.prop = Proportion of total sum of squares accounted for by pure term.)

MODEL A

SOURCE	SSQ	DF	MSQ	F	SIGNIF.L	SSQ.prop
Linear	5.435	2	2.718	24.4	>99.9	51.5 o/o
Deviations from linear	5.129	46	0.112			
Pure Quadratic	4.668	3	1.556	145.4	>99.9	44.2 o/o
Deviations from quadratic	0.461	43	0.011			
Pure Cubic	0.289	4	0.072	16.4	>99.9	2.7 o/o
Deviations from cubic	0.172	39	0.004			
Total	10.564					

Table 1 (continued)

	SSQ	DF	MSQ	F	SIGNIF.L	SSQ.prop
MODEL B						
SOURCE						
Linear	36.421	2	18.211			35.0 o/o
Deviations from linear	67.676	46	1.471	12.38	>99.9	
Pure Quadratic	49.772	3	16.591			47.8 o/o
Deviations from quadratic	17.904	43	0.416	39.84	>99.9	
Pure Cubic	5.546	4	1.387			5.3 o/o
Deviations from cubic	12.358	39	0.317	4.38	>99	
Total	104.097					
MODEL C						
SOURCE						
Linear	3.986	2	1.993			12.7 o/o
Deviations from linear	27.359	46	0.595	3.35	>95	
Pure Quadratic	6.541	3	2.180			20.9 o/o
Deviations from quadratic	20.818	43	0.484	4.50	>99	
Pure Cubic	8.369	4	2.092			26.7 o/o
Deviations from cubic	12.449	39	0.319	6.55	>99.9	
Total	31.345					

cubic components are all significant (greater than 95% significance) for all models. Closer examination of the Model A statistics show that pure linear and quadratic terms are strongly significant and account for a fair proportion (51.5 and 44.2%) of the total sums of squares of the map data (as would be expected for a simple conical surface with large apex angle). This is contrasted with the pure cubic term which is again highly significant, but accounts for only 2.7% of the total map variability. While one accepts that the residual difference between a conical and a paraboloid surface may contain a dominantly cubic component, which is therefore significant, the low proportion of regional variability accounted for by this element suggests that this is a systematic local factor (located at the apex of the cone) rather than one of large-scale regional significance. It seems that while such F test results do reveal significant trend terms, attention should also be directed at the proportion of total sums of squares satisfied by these terms in judging the scale of their contribution.

In the case of Model B, total variation is again dominated by the cone datum plane, though sine-wave modifications are an important additional factor which are partly accounted for by pure cubic terms and could therefore be viewed as local or regional in significance.

Variation in Model C is largely accounted for by the sine-wave configuration with a dampened contribution from the high apex angled conical datum. The regional pattern can be thought of as a combination of pure linear, quadratic and cubic effects, as illustrated by both the F test significance level values and the proportion of map variability assignable to each component.

Summary of conclusions derived from artificial model work

The lessons to be learned from these studies which must be borne in mind in the interpretation of trend surfaces of geological variables are therefore:

(1) if there is a tendency for linearity (of even moderate to low strength) in the arrangement of data points, a component of elongation of the 'true' surface is to be expected sub-parallel to the best-fit line passing through the data point population.

(2) the quantitative degree of elongation will vary according to the geometry of the variable surface and while no systematic estimate of this fault can be made, its magnitude seems related to the steepness of trends represented by the surface.

(3) if the surface accounts for an indifferent to moderate proportion of total map variability, the true surface will tend to be displaced towards a position marking the mean co-ordinate of an elongate data point distribution.

(4) any tendency towards local clustering with the point population first becomes noticeable in cubic surfaces when the complex terms take account of this local variation in information. This suggests that unless the points have a high degree of homogeneity on the small scale, analysis should be preferentially directed at linear and quadratic surface map patterns.

(5) analysis of variance by an <u>F</u> test appears to be an aid in estimating the significance of trend surfaces, though

the scale of this character is best judged by reference to the proportion of the map variability accounted for by each term.

The data point population used in the generation of these artificial model surfaces represents the worst set (from the point of view of potential distortion) used in the study of areal variation of geological variables described in the next chapter. However, such an arrangement of points is not entirely atypical, because the broad orientation of the Coal Measure tract as a NW-SE belt across the map area imparts some degree of linearity to any selected population of points. The data points were selected to ensure as homogeneous a scatter as possible in so far as this was compatible with availability of data. However, the sparseness of data in some areas, relative abundance in others, inevitably led to some degree of clustering. Therefore, the general conclusions drawn from work with these artificial models find their application in the geological studies that follow.

Chapter 3

TREND SURFACE ANALYSIS OF AREAL VARIATION WITHIN THE AYRSHIRE COAL MEASURES

Choice of Features Studied

The area used in trend surface analysis study of geological variation was set to include the major part of the Ayrshire Coalfield as defined by the Geological Survey Regional and Economic memoirs, with the exclusion of only minor Coal Measure developments at the eastern and northern margins. The geographic and geological base map underlying the following trend surfaces is shown in Appendix I and arranged in fold-out form to enable easy comparison between the surfaces and features of geographic and geological interest.

As trend surface analysis is the study of two-dimensional (geographic) variation of characters, the dimension of time must be sensibly constant over the area. Stated another way, observations must be made at horizons that are accepted as essentially non-diachronous or within units bounded by such horizons. Potential 'time planes' in the Coal Measures are marine bands and coal seams. While such horizons cannot be strictly synchronous in the absolute time sense, in the context of 'geological time' they are likely to be only feebly diachronous. It was stated earlier (p. 8) that the marine and *Lingula* bands of the Ayrshire Coal Measures are local in development so that the boundaries they represent cannot be used over more than a limited area. Reference to the stratigraphy of the sequence in Fig.8 shows that only four coals can, at present, be correlated over the entire region, these being the Ell, Main,

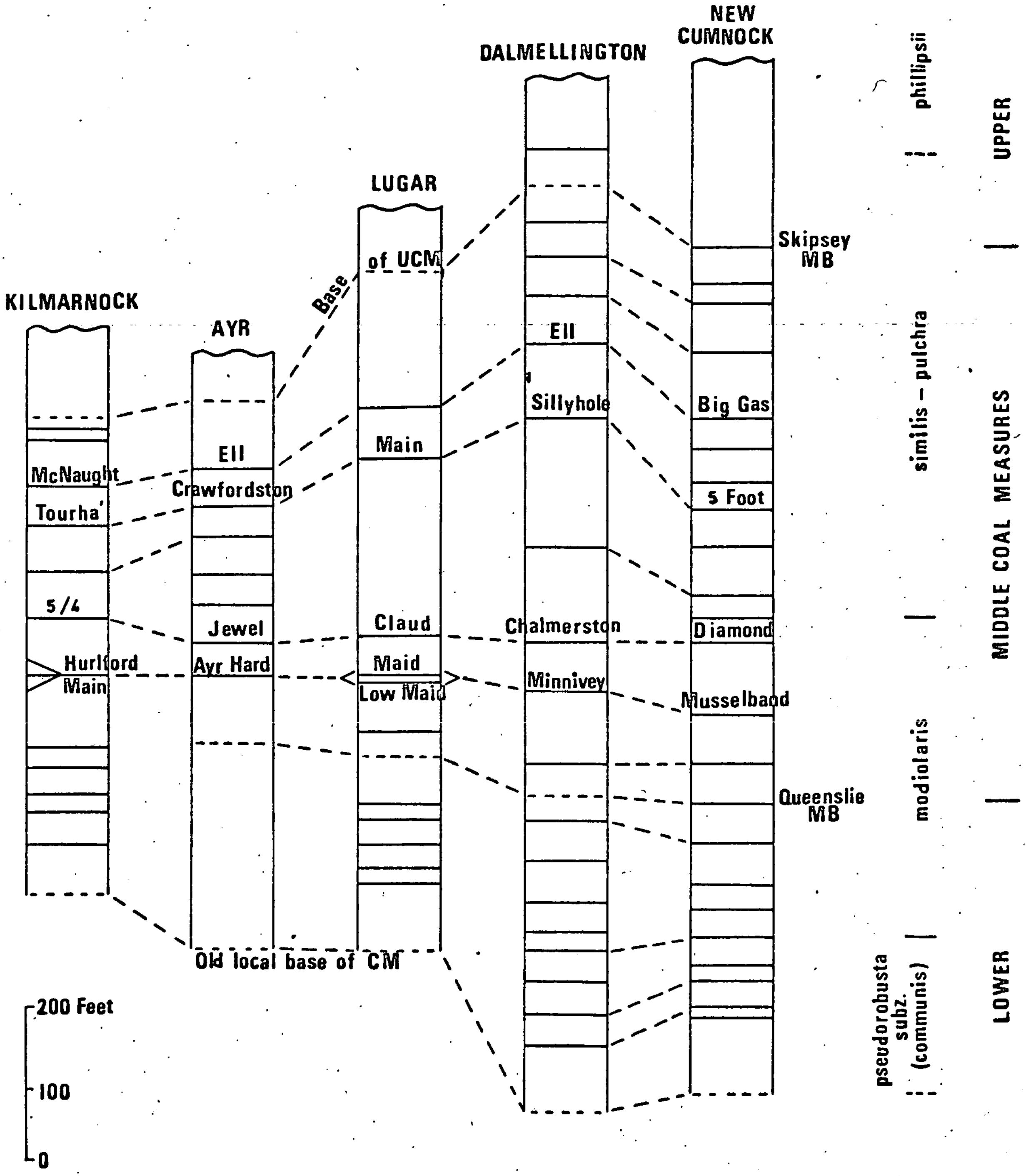


Fig. 8 Stratigraphy of the Ayrshire Coal Measures after Trueman (1954) with modifications after Mykura (1967). For full coal nomenclature, see Trueman.

Jewel and Ayr Hard coals (or local variant names), of similis-pulchra and modiolaris zone ages.

These coals were used as boundary planes to describe two rock units, the higher defined by the Ell and Main coals, and the lower by the Jewel and Ayr Hard coals. Observations made within these units were taken from borehole records logged by geologists from either the Geological Survey or the National Coal Board. (In certain cases, other bores were used where the measured attribute was a function of position or thickness of named coals correlatable on geological grounds).

Trend surface maps were computed for the following variables:

1. Depth of the Main Coal below sea level (structural contour).
2. Thickness of the interval between the Ell and Main coals (isopachyte).
3. Thickness of the interval between the Jewel and Ayr Hard coals (isopachyte).
4. The proportions of the interval (calculated as percent) represented by sandstone, siltstone and shale between the Ell-Main and Jewel-Ayr Hard coals (lithofacies).
5. The thickness of the Ell, Main and Jewel coals (isopachyte).

1. Structure (Horizon of Main Coal)

Measurements of the depth of this coal below mean sea level were made for 55 observations whose locations were chosen to represent a reasonable distribution about the map area. Hand-contouring of such data would result in a structure contour map of this seam which would be a record of tectonic movements since the time represented by its formation. Such a map would be a complex mixture of regional and local effects and the aim of this exercise was to separate the components at two levels, the higher representing structures regional to Ayrshire and registered by low order trend surfaces, the lower diagnostic of structures local to the map area and brought out in residuals from low order surfaces and certain complex components of higher order surfaces.

The computed surfaces to cubic level, together with the data point distribution and contoured quadratic residuals, are set out in Fig.9. Analysis of variance F tests were performed on these surfaces and the computational parts and results, as well as coefficients of determination of individual pure terms, set out in Table 2. Examination of the statistics shows that only the pure quadratic term proved to be significant, being above the 99.9% level. It therefore seems likely that the quadratic surface is the valid representation of the regional trend and has the form of a large basin trending NNW-SSE.

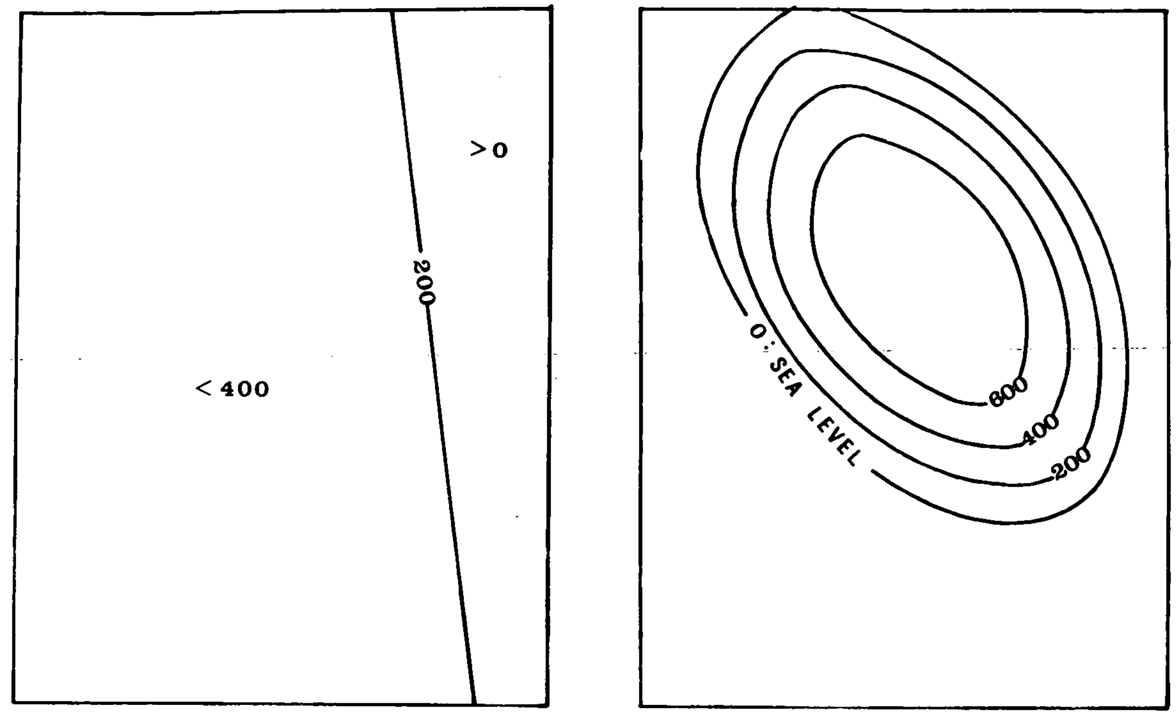
The patterns of these trend surfaces are reminiscent of those produced from the artificial models, suggesting that checks derived from them may be usefully applied to the structure surface. The proportion of the total sums of squares accounted for by these surfaces is low (33.6% at cubic level) and it will be remembered that in such a case there was a displacement of the predicted structure from its true position towards the mean co-ordinate position of the data points. The gross orientation of data points used in the structural analysis suggests an analogous distortion of these surfaces is possible. However, contoured quadratic residuals show a systematic negative area coinciding with the centre of the regional structure, demonstrating that in this case, the displacement of the surface is minor or absent. The lack of this type of distortion

Table 2

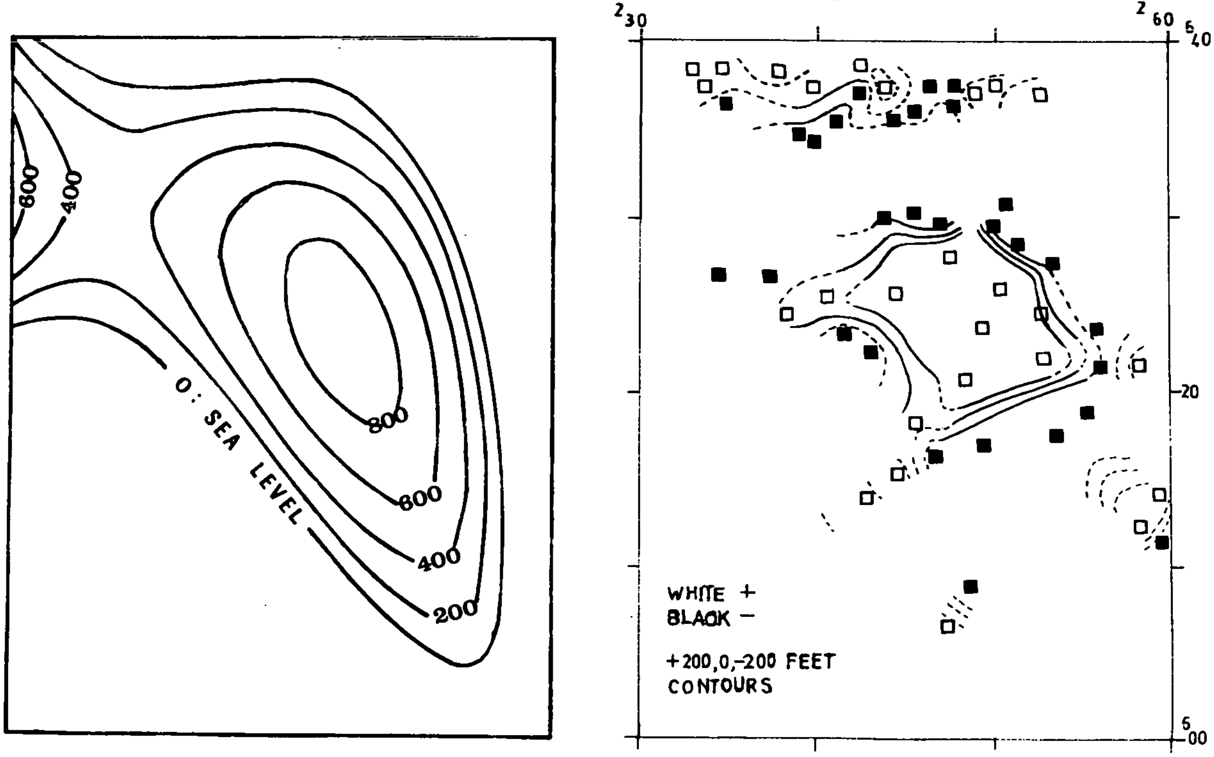
ANALYSIS OF VARIANCE F TESTS OF MAIN COAL STRUCTURE CONTOUR TREND SURFACE DATA

(SSQ = Sum of Squares ; DF = Number of degrees of freedom ;
MSQ = mean square ; F = F ratio ; SIGNIF.L = o/o Significance level ;
SSQ.prop = Proportion of total sum of squares accounted for by pure term.)

SOURCE	SSQ	DF	MSQ	F	SIGNIF.L	SSQ.prop
Linear	49017	2	24508.5			0.[illegible]2 o/o
Deviations from linear	26786000	52	515115.4	0.05	<5	
Pure Quadratic	7642283	3	2547427.7			28.5 o/o
Deviations from quadratic	19144000	49	390693.9	6.5	>99.9	
Pure Cubic	1369800	4	342450.0			5.1 o/o
Deviations from cubic	17774000	45	394978.0	0.9	<75	
Total	26835017					



linear quadratic



cubic quadratic residuals

FIG. 9 TREND SURFACES OF MAIN COAL DEPTH (FEET) B.S.L.

is explained in that the centre of the structure and the point distribution roughly coincide so that appreciable displacement is not possible.

The best-fit line drawn through the data point distribution would roughly parallel the long axis of the trend surface regional structure and experience from the artificial models suggests that there may be an elongation effect along this line. However, the Mauchline basin, which contributes significantly to the regional feature, is of NW-SE trend (Mykura, 1967, p.88) so that any sense of elongation is likely to be an accentuation of a real geological feature.

A further encouraging feature regarding the quadratic and cubic maps is that the intersection of these surfaces with a topographic level typical of the region, would give a very reasonable estimate of the broad outcrop of the Main coal, an empirical demonstration that the surfaces are fair regional models.

However, while the quadratic component is significant and the computed maps rational, the proportion of sums of squares accounted for by these surfaces is low. It follows that the majority of variance is contained in higher degree terms which must represent a combination of structural features local to the total map area and some degree of 'noise.' The structure of the area is therefore dominated by these local phenomena caused by relatively small-scale folding and faulting, though it is underlain by a significant regional basin structure. Although the 'fit' of the linear surface is remarkably low (0.2%), indicating that little or no interpretation can be based on the surface configuration, it is striking that the mapped plane is of very low angle, implying that there is no pronounced asymmetry to the regional structure.

Examination of the quadratic residual contour pattern (Fig.9) shows the occurrence of local basins in the Mauchline Basin, probably within the Kerse Loch-Littlemill Fault zone, at Dalleagles and Dalmellington in the south, and in the Kilmarnock area, north of the Inchgotrick Fault.

2. Thickness of the Ell-Main Interval

The observation points used in the trend surface analysis of the structure of the Main Coal were set as the data point population for the variable of the thickness between the Main and the overlying Ell Coal, to enable systematic study of the relationship between structure and thickness of sediment. Analysis of variance F tests are set out in Table 3, while the computed surfaces to cubic level and residuals from the cubic are shown in Fig.10.

The linear surface accounts for 62.3% of the total variance, is significant above the 99.9% level, and is the dominant theme of regional variation. The trend predicts a direction of regional thinning of N 14° E which accords well with the generalised observation of Mykura (1967) p.74 that, "the strata between the Main and Ell coals .... shows a fairly consistent thinning to the north-north-east." The remainder of the total population variability appears to be contained in variations of a local character as the pure quadratic term accounts for only 3.2% and is insignificant, while the significant pure cubic term provides 8.1%.

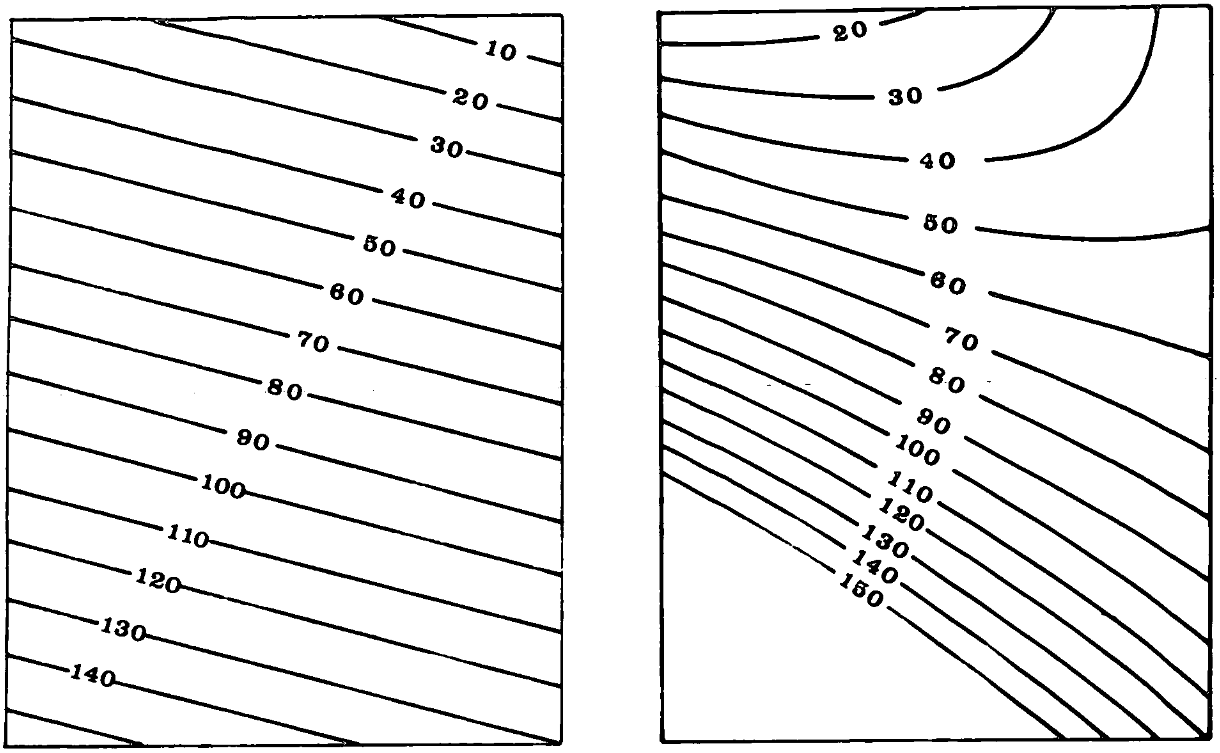
This local variation is represented to some degree by the residuals from the cubic surface (Fig.10). The geometry of the residual contours shows a fair parallelism with the trace of faults of local significance to the region (see Appendix I) and a reas-

Table 3

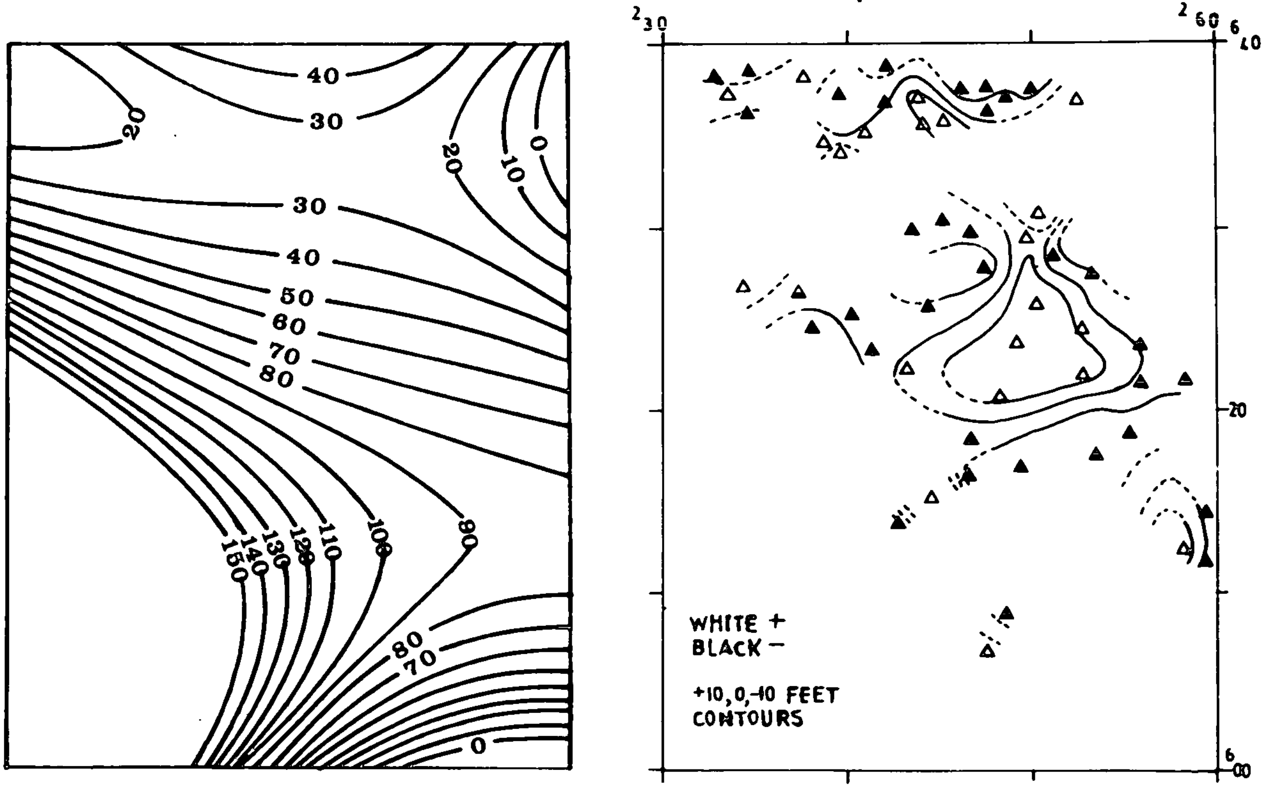
ANALYSIS OF VARIANCE *F* TESTS OF ELL - MAIN INTERVAL THICKNESS TREND SURFACE DATA

(SSQ = Sum of Squares ; DF = Number of degrees of freedom ;
MSQ = mean square ; *F* = *F* ratio ; SIGNIF.L = o/o Significance level ;
SSQ.prop = Proportion of total sum of squares accounted for by pure term.)

SOURCE	SSQ	DF	MSQ	*F*	SIGNIF.L	SSQ.prop
Linear	40498	2	20249.0	43.0	>99.9	62.3 o/o
Deviations from linear	24481	52	470.8			
Pure Quadratic	2104	3	701.3	1.5	<90	3.2 o/o
Deviations from quadratic	22367	49	456.5			
Pure Cubic	5243	4	1310.8	3.4	>97.5	8.1 o/o
Deviations from cubic	17124	45	380.5			
Total	64979					



linear quadratic



cubic cubic residuals

FIG.10 TREND SURFACES OF ELL-MAIN INTERVAL THICKNESS (FEET) reasonable coincidence between positive residual areas and the 'small-scale' structural basins of the quadratic residuals of the Main Coal depth (Fig.9). Such features suggest the possibility of a relation between local structure and unit thickness.

Relationship between thickness and potential structural control

The general thesis that thickness of sedimentation had some degree of structural control in the Carboniferous of Ayrshire has been demonstrated in earlier work (see p. 4). The study of a possible tectonic factor in the thickness of the Ell-Main interval seeks to answer the following questions:

1. While there is a known structural control in the deposition of the relatively large units of Upper Carboniferous age, does this broad control extend to relatively thin intervals of the order of the Ell-Main unit (average thickness 54 feet)?
2. If present, is this control of regional and/or local significance (relative to Ayrshire as a whole)?

The choice of the same data point distribution for trend surface computation of the depth of the Main Coal and for the Ell-Main interval thickness enables studies of the correlation of the two variables to be made. A calculation of the correlation coefficient, r, between the raw values of 'structural depth' and 'thickness' gave a feeble positive correlation of 0.09, demonstrating no significant relation at this level. Correlation coefficients were calculated for corresponding data point values of the two variables for trends and residuals up to quintic degree and these are indicated by the continuous lines of Fig.11. Examination of this figure

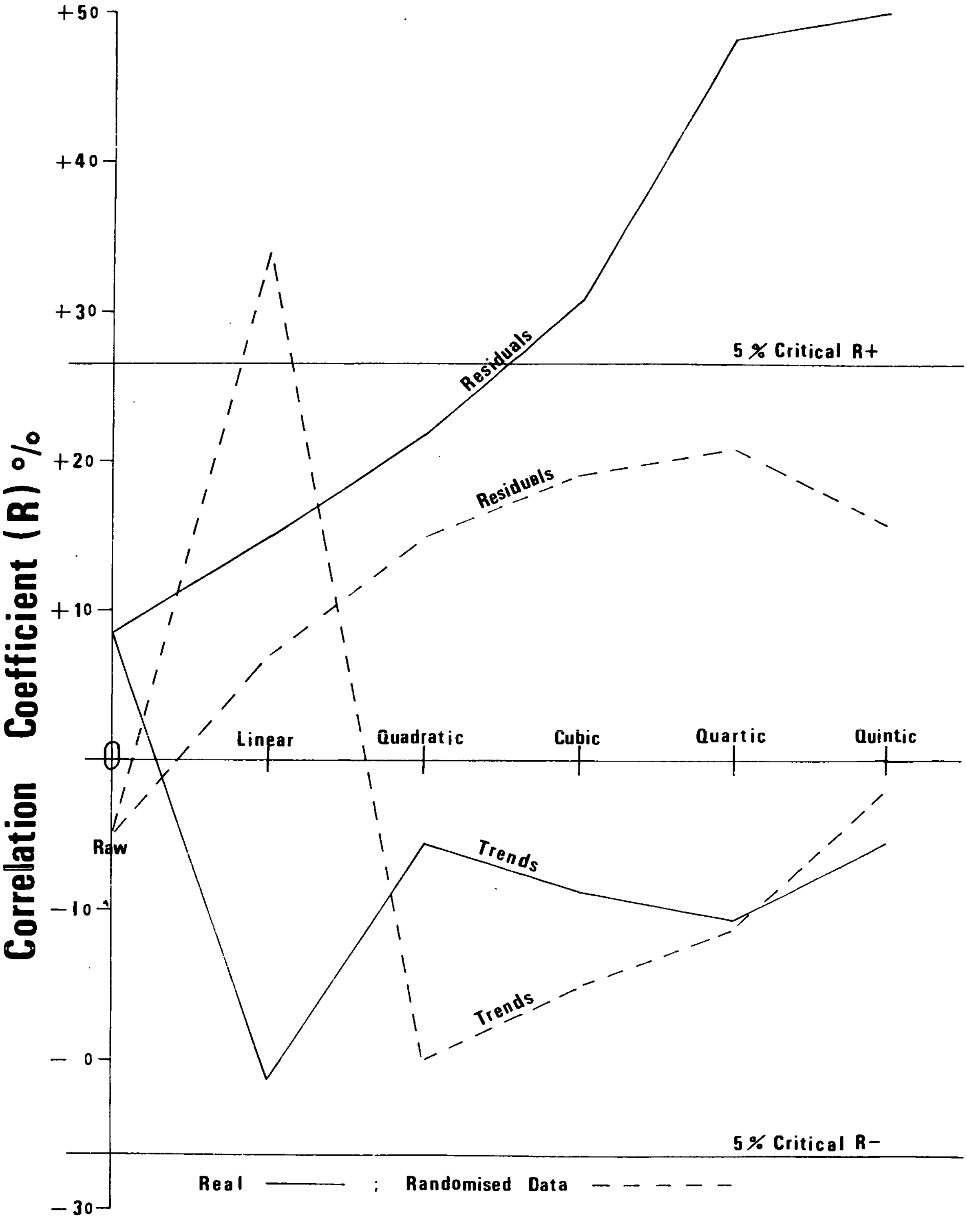


FIG. 11 Correlation coefficients (R) of trends and residuals of real and randomised data : E11 - Main unit thickness v. structural level of Main Coal (see text)

shows a feebly negative (and insignificant) correlation in trend values throughout, establishing that there is no association between the thickness of the unit and the structural development on a regional scale. Such a conclusion is hardly surprising when it is recalled that the regional structure is described essentially by a quadratic surface with utterly insignificant pure linear term content and weak pure cubic term modifications, while the regional pattern of thickness variation is dominantly one of linear degree with muted pure quadratic and cubic additions.

Contrasted with this aspect, the correlation between the variable residuals shows fairly systematic improvement in positive character as the power of the complementary surface is increased, reaching a value of 0.50 at quintic level. It was suspected that a certain amount of this enhancement of residual correlation with higher power was artificial. This would express itself by the attempt of higher surface terms to describe more extreme residuals left from a lower surface, in preference to smaller residuals. The result would be a truncation of the 'tails' of the distributions of the residuals about the surfaces and so a spurious increase in correlation between the two variables in the residual series. To allow for this possible factor, the raw observations of each variable were randomised between data points and trend surfaces were computed for this 'random data.' Correlation coefficients were calculated as for the real data and these are shown by the dotted line of Fig.11. The random series show an increase in positive correlation with degree of residual, though rather less than for the real residuals, reaching a maximum value of 0.21 for quartic residuals. This suggests, therefore, that there does exist some systematic component of geological meaning in the higher residuals of the real data. Such a possibility was examined more closely by plotting the critical absolute value at the 5% point of the correlation coefficient for two variables at the appropriate number of degrees of freedom (53), shown at the lines $r = \pm 0.27$. These set an 'area of insignificance' such that, in the case of the residuals, the correlation coefficients of the real data become significant after the quadratic level, whereas the random residual series is one of insignificance throughout. However, it will be noticed that the correlation coefficient of the randomised data linear trend surfaces also has a small 'significance' on this criterion and presumably reflects the fact that these correlation coefficient values are only an estimate of the true universal population values, being based on a population of 55 points. To counter this error, 95% confidence limits envelopes were drawn for each residual sequence (Fig.12) and these show that while the real cubic residual r value has an acceptable probability of being significant, this is very high for the quartic and quintic orders, where the entire confidence limit belt exceeds the absolute level of significance.

The conclusions to be derived from these arguments is that for the unit studied (roughly equivalent to two seatearth-to-seatearth cycles) the thickness is unrelated to the large-scale regional structure of the area. On a regional scale, the unit tends to have a wedge-like development (described by the linear term) which may reflect the palaeoslope underlying deposition. This cuts across an effectively quadratic regional structural surface, possibly mainly the product of tectonic movements of post-Carboniferous age. On a scale local to the whole map area, however, there is a

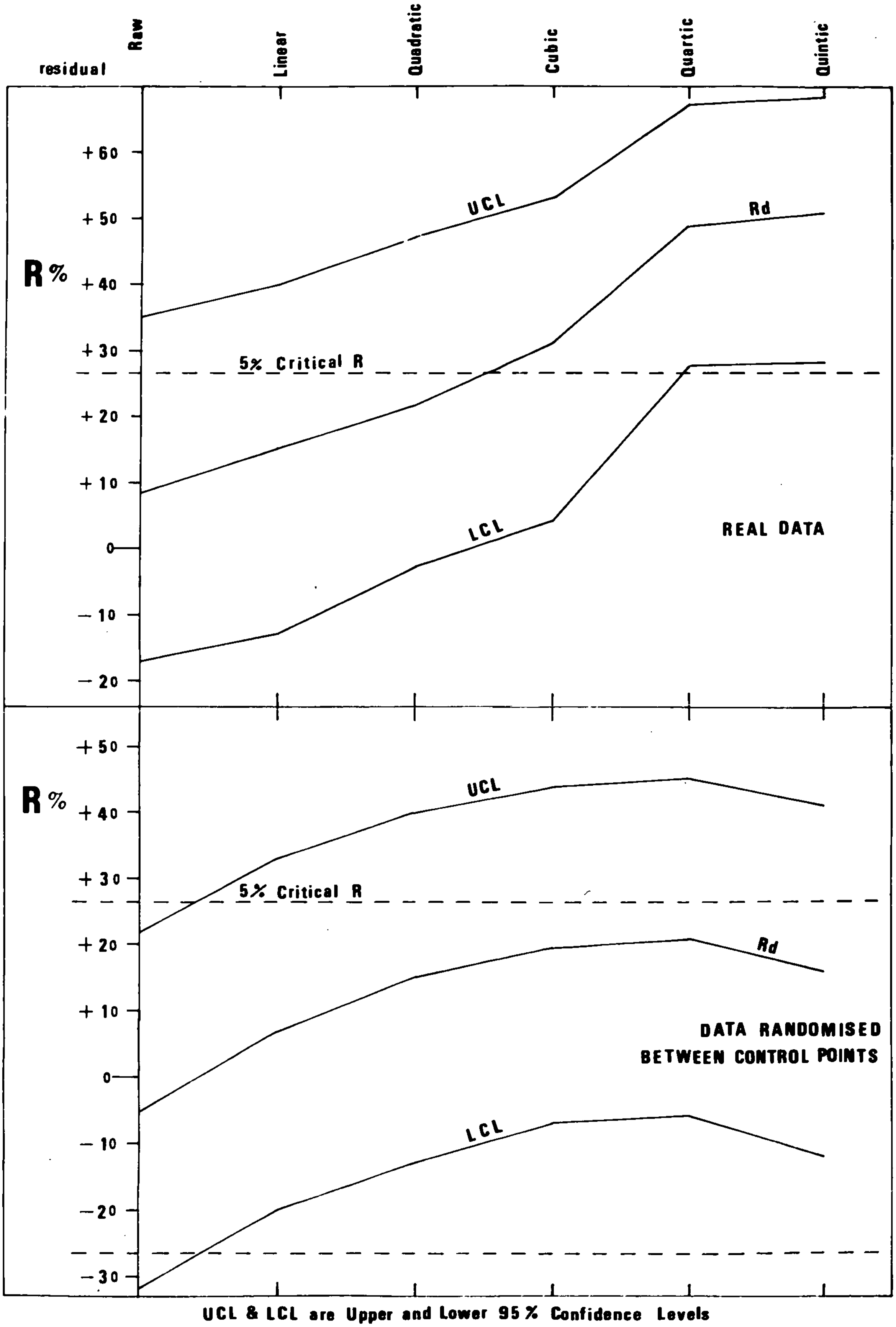


FIG. 12 Confidence levels for real residual correlation coefficients of Fig. 11 (see text)

significant correlation between the thickness of the unit and the structural depth of its base and comparison between residual maps of the two variables indicates the presence of small basins in various parts of the area which were probably tectonically active during deposition.

3. Thickness of the Jewel-Ayr Hard Interval

Measurements were made of the thickness of the interval banded by the Ayr Hard and Jewel coals at 57 borehole locations. The computed surfaces together with the contoured residuals from the cubic trend are shown in Fig.13 while the analysis of variance F tests are set out in Table 4.

The surfaces of this interval show marked differences in character from those of the Ell-Main unit. In this case, the linear surface is one of a thinning to the south-west, though it should be noted that the proportion of the sum of squares accounted for (12.3%), while significant, is substantially lower than for the linear surface of the Ell-Main unit, while the wide spacing of the contours shows this as a gentle trend. Further, the pure quadratic component is more significant and absorbs a further 29.9% of the total variability, in strong contrast to that of the Ell-Main interval where it is insignificant and adds only 3.2%. In terms of analysis of variance results, the pure cubic elements of the two intervals are similar.

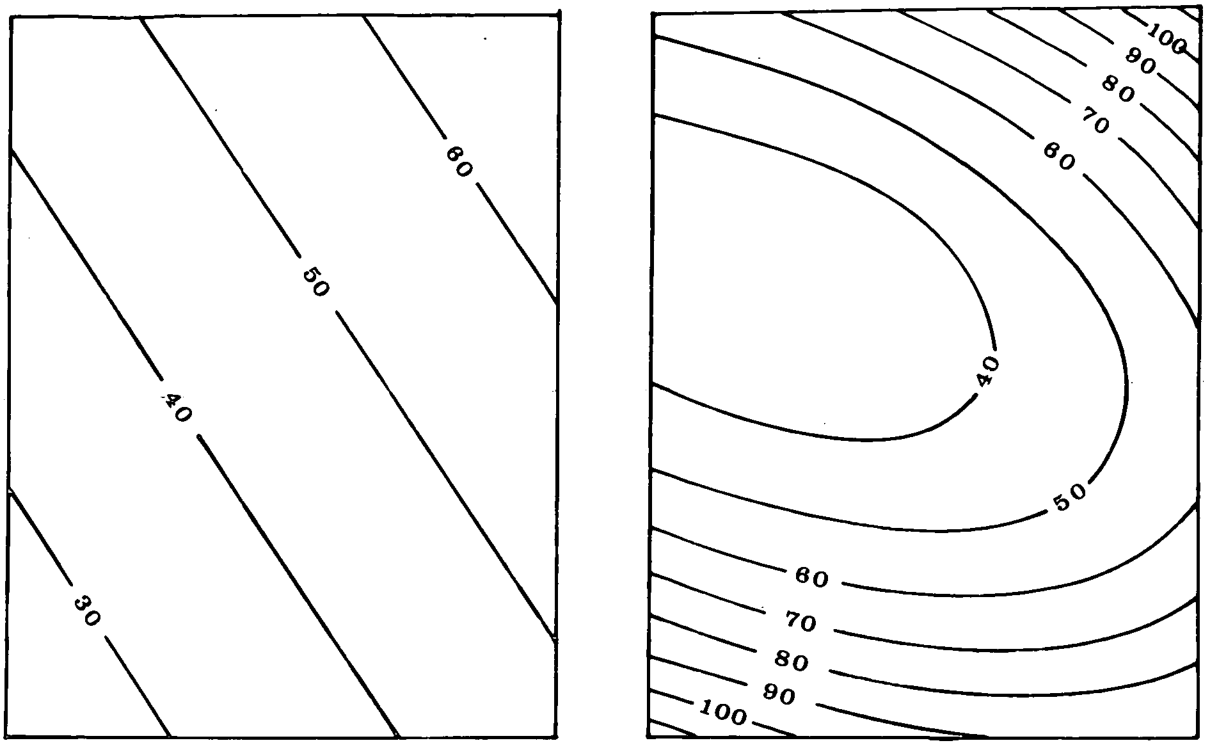
The conclusion that follows is that the thickness variation of this unit is dominated by its pure quadratic term, though it has significant pure linear and cubic componemts. (This differs from the Ell-Main unit which is primarily linear in geometry). Reference to the quadratic surface map suggests that there is a thick

Table 4

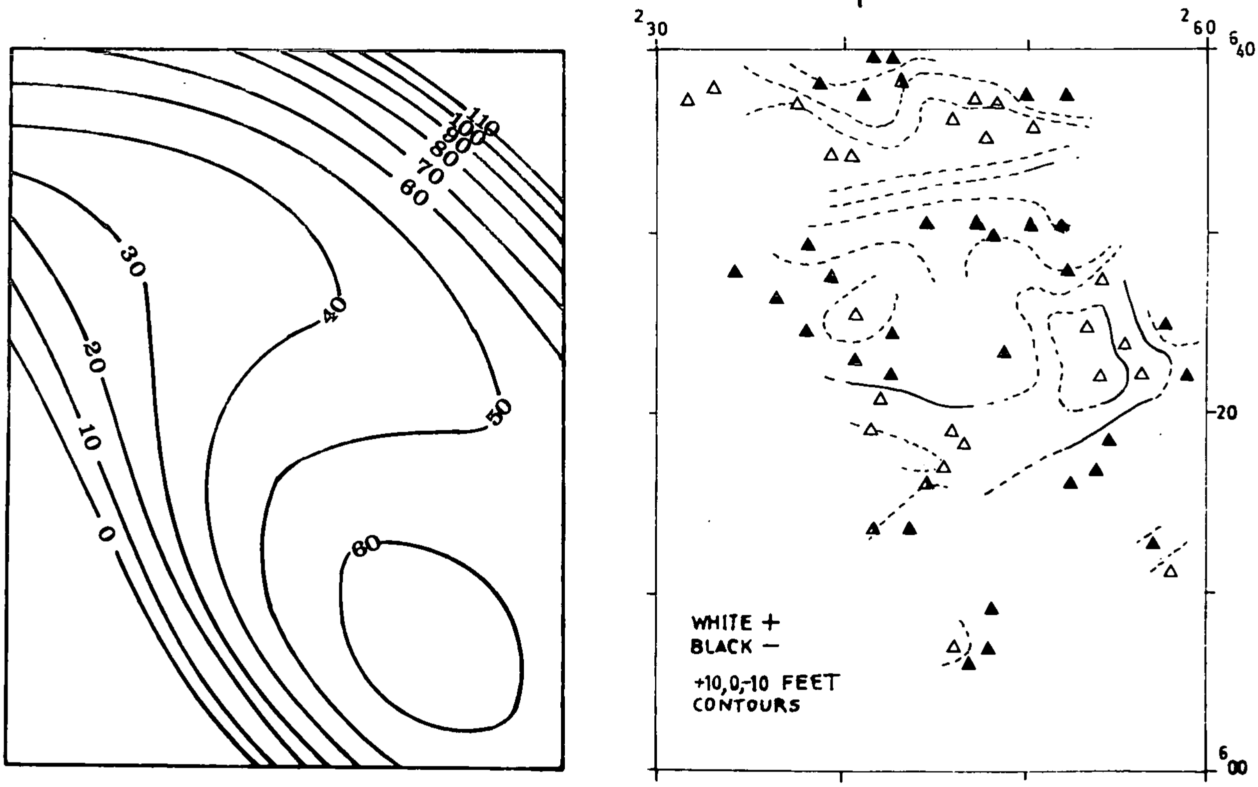
ANALYSIS OF VARIANCE *F* TESTS OF JEWEL - AYR HARD INTERVAL THICKNESS TREND SURFACE DATA

(SSQ = Sum of Squares ; DF = Number of degrees of freedom ;
MSQ = mean square ; *F* = *F* ratio ; SIGNIF.L = o/o Significance level ;
SSQ.prop = Proportion of total sum of squares accounted for by pure term.)

SOURCE	SSQ	DF	MSQ	*F*	SIGNIF.L	SSQ.prop
Linear	1992	2	995.8	4.0	>97.5	12.3 o/o
Deviations from linear	14144	57	248.1			
Pure Quadratic	4829	3	1609.8	9.3	>99.9	29.9 o/o
Deviations from quadratic	9314	54	172.5			
Pure Cubic	1666	4	416.6	2.7	>95	10.3 o/o
Deviations from cubic	7648	50	152.9			
Total	16136					



linear quadratic



cubic cubic residuals

FIG. 13 TREND SURFACES OF JEWEL-A.H. INTERVAL THICKNESS (FEET) development at both the south-west and north-east margins, with a correspondingly thinner area in the centre and west. Mykura (1967) p.55 noted that, "the area of overlap or attentuated deposition near Monkton which was a major feature in the Lower Coal Measures was still in evidence up to the formation of the Ayr Hard Coal." Comparison with the geological base map of these surfaces (Appendix I) shows that the sense of thinning in the geometry of the quadratic surface centres on the Monkton area. This suggests that the progressive overlap of the 'Millstone Grit lavas' through Lower Coal Measure times was still a factor of regional significance in late modiolaris times (Jewel-Ayr Hard), though dwindling to insignificance by the time of the deposition of the younger Ell-Main unit.

Examination of the contoured residuals from the cubic surface for the Jewel-Ayr Hard interval (Fig.13) shows a configuration that has some degree of broad similarity with the equivalent for the Ell-Main unit (Fig.10), though they differ in detail, indicating that while local basin subsidence is likely to have been active, the pattern was a highly fluid one.

4. Areal Clastic Variation of the Ell-Main and Jewel-Ayr Hard Units

A study of the lithological variation of these units was based on borehole data for which the sandstone, siltstone and shale proportions were calculated as percentages for each observation point. A population of points was assembled for each interval and trend surfaces computed for each lithological variable. The resulting six sets of trend surfaces (Figs. 14 to 19) are considered collectively so that generalisations can be made between units while the percentage form of the data makes the total variation a closed system so that conclusions from the variable surfaces within each unit are partly interdependent.

Comparison of the linear surfaces for the three lithologies reveals a consistent pattern in both units. This shows an increase in sandstone in a north-easterly to north direction which is closely paralleled by an increase in siltstone and a decrease in shale along virtually the same bearing. Consideration of the proportion of total variability accounted for by the successive pure degree terms for each variable (Fig.20) shows that the areal variation of shale content is mainly linear with minor but significant pure quadratic and cubic components. Sandstone variation consists of a limited, but significant, linear element together with some degree of pure cubic contribution, while siltstone variation geometry appears somewhat haphazard as might be expected for a lithofacies development sandwiched between the depositional environments represented by sandstone and shale. The intimate association between the sandstone and siltstone fractions shown by the linear surfaces coupled with their low coefficients of determination compared with the shale linear surface, suggests an environmental model of relatively irregular sand lobes or sheets with associated swathes of silt, active within a regional 'platform' background of mud deposition. The orientation of these linear surfaces indicates an overall derivation of coarse material from a north-easterly direction.

Examination of the residuals of these variables from their highest significant (from analysis of variance) trend surface shows a patchy development of facies belts and areas, none of which seem to be strongly related to the pattern of the local tectonics as is suggested for the units' gross thickness.

Table 5

ANALYSIS OF VARIANCE *F* TESTS OF ELL - MAIN INTERVAL o/o CLASTICS TREND SURFACE DATA

(SSQ = Sum of Squares ; DF = Number of degrees of freedom ; MSQ = mean square ; *F* = *F* ratio ; SIGNIF.L = o/o Significance level ; SSQ.prop = Proportion of total sum of squares accounted for by pure term.)

o/o SAND

SOURCE	SSQ	DF	MSQ	*F*	SIGNIF.L	SSQ.prop
Linear	3889	2	1944.5	5.46	>99	19.2 o/o
Deviations from linear	16365	46	355.8			
Pure Quadratic	1178	3	392.7	1.11	<75	5.8 o/o
Deviations from quadratic	15187	43	353.2			
Pure Cubic	3129	4	782.3	2.53	<95	15.4 o/o
Deviations from cubic	12059	39	309.2			
Total	20254					

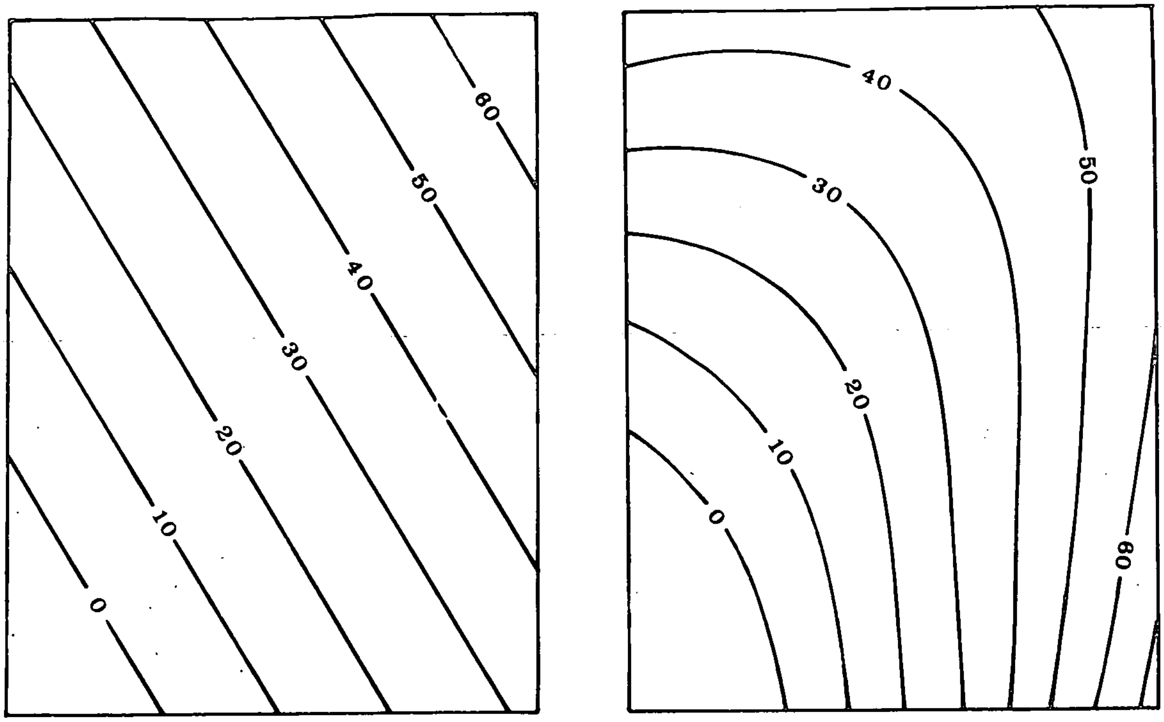
Table 5 (continued)

o/o SILTSTONE

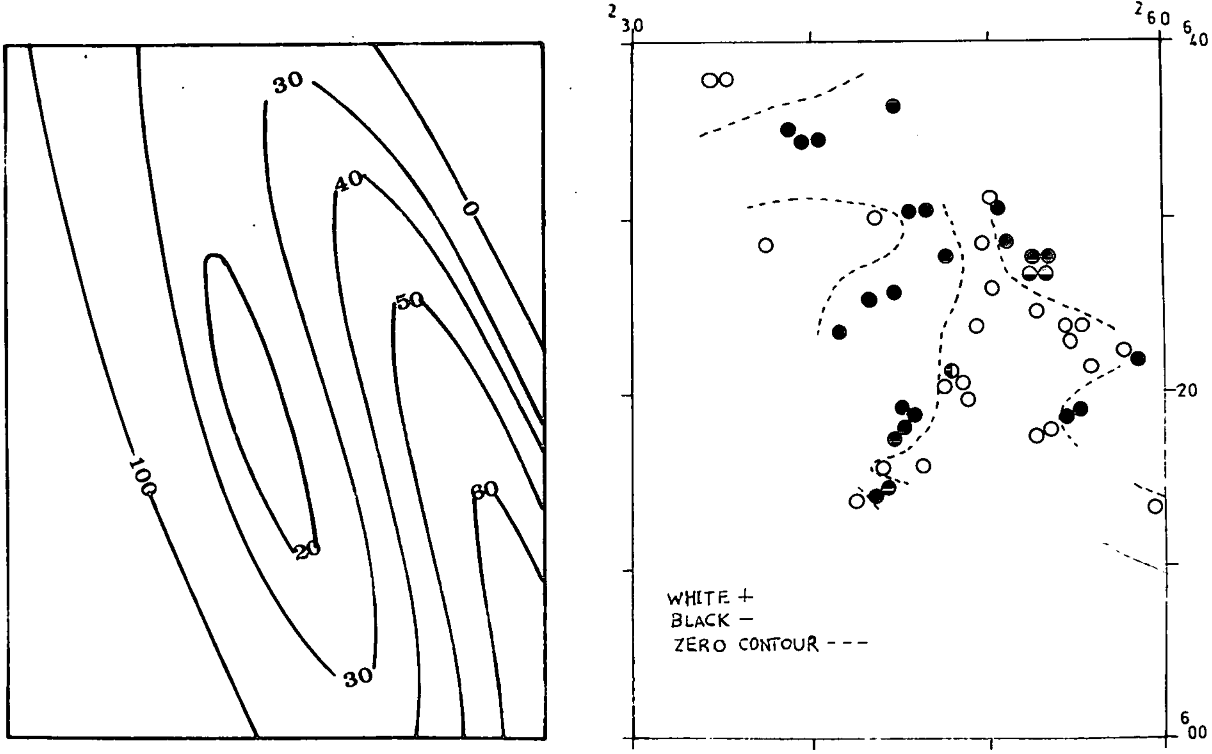
SOURCE	SSQ	DF	MSQ	F	SIGNIF.L	SSQ.prop
Linear	1729	2	864.5	3.6	>95	13.4 o/o
Deviations from linear	11131	46	242.0			
Pure Quadratic	1839	3	613.0	3.1	>95	14.3 o/o
Deviations from quadratic	9292	43	197.9			
Pure Cubic	184	4	46.0	0.2	<10	1.4 o/o
Deviations from cubic	9108	39	233.5			
Total	12860					

o/o SHALE

SOURCE	SSQ	DF	MSQ	F	SIGNIF.L	SSQ.prop
Linear	10470	2	5235.0	22.7	>99.9	49.6 o/o
Deviations from linear	10623	46	230.9			
Pure Quadratic	2815	3	938.3	5.2	>99.5	13.3 o/o
Deviations from quadratic	7808	43	181.6			
Pure Cubic	2154	4	538.5	3.7	>97.5	10.2 o/o
Deviations from cubic	5654	39	145.0			
Total	21093					

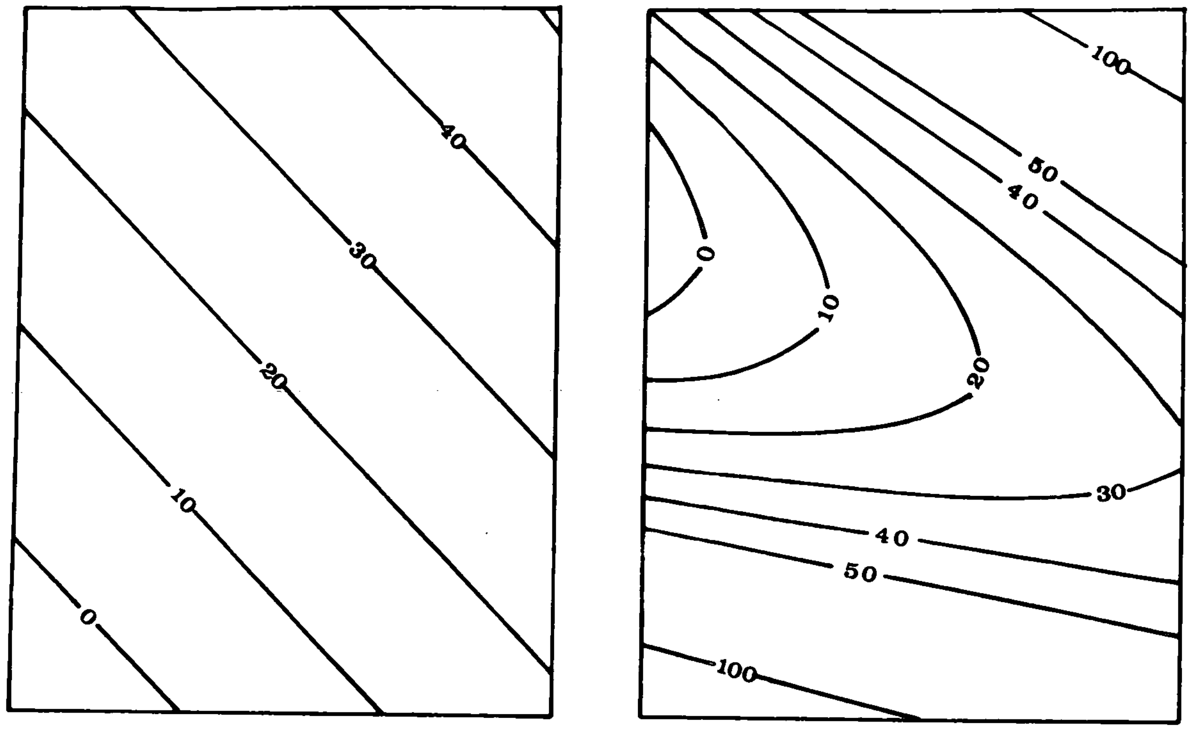


linear quadratic

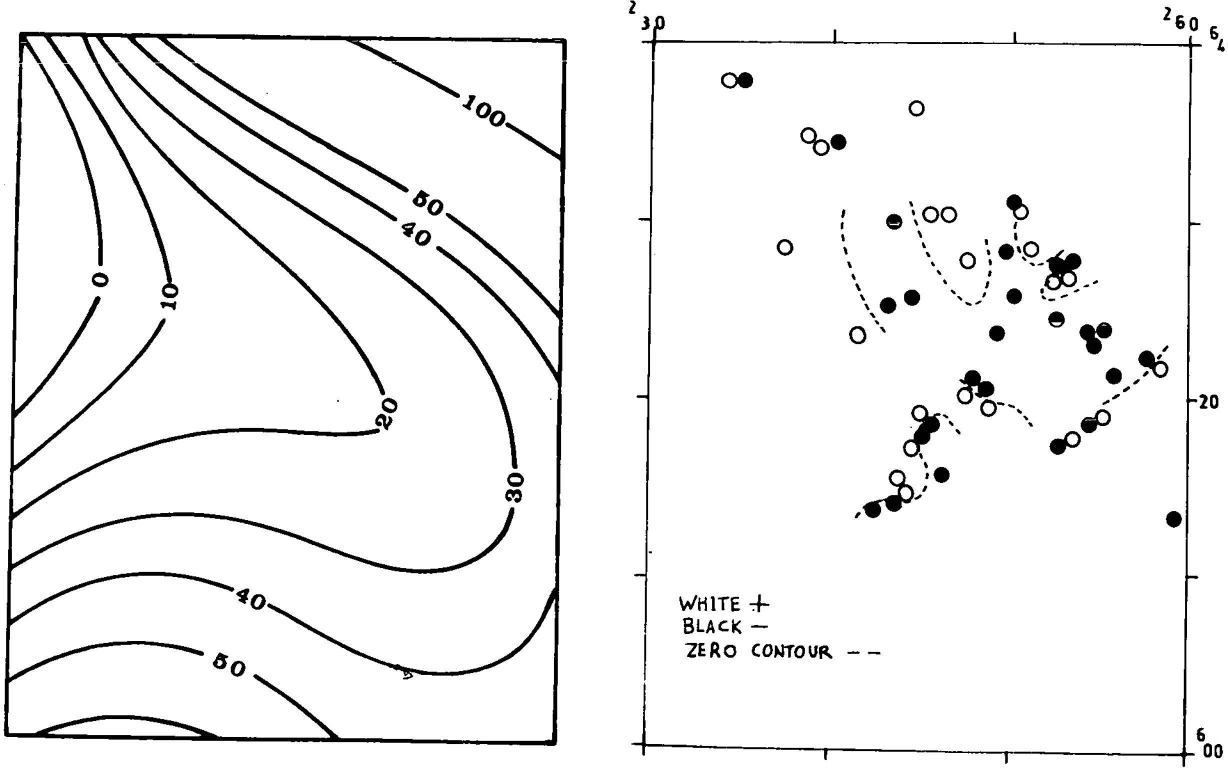


cubic linear residuals

FIG. 14 TREND SURFACES OF ELL-MAIN INTERVAL %SANDSTONE

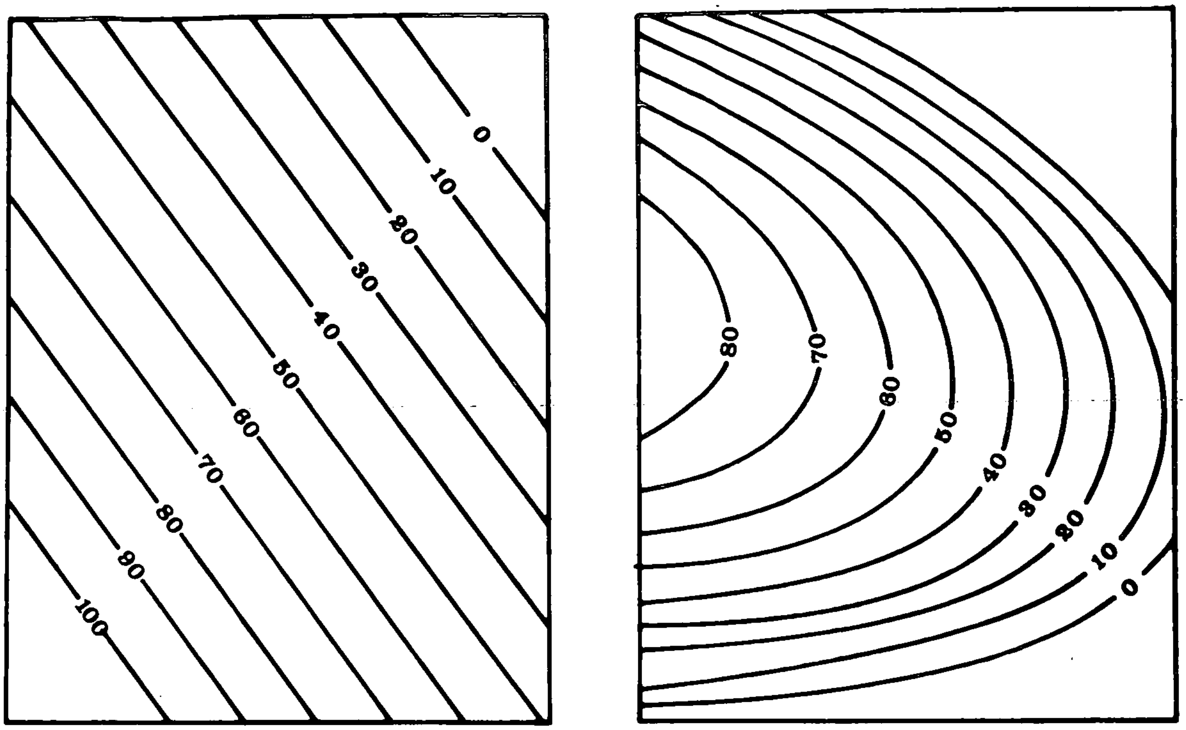


linear quadratic

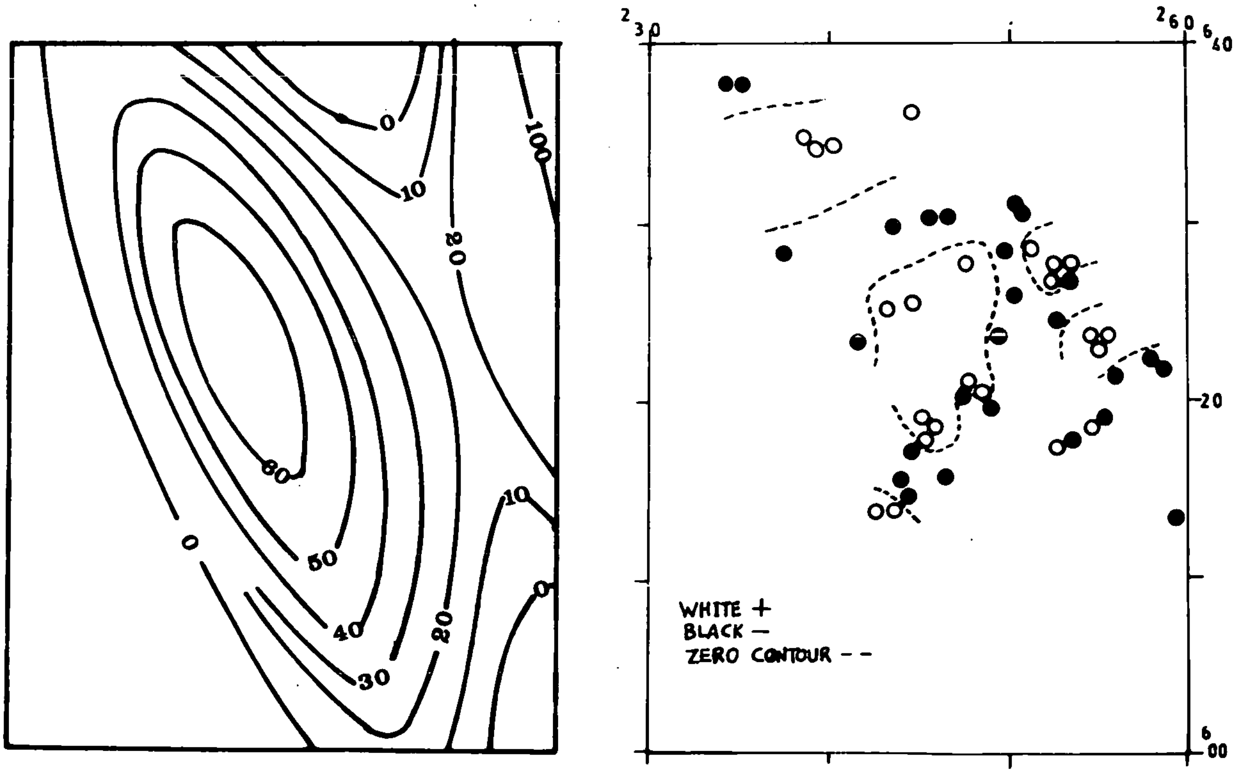


cubic quadratic residuals

FIG.15 TREND SURFACES OF ELL-MAIN INTERVAL %SILTSTONE



linear quadratic



cubic cubic residuals

FIG.16 TREND SURFACES OF ELL-MAIN INTERVAL %SHALE

Table 6

ANALYSIS OF VARIANCE F TESTS OF JEWEL - AYR HARD INTERVAL o/o CLASTICS TREND SURFACE DATA

(SSQ = Sum of Squares ; DF = Number of degrees of freedom ;
MSQ = mean square ; F = F ratio ; SIGNIF.L = o/o Significance level ;
SSQ.prop = Proportion of total sum of squares accounted for by pure term.)

o/o SANDSTONE

SOURCE	SSQ	DF	MSQ	F	SIGNIF.L	SSQ.prop
Linear	754	2	377.0	4.0	>97.5	10.6 o/o
Deviations from linear	6366	67	95.0			
Pure Quadratic	259	3	86.3	0.9	<75	3.6 o/o
Deviations from quadratic	6106	64	95.4			
Pure Cubic	1059	4	264.8	3.2	>97.5	14.9 o/o
Deviations from cubic	5048	60	84.1			
Total	7120					

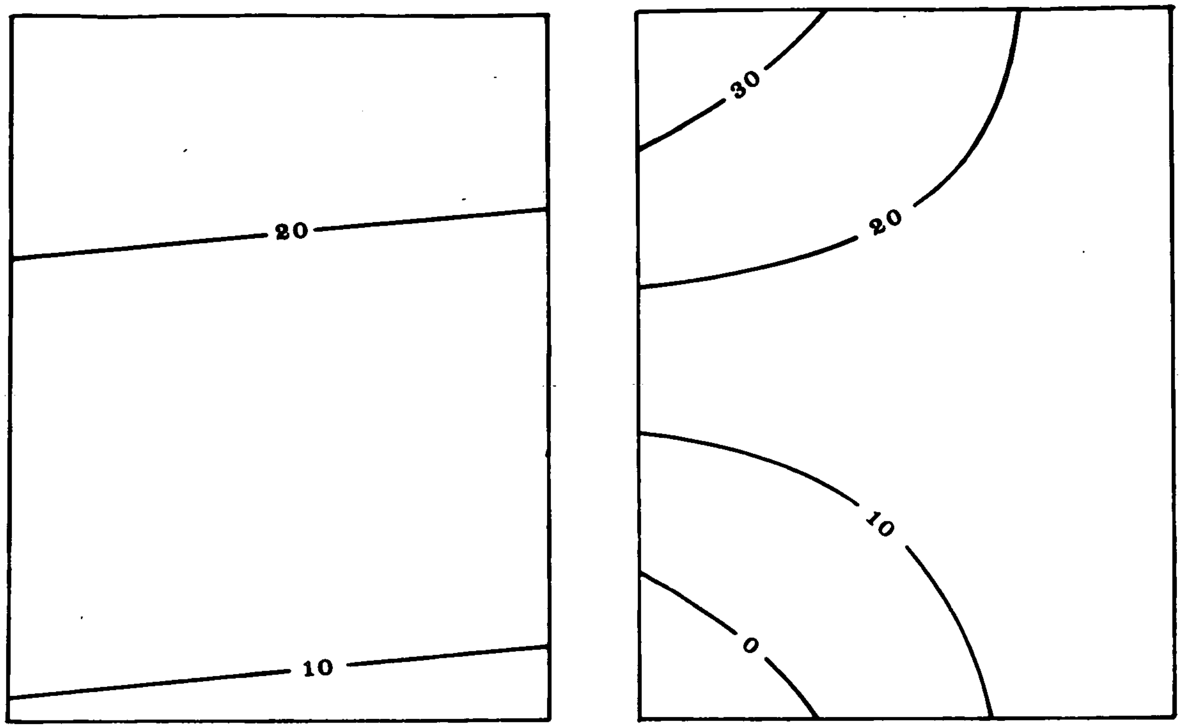
Table 6 (continued)

o/o SILTSTONE

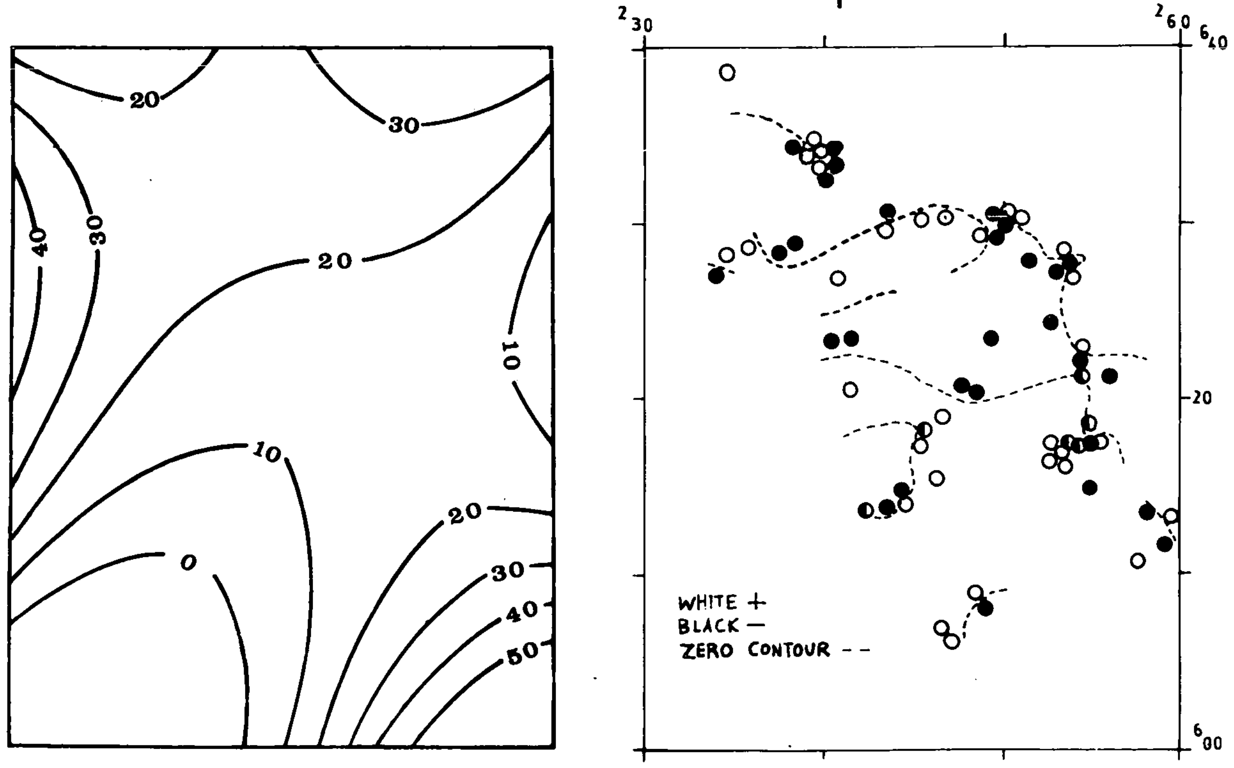
SOURCE	SSQ	DF	MSQ	F	SIGNIF.L	SSQ.prop
Linear	2446	2	1223.0	9.1	>99.9	21.4 o/o
Deviations from linear	8984	67	134.1			
Pure Quadratic	132	3	44.0	0.3	<25	1.2 o/o
Deviations from quadratic	8852	64	138.3			
Pure Cubic	1090	4	272.5	2.1	<95	9.5 o/o
Deviations from cubic	7763	60	129.3			
Total	11430					

o/o SHALE

SOURCE	SSQ	DF	MSQ	F	SIGNIF.L	SSQ.prop
Linear	5898	2	2949.0	15.5	>99.9	31.7 o/o
Deviations from linear	12708	67	189.7			
Pure Quadratic	642	3	214.0	1.1	<75	3.5 o/o
Deviations from quadratic	12066	64	188.5			
Pure Cubic	3871	4	967.8	7.1	>99.9	20.8 o/o
Deviations from cubic	8195	60	136.6			
Total	18606					

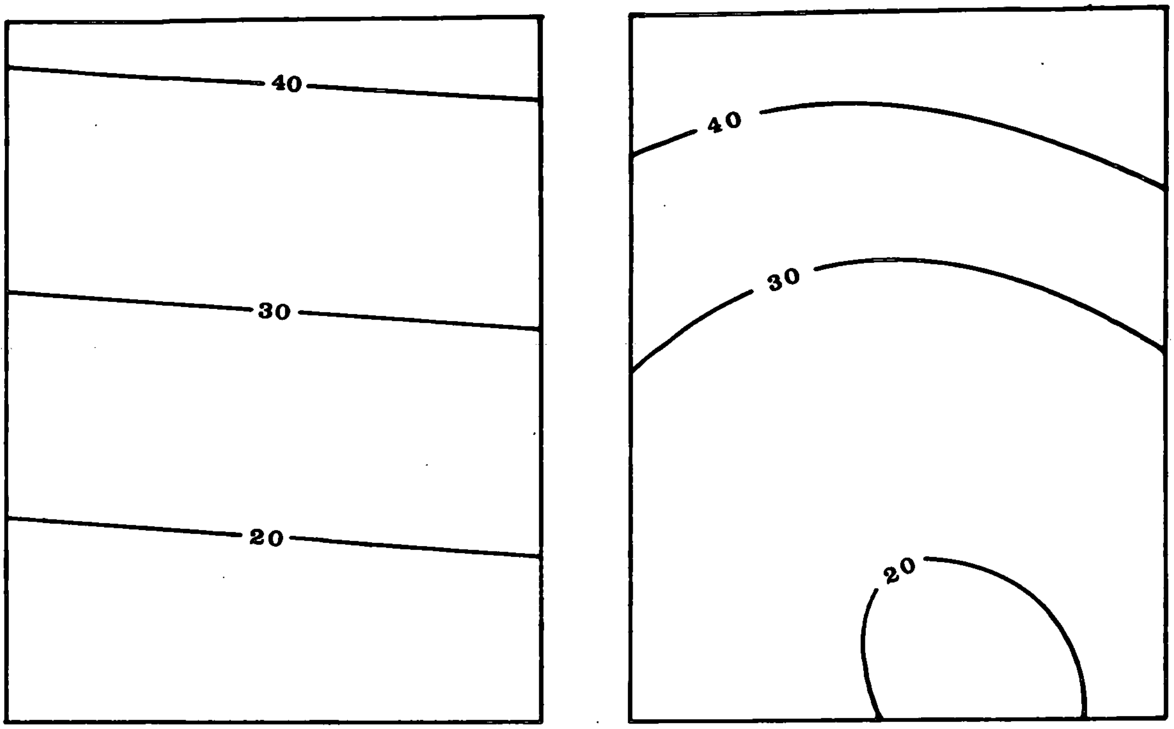


linear quadratic

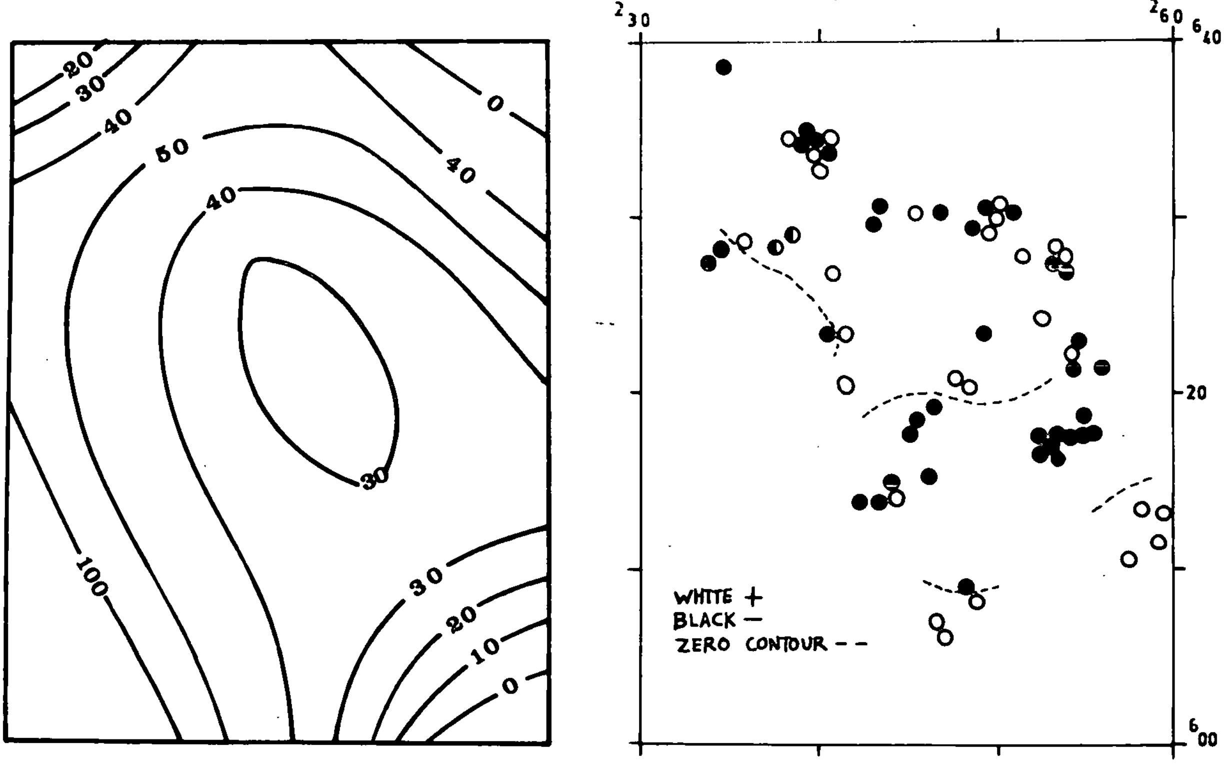


cubic cubic residuals

FIG.17 TREND SURFACES OF JEWEL-A.H. INTERVAL % SANDSTONE

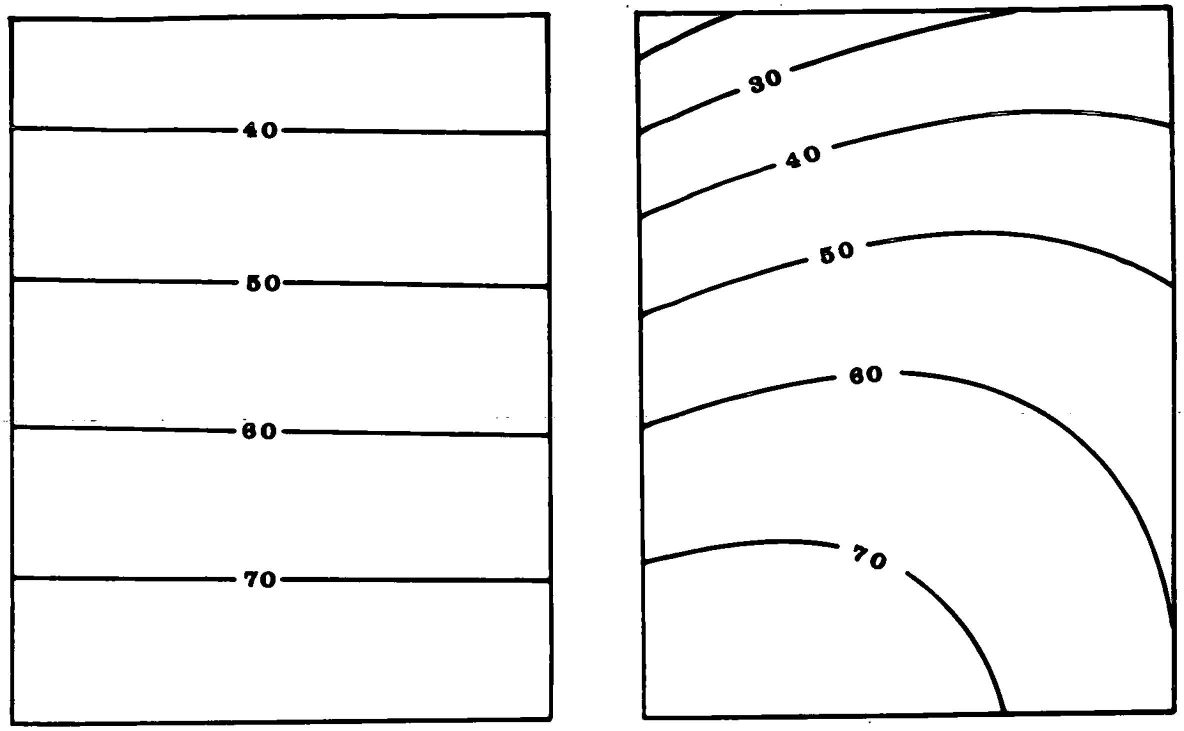


linear quadratic

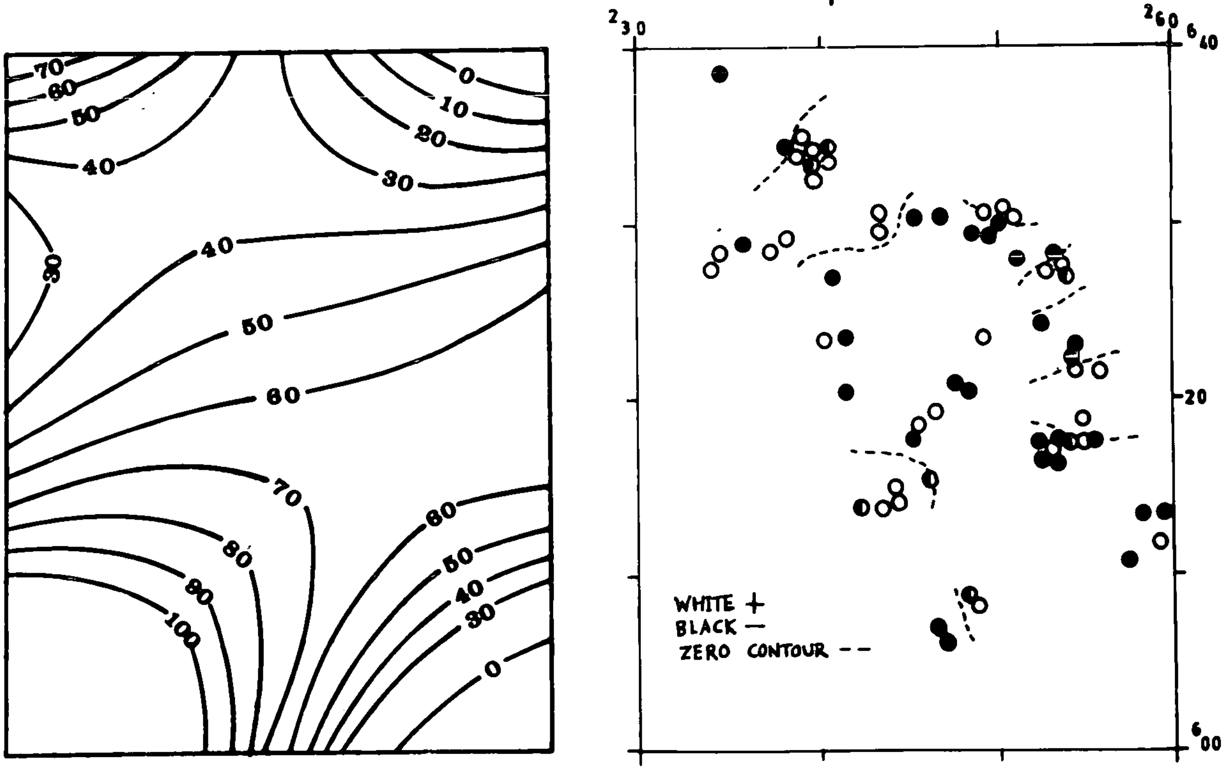


cubic linear residuals

FIG. 18 TREND SURFACES OF JEWEL-A.H. INTERVAL %SILTSTONE

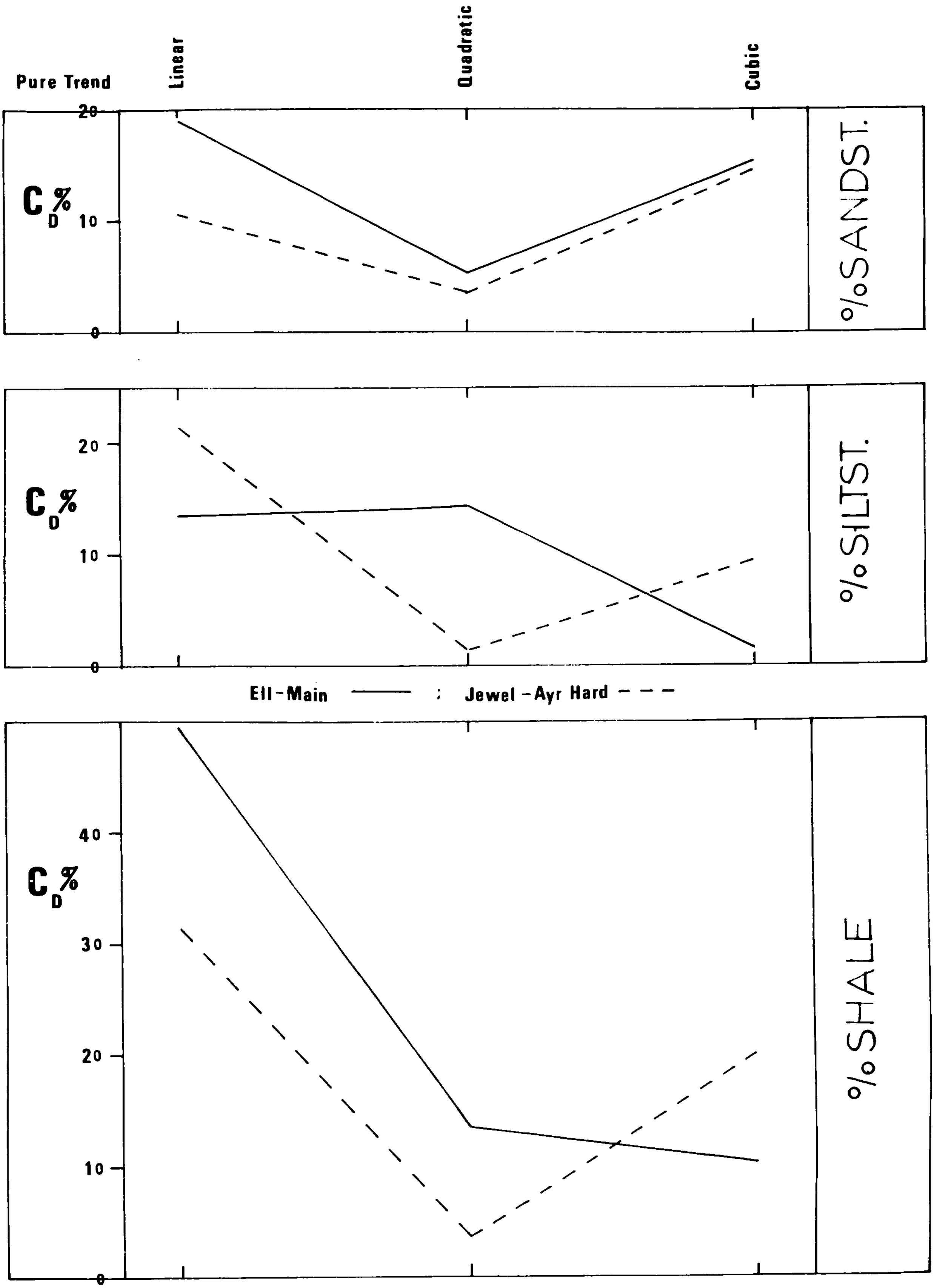


linear quadratic



cubic cubic residuals

FIG. 19 TREND SURFACES OF JEWEL-A.H. INTERVAL % SHALE


Pure Trend
Linear
Quadratic
Cubic
$C_D\%$
0
10
20
%SANDST.
$C_D\%$
0
10
20
%SILTST.
Ell-Main
Jewel-Ayr Hard
$C_D\%$
0
10
20
30
40
%SHALE

5. Thickness of Coals

Data was compiled of the thickness of the coals that bound the units studied, with the exception of the Ayr Hard Coal which shows pronounced major splitting into the Maid coals in the central area, and the Parrot, Turf and Wee coals in the north, making difficult its rationalisation as a discrete coal. Trend surfaces, therefore, were computed of the areal thickness variation of the Ell, Main and Jewel coals and these are shown in Figs.21, 22 and 23.

Analysis of variance F tests (Table 7) show that pure linear, quadratic and cubic terms are all represented as significant components of the regional variation, though the coefficients of determination are generally fairly low and there is no constant pattern that has generalised meaning for all three coals. The general character of this series is reminiscent of the statistics and surfaces of artificial Model C (p.25), where there is a mixture of weak simple regional components and more complex factors, and it is suggested that the areal development of coal is governed by a model of this sort.

Contoured residuals from the cubic surfaces of these coals show patterns of rather amorphous, sometimes belt-like, areal distribution, analogous in form to residuals of the clastic lithology proportions, though there is no obvious spatial relationship between the two. Similarly, there appears to be no clear-cut correspondence between the coal thickness positive residuals and the local structural basins. It is inferred that the variation of the thickness of these coals throughout the area is primarily a localised phenomenon, probably controlled by factors of sedimentary facies, subsidence and palaeoecology at this scale.

Table 7

ANALYSIS OF VARIANCE *F* TESTS OF COAL THICKNESS
TREND SURFACE DATA

(SSQ = Sum of Squares ; DF = Number of degrees of freedom ;
MSQ = mean square ; *F* = *F* ratio ; SIGNIF.L = o/o Significance level ;
SSQ.prop = Proportion of total sum of squares accounted for by pure term.)

ELL COAL

SOURCE	SSQ	DF	MSQ	*F*	SIGNIF.L	SSQ.prop
Linear	2856	2	1428.0	15.6	>99.9	28.1 o/o
Deviations from linear	7314	80	91.4			
Pure Quadratic	572	3	190.7	2.2	<95	5.6 o/o
Deviations from quadratic	6742	77	87.6			
Pure Cubic	1233	4	308.3	4.1	>99	12.1 o/o
Deviations from cubic	5510	73	75.5			
Total	10170					

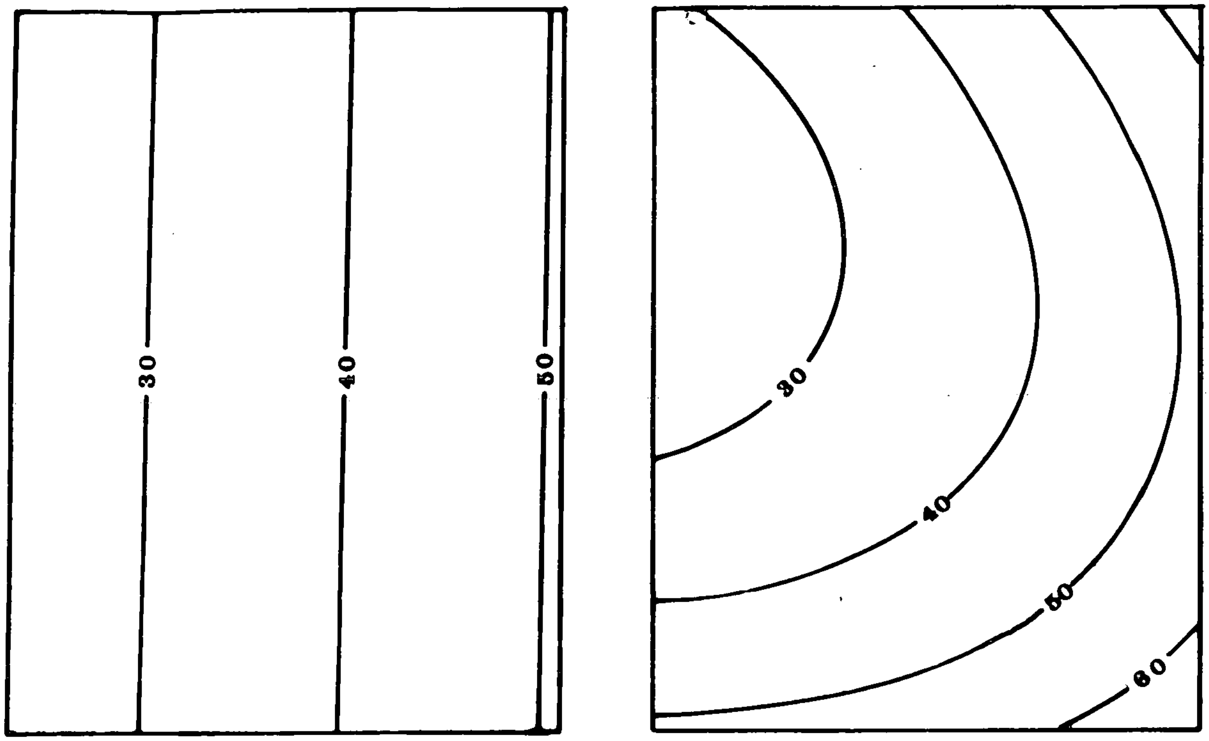
Table 7 (continued)

MAIN COAL

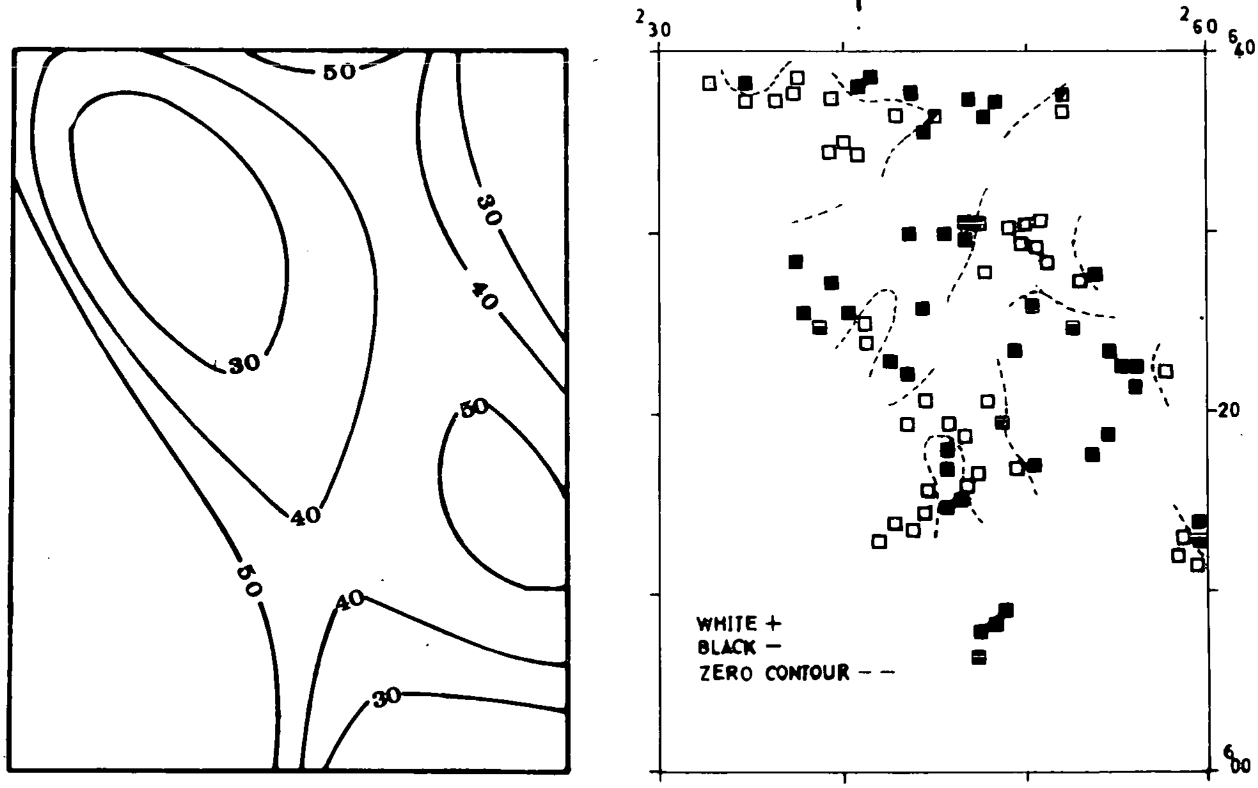
SOURCE	SSQ	DF	MSQ	F	SIGNIF.L	SSQ.prop
Linear	4986	2	2493.0	9.7	>99.9	20.2 o/o
Deviations from linear	19746	77	256.4			
Pure Quadratic	3518	3	1172.7	5.3	>99.5	14.2 o/o
Deviations from quadratic	16228	74	219.3			
Pure Cubic	5358	4	1339.5	8.6	>99.9	21.7 o/o
Deviations from cubic	10870	70	155.3			
Total	24732					

JEWEL COAL

SOURCE	SSQ	DF	MSQ	F	SIGNIF.L	SSQ.prop
Linear	51	2	25.5	0.1	<25	0.3 o/o
Deviations from linear	16577	78	212.5			
Pure Quadratic	9810	3	3270.0	36.2	>99.9	59.0 o/o
Deviations from quadratic	6767	75	90.2			
Pure Cubic	2598	4	649.5	11.1	>99.9	15.6 o/o
Deviations from cubic	4169	71	58.7			
Total	16628					

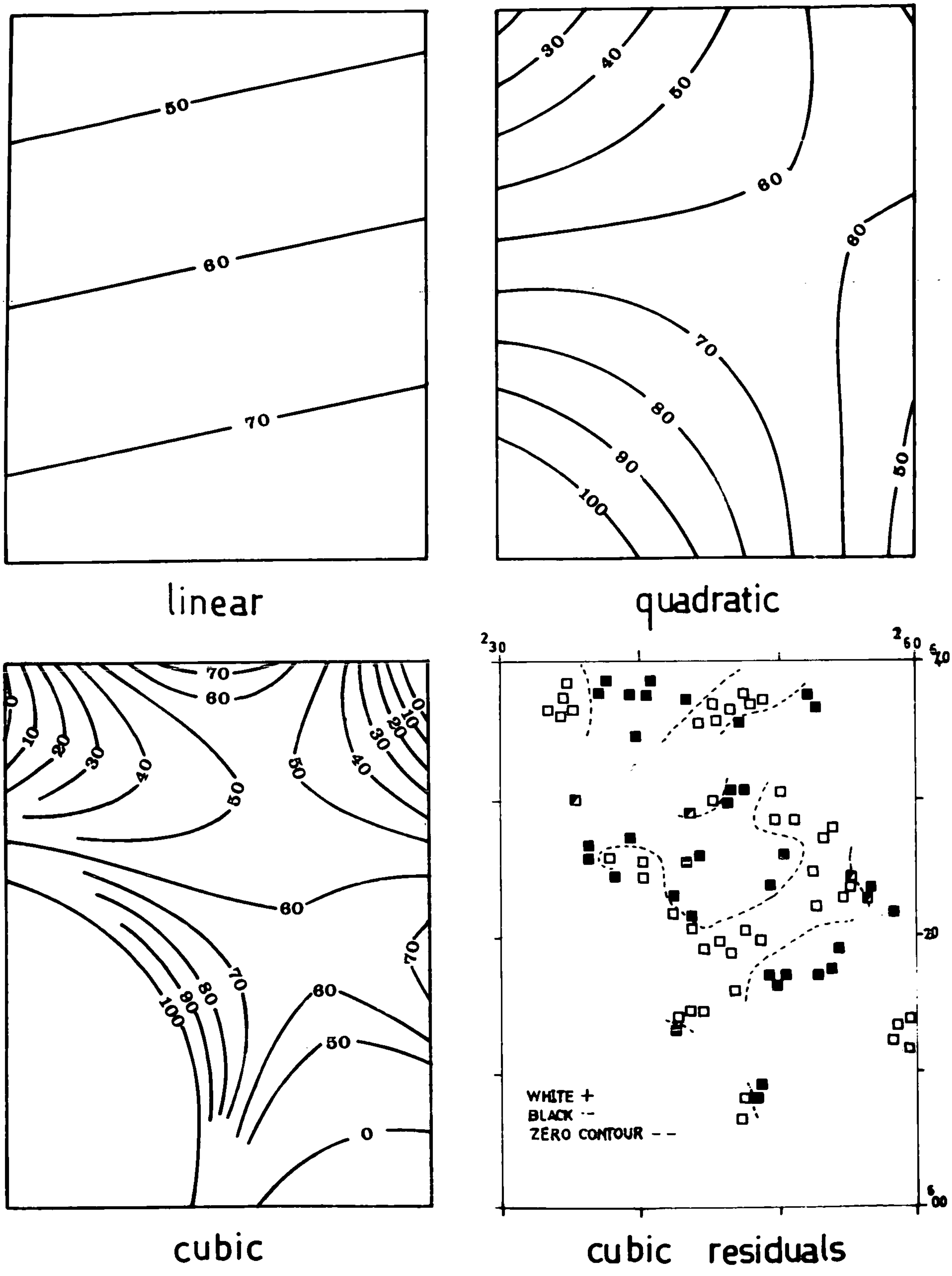


linear quadratic



cubic cubic residuals

FIG. 21 TREND SURFACES OF ELL COAL THICKNESS (INCHES)



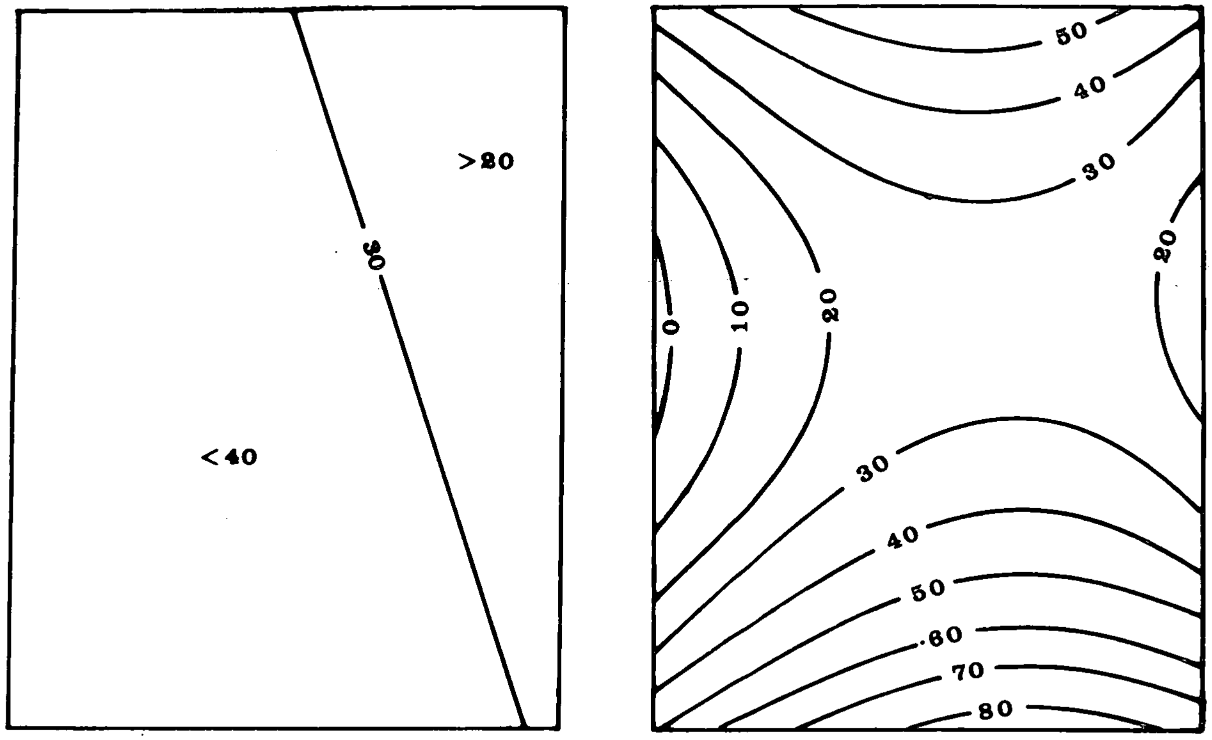
linear

quadratic

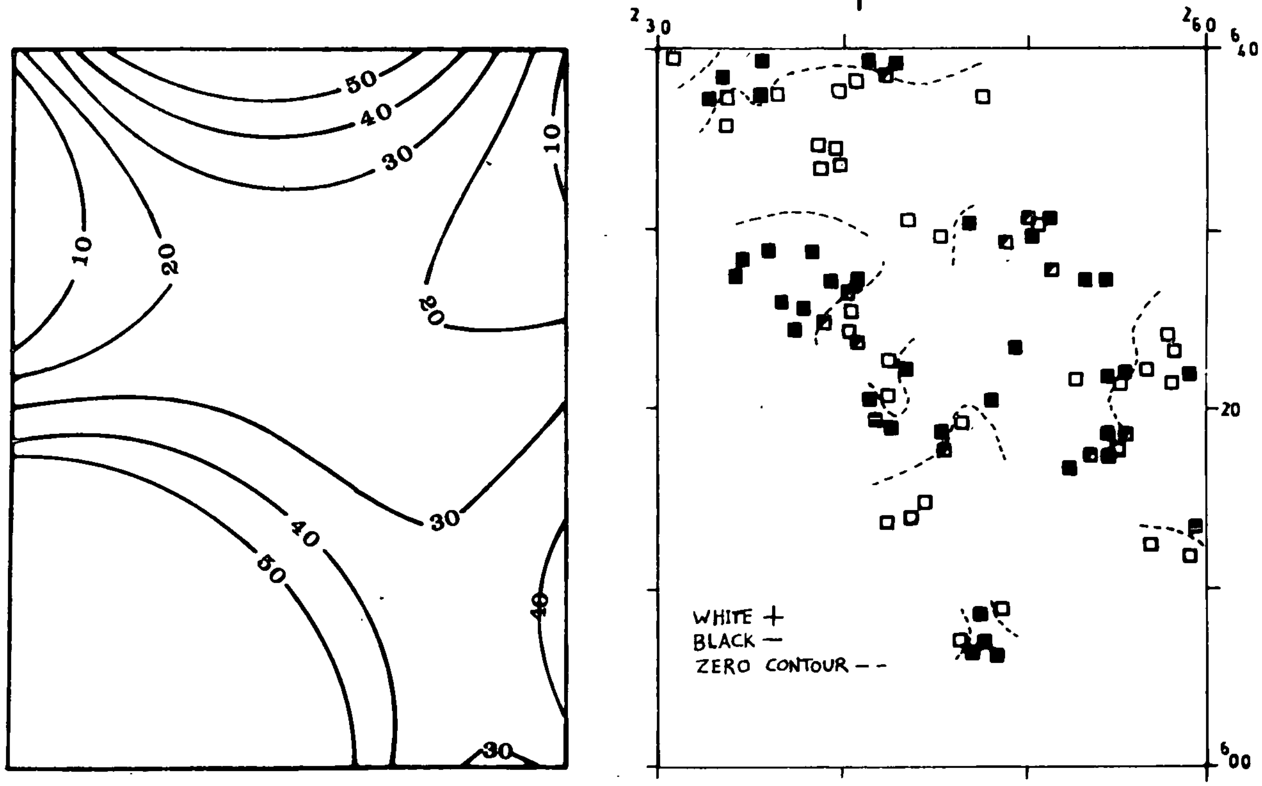
cubic

cubic residuals

FIG. 22 TREND SURFACES OF MAIN COAL THICKNESS (INCHES)



linear quadratic



cubic cubic residuals

FIG. 23 TREND SURFACES OF JEWEL COAL THICKNESS (INCHES)

Conclusions

1. The regional structure is described by a large symmetrical syncline trending NNW-SSE with systematic basins of local character set in its flanks and centre.
2. In upper modiolaris times, the sediments of the Jewel-Ayr Hard interval appear to have been attentuated over the Millstone Grit lava pile in the Monkton area to the west, a factor of regional significance persisting from the Lower Coal Measures when these lavas were progressively overlapped. This feature faded in effect with time so that the regional development of the younger (similis-pulchra) Ell-Main is represented significantly by a linear wedge, increasing in thickness towards the south-south-west. The thickness of the Coal Measure sequence as a whole, as well as the number and areal extent of the marine bands, also increases in much the same direction (see p. 8), indicating that this is both a regional and long-term character and reflects a pattern of regional subsidence that can be represented as a plane tilting toward the south-west.
3. On the regional scale, there is no relationship between the broad structure that underlies the coalfield and the thickness of the Ell-Main unit and it seems likely that the age of the major folding is mainly of post-Carboniferous age. However, on a scale local to the area, there is a good correlation between thickness variation and structural development, implying active local subsidence of small basins, which modifies the linear regional pattern of subsidence. In the case of the older Jewel-Ayr Hard unit, regional variation is complicated by the apparent overlap attenuation in the west. However, the similarities of

the residual configuration with that of the Ell-Main unit suggest that local basins of subsidence were more or less continuously active, though somewhat fluid in their areal pattern.

4. On the large scale, the derivation of the coarse material (sandstone and siltstone) in the units studied was from the north and north-east. The statistics of the surfaces suggest the development of variable lobes or sheets of sands with associated silts across a platform of muddy facies as a suitable environmental model. At a smaller scale, the form of the residuals shows complex patterns of facies belts with no obvious relation to the supposed contemporaneously subsiding small basins.
5. The regional variations of the thickness of the coals bounding these units show no simple motif and contain significant components of both a regional and local scale. The residuals appear to have no explicit association with lithofacies or subsidence areas, but it is suspected that they are the product of a complex interplay of these and other factors at a local level.

Chapter 4

SEDIMENTATION TIME-TREND FUNCTIONS

Introduction

In trend surface analysis, Coal Measures attribute variation was studied in an essentially two-dimensional (geographic) framework, with a supression (but not elimination) of the time dimension. This variation can also be studied in terms of continuous vertical change (i.e. as a function of time), while the two-dimensional locus is kept constant.

Such vertical profiles can be examined on several scales. On the small scale, for instance, bed transition character and cyclic properties can be considered. (Small-scale work forms the basis for Markovian process work described in the next section). This chapter is concerned with the larger scale aspect, where long-term changes in the attributes are separated from the fluctuations of small scale character.

The application of mathematical techniques to the study of long-term variation of geological successions is comparatively recent, interpretation of such characters being formerly entirely based on an intuitive assessment of a bulk of raw data. The purpose of mathematical treatment is to gain information not readily appreciated by the human eye in the original observational material, and this information is usually expressed as 'trends' or 'periods' of various time magnitudes. The methods have been borrowed from among such diverse fields as business market analysis and radio communications theory, selected according to the study aims of the worker. These aims fall into two main categories of investigation. The first is as a tool for stratigraphic correlation (e.g. Vistelius, 1961) and the second as a means of analysing rock successions for periodicity of geological significance (e.g. Schwarzacher, 1967; Carss, 1967). In the latter approach, stationarity within the succession is assumed and this stipulation is broadly upheld if the mean and autocorrelation function are time-invariant (Schwarzacher, 1967, p.6) This property is violated by the presence of a definite long-term trend and, as the study of such trends is the purpose of this section, techniques that do not depend on the condition of stationarity are used here.

Vistelius (1961) has considered the problem of separating a 'systematic trend component' from a 'random (local) component' in work on sedimentary sequences and for this applies Spencer's formula to numerically rendered observations of the sequence studied. (The method is also included in Davis and Sampson's time-trend package for computer [Davis and Sampson, 1967]). The computed result is a smoothed profile produced by a moving average, in which the smoothed value at the ith observation point is calculated by ascribing the heaviest weighting to the ith observation and giving decreasing weight to the increasingly peripheral observations relative to i (ten observations on either side). Spencer's formula is:

$$\begin{aligned} U/_o = 1/350\,(&60U_0 + 57U_{-1} + 57U_{+1} + 47U_{-2} + 47U_{+2} \\ &+ 33U_{-3} + 33U_{+3} + 18U_{-4} + 18U_{+4} \\ &+ 6U_{-5} + 6U_{+5} - 2U_{-6} - 2U_{+6} \\ &- 5U_{-7} - 5U_{+7} - 5U_{-8} - 5U_{+8} \\ &- 3U_{-9} - 3U_{+9} - U_{-10} - U_{+10}) \end{aligned}$$

where $U/_o$ = smoothed value at ith point (i = o),

U_x = raw value at (i + x)th point.

The long-term component is then $(U/_0)$ and the short-term is $(U/_0 - U_0)$. The scale of these two components is then dictated by:

(i) the size of the distance between successive observations;

(ii) the numerical scale selected for the observational data;

and (iii) the scale of the method, in this case twenty-one observations (as opposed to Sheppard's five term smoothing equation).

The spacing of observations depends on the scale of the long-term trend required. As 'long-term' has no discrete meaning, the scale is stipulated by the needs of the worker. In this study, two trends were extracted. One, which can bo considered as a 'medium-term' trend was based on an observation interval of one foot, and the second, a 'long-term' trend based on ten feet.

The method can be applied to the variation of any attribute, provided numerical values can be ascribed to observations of the attribute at the data points. The smoothing formula is used here to interpret long-term sedimentation patterns from logged borehole sections. The basic data for this approach was assembled by listing the clastic characters of the lithologies found in the object successions. (More subtle sedimentological criteria are not practicable, by virtue of the fact that, beyond stating the nature of the lithologies, further potentially useful log information is negligible). The rock-types must be translated as a numerical system for the trend calculation procedure to be applied, and this system must be designed on geologically meaningful grounds. The scale selected is shown in Table 8 and the arguments used in its construction set out in Appendix D.

ROCK TYPE		CODED VALUE
Conglomerate		39
Sandstone	Coarse grain size	26
	Medium - coarse	24
	Medium	23
	Fine - medium	21
	Fine	20
Silty sandstone		17
Sandy siltstone		13
Siltstone		9
Muddy siltstone		7
Silty mudstone		5
Mudstone		2
Coal		0

(Definitive lithologies - intermediate rock types coded by interpolation between these values.)

Table 8 CLASTIC CODING SCALE USED IN SMOOTHING OPERATIONS

In the following procedure, Spencer's formula was used to calculate smoothed values that represent a 'first order' profile. These values were themselves treated as raw data and the smoothing formula again applied to obtain a second order profile. A repetition of this method produces a third order profile. The advantage of this reiterative approach can be seen by reference to the artificial example of Fig.24. While the first-order trend line retains small kinks due to the continued effect of incompletely smoothed localised components, higher orders show smoother profiles and tend to attain a degree of stability, in that the difference between successive higher orders is less than between low orders. This 'stability' is effectively reached at third order.

One unfortunate feature of Spencer's formula is that, in its application, ten values are lost at either end of the smoothed sequence. In applying this for third order, sixty observations are lost. This is compensated in computation to some degree by inserting ten artificial auxiliary observations at both ends of the sequence. The values in each set of auxiliary observations were set as the arithmetic average of the ten neighbouring real observations and these values recalculated for each order of smoothing. This is a compromise solution to this problem, but is not unrealistic and the result is a slight distortion at the ends, while the main body of the sequence remains unaffected.

The programme SMOOTHBORE was written to perform these smoothing calculations on suitably coded borehole data, of which details are given in Appendix 3. The computed third-order smoothed values of the medium and long-term trends were fed off-line to the Calcomp 564 digital graph plotter, which drew continuous profiles of the smoothed

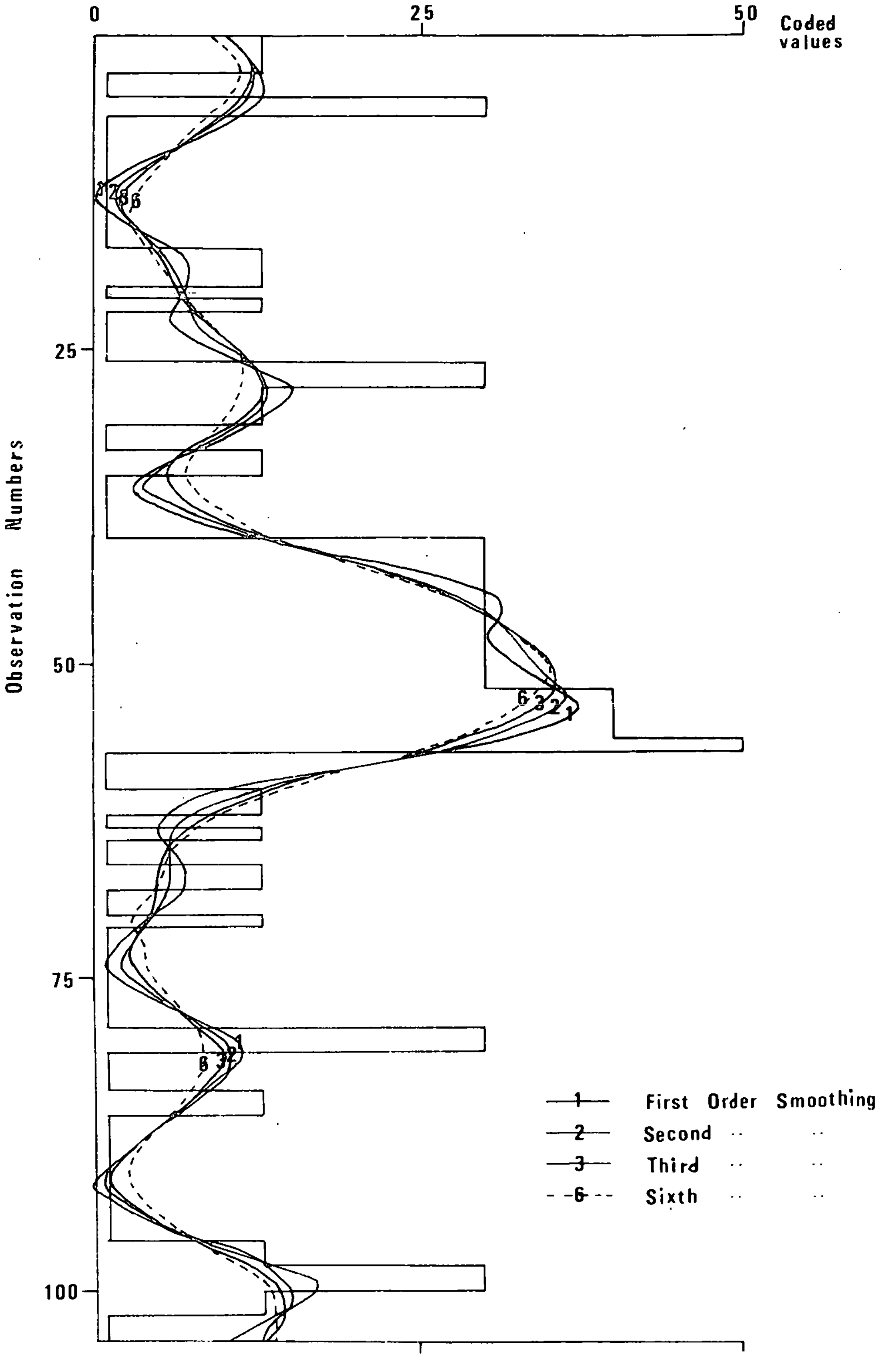


FIG. 24 SPENCER'S FORMULA SMOOTHINGS OF ARTIFICIAL DATA

data.

Tests of the results of this programme must necessarily be empirical and designed to assess whether the computed trend geometry is geologically meaningful or a product of the mechanics of computation and/or the assumptions of the method. Accordingly, two neighbouring boreholes of similar stratigraphic range were smoothed and compared. They are Dalmellington No.231 and West Tarelgin No.1 (Sheet NS 41 NE) separated by a distance of 0.61 miles. Now, while differences of a small scale can be expected due to impersistent rock units and operator error in recording, the long-term geometry should be essentially the same. Reference to Fig.25 shows that this is so, and therefore that the method is an objective analysis of trends of potential geological significance.

Viewed in medium-term character (at the one foot level), the profiles show the wildly fluctuating trace that is to be expected from an alternation of relatively thin beds with a large numerical range in coding. However, on a larger scale, definite long-term trends can be seen in the broad change of the oscillation ranges of these local components and this is quantified in the long-term (ten foot level) smoothing profile. This ten foot sampling interval trace shows major trends, but also retains features of local significance. The distinction between the two types is obviously one of scale and 'sand highs' and 'shale lows' that can be considered of long-term significance are those whose length is of the order of many cycles (here taken as a seatearth to seatearth unit). Local components can be broadly considered as restricted to one cycle so that, for instance a thick sandstone within one cycle can produce a localised high trend configuration which is essentially a function of a short-term facies

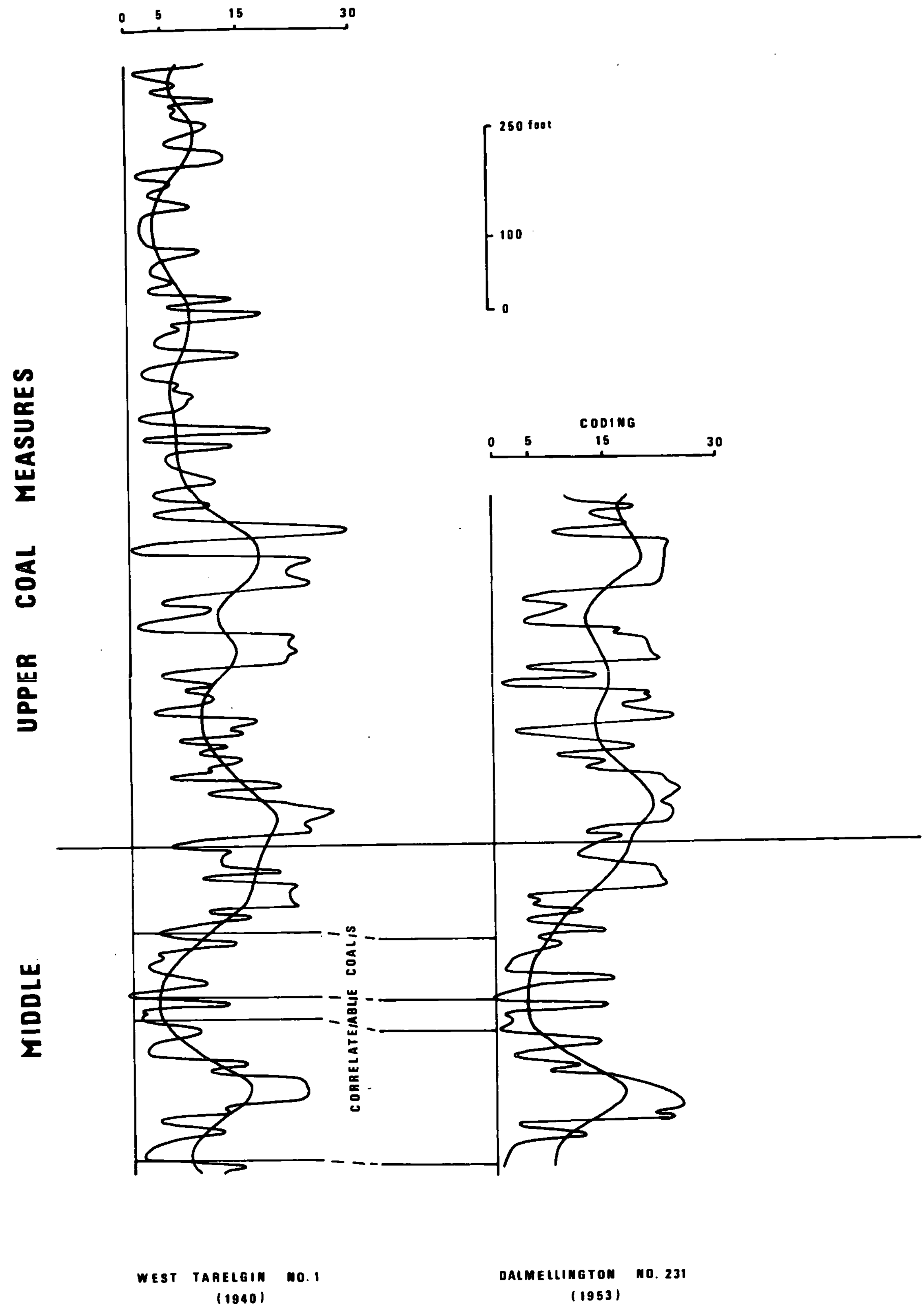


Fig. 25 Smoothed profiles of neighbouring bores

development. The two types are illustrated by comparison of the bores of Fig.25 with those of Fig.27. The broad long-term sand high of the lower part of the Upper Coal Measures is shown on all bores, but the prominent peak produced by the thick sandstone body above the Jewel coal shown on the West Tarelgin No.1 and Dalmellington No.231 bores does not appear on the others and represents a sand facies of localised lateral and vertical extent.

Interpretation of Long-term Changes

The scale of long-term profile fluctuations indicates a correspondingly large-scale causative mechanism external to the depositional environment. The possible nature of this control is discussed under the following headings

(i) Changes in sea level

Examination of the computed profiles that follow (Figs.27, 28 and 29) for relationship of marine bands with major fluctuation geometry suggests that the two are independent. Marine bands appear to be associated with localised facies changes minor to the long-term trend. The widespread extent of many of their correlatable equivalents to the south, some reaching across the whole of Europe, indicates that they are caused by eustatic rises in sea level. It is interesting to note that the occurrences of marine and Lingula bands tend to cluster in the basal part of the Lower Coal Measures and at the Middle/Upper Coal Measure boundary in both Ayrshire and other British coalfields. Coupled with this is the generalised observation that the grade of sedimentary material tends to be coarser at these two levels (a point developed more fully later). It has been suggested by Armstrong (1969) that eustatic rises in sea level are related to sympathetic uplift in both oceanic rises (causing displacement of sea water) and orogenic activity within continents (leading to renewed erosion and coarser detrital sedimentary facies). If this theory has any validity, then the emplacement of marine bands by rises in sea level, as well as the change in grade of clastic material, may both be effects of tectonic activity.

(ii) Tectonic movements

The role of contemporary fold and fault movement as Coal Measure depositional controls has already been referred to (p. 4) though their timing has not been discussed. It seems probable, however, that many such movements both within the basins and the hinterland source areas must have had some degree of synchronisation with early Hercynian movements in the south. For some years now, a history of significant syntectonic movements has been recognised in the development of the coalfields of the Subvariscan and Pennine provinces (e.g. Moore and Trueman, 1939; Trueman, 1947; Moore and Blundell, 1951; Wills, 1956). It has been suggested that the sequence of events is as follows. Tectonic activity (equivalent to the Erzgebirgian of Europe) caused minor local unconformities and thin stratal developments in the Lower Coal Measures, but this gave way to the comparatively undisturbed period of the Middle Coal Measures. However, 'Malvernian' phase movements occurred in the late Middle and early Upper Coal Measure times, with marked unconformities and depositional breaks in all the southern coalfields, though the precise timing varied from basin to basin, so that the movements in South Wales and the English Midlands were of phillipsii age (Wills, 1956), while in the Bristol Coalfield, movements started earlier, in late similis-pulchra times, though persisting into phillipsii times

(Moore and Blundell, 1951). Such tectonic activity is likely to have resulted in uplift and increased erosion of the Midland Barrier itself (Wills, 1956, p.72), leading to a greater contribution of coarse clastics to the flanking basins, though Trueman (1947, p.lxviii) suggests that current directions and thickness variation indicates that much of the coarse material of this age in South Wales was derived from the south, perhaps from the erosion of a rising Variscan fold belt. At all events, movements of this time can generally be related to an increase in coarse clastic sedimentation as a result of erosion of rising areas. At the end of phillipsii times, the movements appear to have gradually faded away and a relative stability attained in tenuis, accompanied in some areas by a return to coal formation.

(iii) Climatic changes

It seems probable that the approximately sub-tropical conditions that are likely to have prevailed during the deposition of the earlier part of the British Coal Measures gave way to a climate of greater aridity in Upper Coal Measure times. This is shown by features in Ayrshire which have analogies with many coalfields in the south. These include mudstone desiccation cracks filled with sand, limy concretions in fine-grained rock, 'pseudo-breccias' and, in the higher parts, the introduction of millet-seed sand grains. It is now widely accepted that most of the reddening of these strata, formerly taken as additional evidence, is essentially diagenetic and of probable early Permian age. However, Mykura (1967, p.79) suggested that at least some of this reddening may be of later Upper Coal Measure age.

The effect of these two latter hypothetical controls, acting either singly or in unison, could account for any long-term trends recorded in the sedimentary history, in that movements would be reflected broadly in the grade of contemporary sedimentary material, while an increasingly arid climate would be expected to profoundly modify the hydrology of the area.

A number of recent boreholes of suitable length for various parts of the Ayrshire Coalfield were coded in the manner described and their smoothed profiles computed. According to their location, these bores were grouped into three classes as descriptors of areas within the region, to obtain not only ideas of the variation through time of major trends but of their likely areal extent. These classes are as follows:

1. Central Area (Mauchline Basin and Littlemill Trough) Fig.27
   Bores: Outmains - Kingencleugh - Slatehole - West Tarelgin No.1 - Ashentree No.1
2. Eastern Area (Auchinleck to Dalleagles) Fig.28
   Bores: Kenstey - Mortonmuir No.16 - Rigg No.1 - Main Coal Group No.10 - Upper Red Group No.3
3. Southern Area (Dalmellington) Fig.29
   Bores: Dalmellington No.237 - Chalmeston No.4/5 Ugd - Auchincross No.14

(The location of the bore sites of these groups is shown in Fig.26).

(1) Central Area

The profiles of this group of bores show the following general characteristics, described in order of time:

(i) A repeated development of relatively thin sandstones in the Lower Coal Measures, declining in a gradual

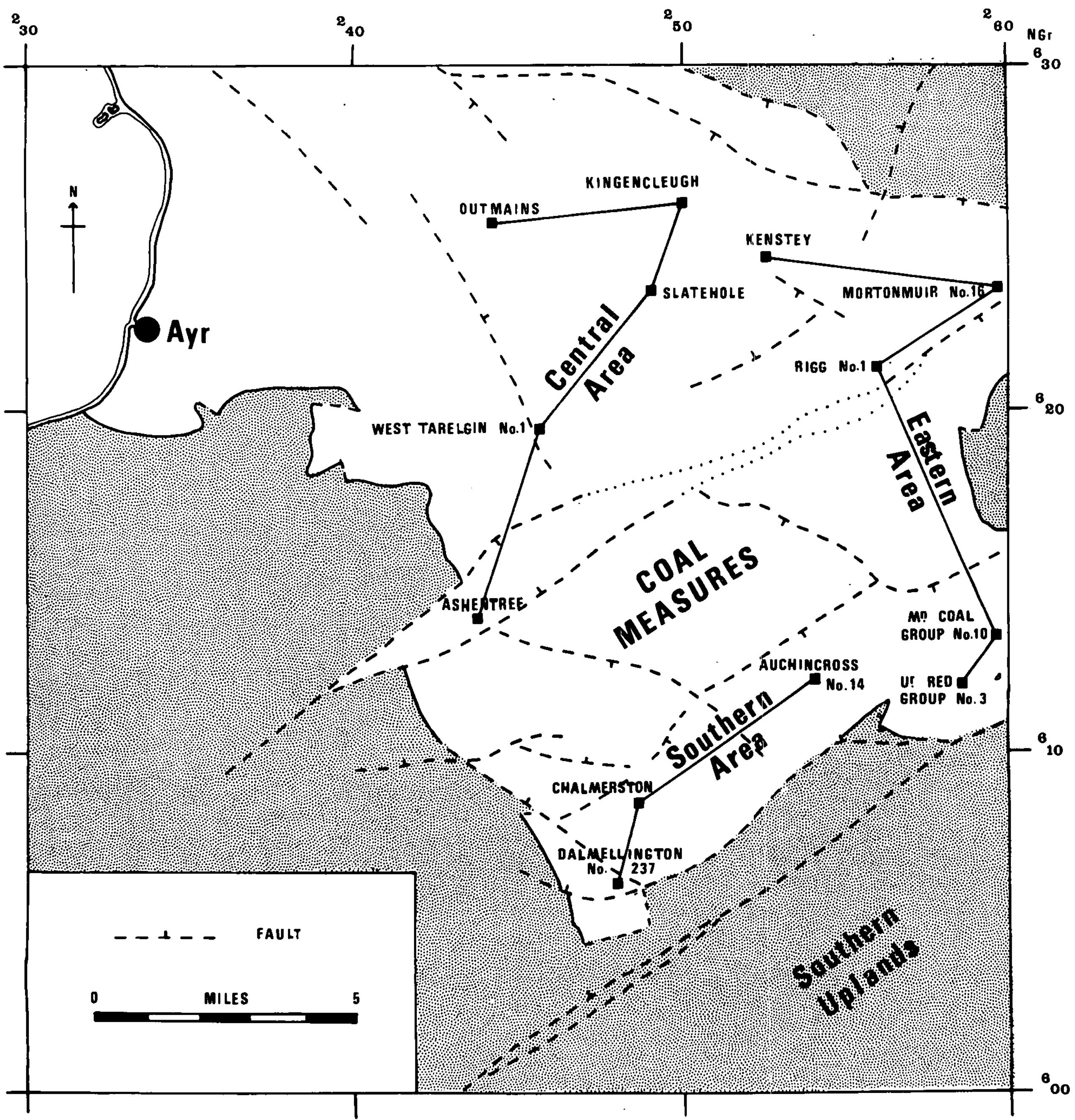


Fig. 26

Location of Smoothed Bore Sections

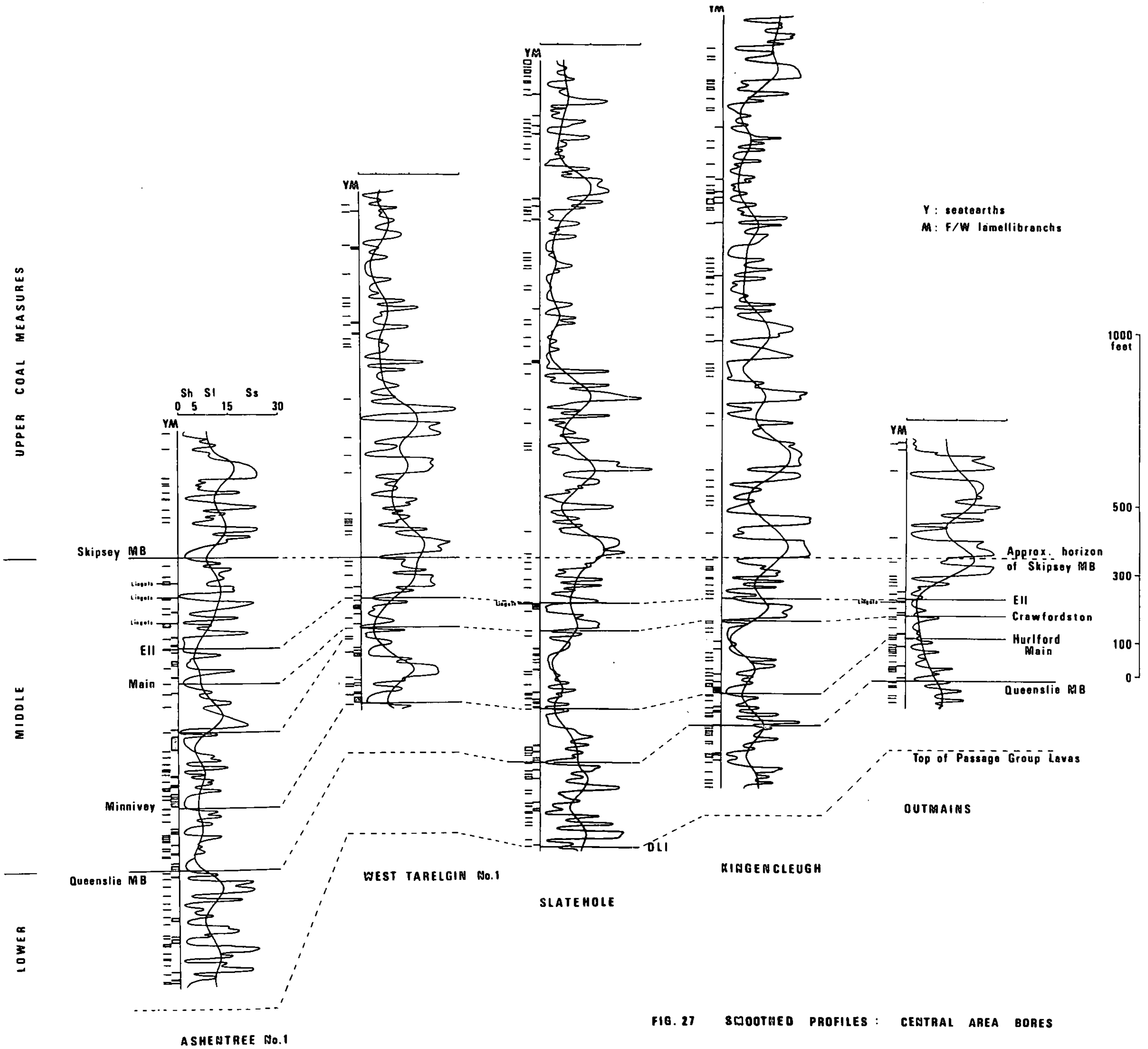


FIG. 27 SMOOTHED PROFILES : CENTRAL AREA BORES

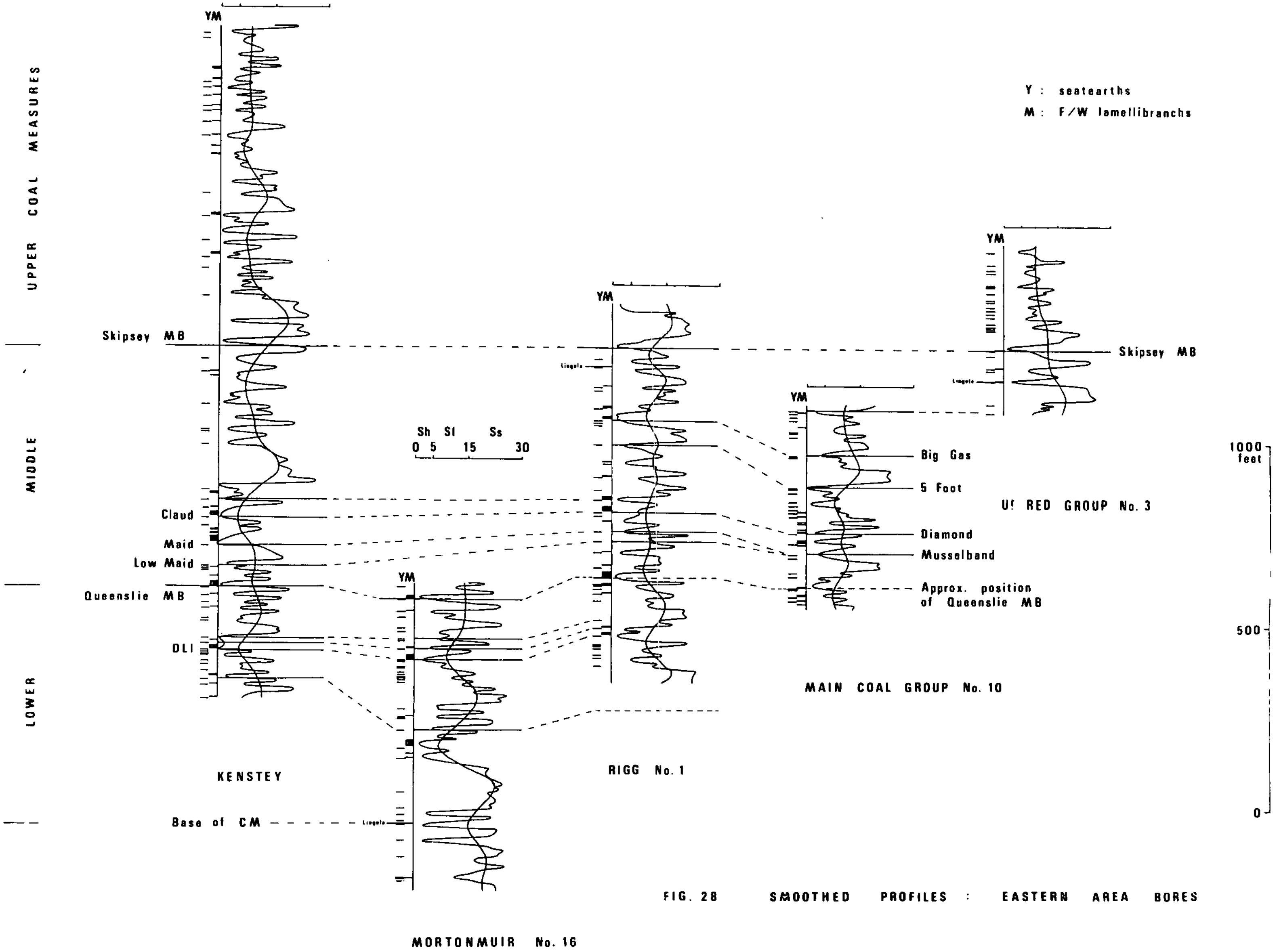


FIG. 28 SMOOTHED PROFILES : EASTERN AREA BORES

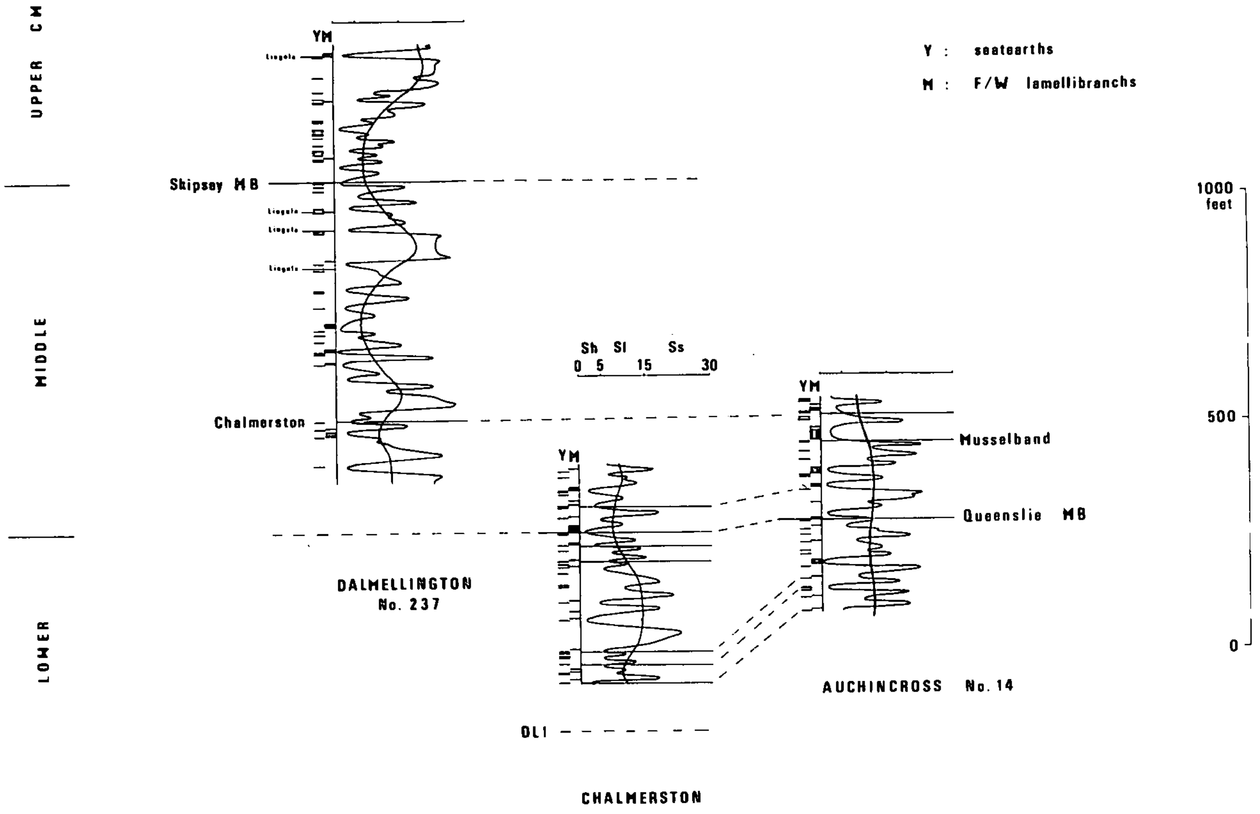


FIG. 29 SMOOTHED PROFILES : SOUTHERN AREA BORES

manner and ceasing as a major trend at approximately the Queenslie Marine Band horizon (slightly later in the more easterly bores).

(ii) A Middle Coal Measure sequence dominated by thick shales and siltstones with occasional laterally impersistent thick sandstones, these last increasing in frequency of occurrence towards the horizon of Skipsey's Marine Band.

(iii) A protracted phase of thick sandstones with conglomeratic horizons, interbedded with siltstones and subordinate shales, starting in late Middle Coal Measure times and gradually dying away within the Upper Coal Measures.

(iv) A quiescent period of thick marls, mudstones and siltstones with rare thin sandstones and containing evidence of a somewhat arid depositional environment.

(v) A terminal phase, immediately preceding the extrusion of the Mauchline Lava Series, of feeble developments of a few thick sandstones within a mudstone/siltstone sequence.

It can be seen that analogies may be drawn between the broad timing of contemporary tectonic movements and relatively stable period in the south (p.51) with the long-term variation in grade of sediment shown by these bores. Climatic modifications of the depositional history may be registered within the extensive phase of thick interbedded marls and siltstones in the higher part of the Upper Coal Measures where common indicators of a prevailing arid climate suggest a decline in water transport activity.

(2) Eastern Area

Although the westerly bores of this group obviously have gradational similarities with the more easterly bores of the central area, significant large scale differences can be seen. Thus, while the sand content of the Lower Coal Measures is similarly significant, there is only a minor decline of this character with time so that the Middle Coal Measures in this area contains frequent, usually thin sandstones. This suggests that the probable north-eastern source of the Lower Coal Measure sands (see p.7, Fig.2) gradually declined in importance, but continued to supply coarse material in the more easterly parts of the coalfield, though largely ceasing to do so after Queenslie Marine Band time in the central and western area.

The major influx of sand that characterises the beginning of the Upper Coal Measures in the west seems to persist, but with diminished effect in the north-east, though it is not at all apparent in the south-east.

(3) Southern Area

In the Dalmellington area, there is no readily appreciable trend variation in the development of sandstones in the Lower Coal Measures these being intermittent and generally thin, though they disappear raggedly in the higher part of the Middle Coal Measures, with the exception of a thick local sandstone body above the Lodgement Coal.

The major sand phase of the Upper Coal Measures appears to be truncated in this area so that the earlier thick sandstones in the north are represented here by a protracted development of a dominantly shale/siltstone sequence with several *Lingula*, and one marine, bands, though thick sandstones appear slightly higher and are probably equivalent to similar bodies in the central area.

Summary

(1) Throughout Ayrshire, there is a relatively high proportion of sandstone in the Lower Coal Measures, usually as a repeated occurrence of moderately thin beds. This characteristic is particularly noteworthy in the eastern part of the area and it is from this direction that the sands appear to be derived. There is a general decline in the sandstone proportion of these strata with time and the termination of this phase is marked in the west roughly by the Queenslie Marine Band horizon though this becomes progressively later moving eastwards so that, in the east of the area, it seems likely that sand derivation from this direction continued to some extent throughout most of Middle Coal Measure times.

(2) In the central and western parts of the region, the Middle Coal Measure sequence is dominated by thick shales and siltstones with the occasional localised development of discrete thick sandstones seemingly unrelated to any prolonged influx of sand.

(3) Towards the end of Middle Coal Measure times, a protracted phase of deposition of thick sandstones with conglomeratic seams and subordinate siltstones began in the central area where the thickest development of this facies is recorded, being feebler (and probably later) in the east and south. This indicates a derivation from the north or west and the relatively abrupt appearance and age of these sandstone bodies suggests that their origin may be related to the action of Malvernian phase tectonic movements, and so renewed erosion, in a source area in this direction.

(4) Information of the later sedimentary history of the Ayrshire Coal Measures is mainly restricted to the central area, but it appears that here at least, a relatively stable period followed, in

which deposition was almost wholly limited to thick marls and silts, with a minor development of a few thick sand bodies prior to the extrusion of the Mauchline Lava Series. Various aspects of these strata suggest a change to a more arid climate and this factor may have been a significant control of the fine-grained motif of this phase.

Chapter 5

LITHOLOGICAL SEQUENCES, CYCLES AND MATHEMATICAL MODELS

Cyclical Rock Associations

In the preceding chapter, rock successions were examined for patterns of a long-term nature for which mechanisms were postulated of correspondingly large-scale processes of tectonism, climate, etc. A study of variation at a lower level is necessary for inference on more local environmental controls. The recognition that different lithologies represent different facies of deposition implies that from a study of the ordering of lithologies in time and space, a theoretical reconstruction is possible of environments of deposition and speculation as to its controls.

This concept has been fundamental to the geological study of sedimentary rock sequences for many years. The economic importance of the Coal Measures has ensured a long tradition of work in this field and has been the source of many theories concerning the internal ordering of rock sequences.

Since the early nineteenth century, the repeated association of certain rock types has been recognised and expressed in various schemes to describe Coal Measure sequences as essentially repetions of these simple associations. The somewhat sporadic appearance of these ideas eventually led to their popularisation, largely due to the work of Weller (1930, 1931). He proposed that the sequential ordering of Pennsylvanian rocks in America was essentially the reiteration of a basic unit which he termed a cyclothem. Each rock type was thought to be arranged in a definite order in relation to one another. It followed that the repetition of this unit led to a type of 'cyclic' pattern.

From that time, an enormous volume of literature has been produced on the subject of cycles and, like most controversial theories has given rise to a proliferation of confusing and ill-defined terms. Duff, Hallam and Walton (1967) have given a review of the terminology that has been used at various times in the literature and point out that one reason for its muddled state lies in the subjective methods used in the study of cyclical associations.

Commonly, such methods result in a simple scheme of rock association which is intended to represent a widely dispersed spectrum of actual rock associations. This produces such puzzling statements as, "with every conceivable modification, the most significant feature in the sequence of rocks making up the productive (i.e. coal-bearing) part of the Coal Measures is the regularity of the simple pattern" (Trueman, 1954, p.10). Many authors attempt to explain deviation of natural associations from their idealised schemes by a philosophy which could be termed, "the missing members concept." Thus Cross and Arkle (1951) state that, "each rock type occurs in its proper order regardless of the presence or absence of other lithologic units of each cyclothem." Application of this can be used to explain the juxtaposition of almost any rock type with any other, and so used to interpret any lithological sequence, random or non-random, as the repetition of any simple scheme.

Other authors, while accepting the impracticability of applying a simple ideal cycle scheme to lithologies, evade the issue by use of subjective environmental interpretation. An example of this is supplied by Edmunds (1968)p.25 who stating that while Reger's cycle "is probably as close to a usable lithologic cyclothem as could be applied in the northern Appalachian coal fields ... an attempt to regularly apply even Reger's cycle results in such constant invoking of exceptions, variations and complex repetitions to render it almost useless." However, he adopts the 'genetic' cycle of Williams and Ferm (1964) and introduces a concept of "missing environments" to explain the deviations of the environmentally interpreted facies associations from the idealised genetic cycle.

A very similar method is used by Zeller (1964) in an entertaining fashion to fit an arbitrary idealised cycle to a 'stratigraphic section' generated from a random numbers table, in almost as convincing a manner as the tortuous interpretations of actual sequences met in the literature.

The attempts to apply idealised cycles have hence gained disrepute in the eyes of many, as the forceful fitting of an abstract generalisation to a highly variable natural situation which it clearly does not satisfy, without resorting to numerous assumptions, which could equally be applied to discovering 'cyclicity' in totally disordered sequences. Suspicion is even directed at the motives of those who would seek to do so by Zeller (1964) who states that (p.631), "science, to an extent matched by no other human endeavour, places a premium upon the ability of the individual to make order out of what appears to be disordered."

Nevertheless, it can be fairly said that while many geologists are not entirely satisfied with the application of rigid ideal cycles to a highly fluid natural situation, most would accept that the sequence of rock types in the Coal Measures is not entirely random but subject to some sort of scheme of order. Clearly, what is needed are objective proofs to resolve what is essentially a subjective belief. Many authors appreciate this so that, for example, Pearn (1964) p.412 writes, "we need to become increasingly aware that the only slightly exaggerated formulation, 'How do you feel about cyclothems?' is simply not a scientifically meaningful question. We need to become increasingly willing to focus our attentions on hypotheses at least potentially susceptible to proof and on methods orientated toward the realisation of that potential."

A significant step in this direction was made by Duff and Walton (1962) who analysed the internal variation of a large number of cyclic units from the Coal Measures of the East Pennine Coalfield and plotted the various types as a distribution. The modal types of such a distribution could then be fairly said to be more 'typical' of the succession than the conceptual ideal cycle of most workers. The presence of certain distinctive lithologies, such as marine bands, was recognised, whose occurrence was infrequent but whose position within cyclic units was statistically systematic. Such lithologies by virtue of their scarcity were unlikely to be represented as components of a modal class whose definition is based on their occurrence. The authors proposed the term 'composite cycle' in which the various lithologies were placed in their preferred position to one another, regardless of frequency. This was essentially an expression of the optimum sequential occurrence of the rock types, based on their relative positions in modal cycles and the statistically significant placings of less frequent lithologies. Such an overall scheme corresponded broadly to the 'ideal cycle' of other workers, but with the important difference that it was arrived at by an objective treatment of field data rather than as a postulation of an unproved conceptual ideal.

The establishment of the idea of modal cycles is valuable in expressing the dominant themes of actual rock associations, but it must be emphasised that the presence of modal cycles does not, in itself, establish a non-random pattern. An artificial sequence in which the order of rock types is deliberately randomised while maintaining their relative proportions will yield 'cycles,' and also 'modal cycles,' whose internal character is dictated by the rock type proportions. (An example of a distribution of 'random' cycles is given in Fig.35).

This point illustrates the common misconception that the acceptance of the presence of cycles of highly variable internal character necessarily implies the acceptance of a non-random pattern of rock sequence. Thus Weller (1964) p.610 states that, "the intermittent occurrence of coal seams in a succession of dominantly detrital strata is obviously cyclic to some degree." The same could be said for a random analogy of this situation, where the tossing of a dice will lead to the 'intermittent occurrence' of a six in a 'succession of dominantly' non-six numbers. The fitting of an ideal cycle to results of a series of dice-throwing trials would admittedly be extremely difficult, but possible through a concept of 'missing numbers' and the admission that there was a wide variation from the postulated ideal cycle. For this analogy to have parity with the geological situation, the numbers could be weighted in frequency of occurrence as rock proportions, and the difficulty of fitting an 'ideal cycle' would be eased.

Another difficulty inherent in the application of the 'cyclic concept' is the selection of the boundary of the cyclic units measured. In the past, almost every rock type has at some time been selected as termination of a cyclic unit on either purely arbitrary grounds or on geological reasoning of varying degrees of validity. If the selection of the cycle boundary is a matter for debate and ultimately of subjective choice, then the objectivity of measuring cycles based on this selection is compromised.

The entire problem of the establishment of some systematic themes to the succession of rock types in the Coal Measures or elsewhere is reduced to the answering of the following questions:

(1) Is the succession of rock types ordered randomly or non-randomly?

(2) If the succession is non-random, can this be expressed in a simple repetitive scheme?

Mathematical Models

The use of mathematical models in stratigraphic section work is comparitively recent, mainly due to the intermittent communication between the disciplines of geology and mathematics. Such models have the advantages that they are dispassionately objective and can be used to establish the presence or absence of statistically operative simple patterns from a seemingly chaotic sequence of geological data. The conversion of a stratigraphic section into a form amenable to its analysis as a mathematical model merely involves structuring the succession of lithologies as a sequence of events in 'time' (without any implications of cyclicity). This sequence of events can only satisfy one of three types of model:

(1) deterministic
(2) partial ordering
(3) independent events.

These three types are not discrete states but members of a spectrum ranging from perfectly ordered (deterministic) to perfectly disordered (independent events). The intermediate class represents a range of schemes of partial ordering where there is a tendency of events to happen in certain sequences not dictated entirely by the extremes of absolute certainty or chance probability. A degree of randomness is implied, and models of this type come within the class of stochastic models. A stochastic process has been defined by Bartlett (1960) p.1 as "some possible actual, e.g., physical, process in the real world, that has some random or stochastic element involved in its structure."

A deterministic process is involved in the application of a rigid ideal cycle, but this seems incapable of describing the highly variable character of rock sequences without invoking numerous exceptions which are not compatible with determinism. On the other hand, the striking frequency of certain rock associations in the Coal Measures appears to belie complete randomness. Some type of stochastic model would therefore be the best hypothetical model for the sequential ordering of Coal Measure lithologies, implying a property ordering disturbed by some degree of randomness. A postulated modelof this kind is consistent with modern notions of the character of processes operative within the natural world. Processes such as sedimentation are good subjects for stochastic model work and so (from a uniformitarian viewpoint) should equally apply to their Coal Measure products.

Markov Models

One type of stochastic model that has features attractive to geologists is that of Markov Chains. Originally conceived by Markov, the Russian mathematician, in his consideration of the alternation of vowels and consonants in Pushkin's poem "Onegin," Markov Chains have been used in a wide range of fields, but only in geology in recent years. Markov Chains were first applied to stratigraphic sections by Vistelius (1949) in work on a Russian flysch sequence but have only recently come into wider use as is shown by a rapidly expanding literature including papers by Allègre (1964), Schwarzacher (1964), Griffiths (1966), Carr et al. (1966), Krumbein (1967, 1968), Potter and Blakely (1968) as well as further papers by Vistelius (Vistelius and Fass (1965a, 1965b) and Vistelius and Feygelson (1965)). Much of this work has been of a somewhat preliminary nature concerned mainly with explanation of the theory and methodology of Markov Chains, application to simple examples and the generation of simple simulation models.

The simplest Markov model is one of first order. The basic structure of this model is one of partial sequential dependency in that the state of a given system at any one time is dependent to some degree on its immediately previous state but on none other. This dependency is often known as the "memory" of the process. If the character of a state is largely determined by that of the immediately previous state, then the memory is strong but short (only one step). This concept of memory can be extended in the consideration of a second order Markov model. On this model, not only may the immediately preceding state of a system have control on its present state, but the state immediately prior to this preceding state also has some influence, over and beyond the combination of two 'first order memories.' In this case the system has a 'second order memory' which may be weak or strong. (In the context of other classes of model, the memory of deterministic processes is perfect and long, but non-existent in independent-events processes).

The theory can be expanded to consider models that have memories of n steps. Models involving long memories are usually complex in application and interpretation, and probably only models with relatively short memories are likely to represent the intermittent rock associations present in Coal Measure sequences.

The suitability of some kind of Markov process as a model for sedimentary rock successions is apparent when it is remembered that the vertical ordering of beds has long been related to the lateral ordering of the facies they represent. Thus Walther (1919) states, "only rock types which can be deposited side by side can overlie each other directly in a vertical sequence." Now while Potter and Blakely (1968) envisage a whole spectrum of possible lateral lithofacies configurations, from a 'regular' (systematic) to a 'crazy-quilt' (random) pattern, almost all modern sedimentary environments possess a highly variable, but certainly not random, pattern. It therefore follows that the vertical variation of rocks eventually produced by the lateral migration of such facies belts will be endowed with some degree of sequential memory. As such, they are suitable subjects for Markov model studies which yield implications not only of environmental change through time, but of the palaeogeographical distribution of lithofacies in terms of some simple underlying pattern.

Methodology of Markov Models

An extensive mathematical literature replete with an exhaustive terminology deals with the theory of Markov Chains, but it is intended here to restrict the terminology used to that which has some possibility of application and meaning in a geological context. This intention is reinforced by the assertion by Hammersley and Handscomb (1964) p.115 that, "a great variety of terminology exists in the literature, and authors (e.g. Feller) even permute the meanings of various adjectives from one edition to another. As a result, all such words as 'recurrent,' 'null,' 'ergodic,' 'transient,' 'persistent,' etc., are so obscured by hopeless confusion that nobody knows what they mean in any given context."

The First Order Markov Model

The analysis of a stratigraphic section for the presence of properties of a Markov (as opposed to Independent Event) model is conducted as follows.

The various rock types that make up the section are considered together as a 'system,' in which the individual rock type constitutes a 'state.' The section is then visualised as a sequence of events, each event being marked by the occurrence of one of these states. It follows that if the section is classified into three rock types, designated as states A, B and C, observations made moving up the section on a sequential series of steps produce a succession of the form ABACBBAC ...

This succession is then analysed in terms of the nature of the transitions involved in moving from one step to the next. These types of transitions are summed and expressed in the form of a 'transition tally matrix:'

$$\begin{array}{cccc} & A & B & C \\ A & n_{11} & n_{12} & n_{13} \\ B & n_{21} & n_{22} & n_{23} \\ C & n_{31} & n_{32} & n_{33} \end{array}$$

in which rows represent the given state and the columns that of the following state. (On this basis, n_{23} represents the total number of transitions of B to C).

This matrix is then converted to a 'transition probability matrix' by summing each row and dividing each cell by its row total:

$$\begin{array}{cccc} & A & B & C \\ A & p_{11} & p_{12} & p_{13} \\ B & p_{21} & p_{22} & p_{23} \\ C & p_{31} & p_{32} & p_{33} \end{array}$$

These cell values are the empirical transition probabilities that one state will immediately precede another in the sequence. (For example, p_{23} is an estimate of the probability of B being followed by C, as against being followed by A or a repetition of B). (Examples of this procedure are given in Krumbein, 1967).

These two matrices contain the necessary information for deciding whether a first order Markov model is applicable. Now, if the character of adjacent events is unrelated, then their ordering is random and the probability of the transition of one state to another equals the probability of the occurrence of the second state in any part of the sequence or

$$P\ (\text{event } i + 1\ /\ \text{event } i) = P\ (\text{event } i + 1)$$

In this case, the sequence is subject to an independent events model, and the transition probability matrix in the three-state system example is equal to:

$$\begin{array}{ccc} P(A) & P(B) & P(C) \\ P(A) & P(B) & P(C) \\ P(A) & P(B) & P(C) \end{array}$$

If, however, the transition probability matrix differs significantly from this, then a partial dependence between the nature of successive events is proved. This is a first order Markovian model with a memory of one step.

Spacing of events

In the application of Markovian models to processes in other fields, observations of the state the system occupies are usually made at equally spaced intervals of time (though such a condition is not compulsory). A time-based method of spacing events on a stratigraphic section is not possible in the present situation of rudimentary theories of sedimentation rates. Therefore, observations must be spaced according to some other criterion.

Krumbein (1967) uses various lengths of interval dividing successive observations within a rock sequence in his analysis for a Markov property. His summary (p.3) of the criteria by which the size of the interval is selected is,

"It is evident that judgement is required regarding the appropriate interval to use. If it is too large, some lithologies are entirely missed; if too small, the probability of leaving any one state in a given sample of observations becomes impracticably small. Experiments with a variety of stratigraphic sections suggests an interval of from 2 to 10 feet."

A selection of a satisfactory interval was found totally impossible, however, for coal measure sequences. An interval smaller than the 'average' bed thickness produced a very strong spurious 'memory' that successive observations would be in the same state rather than in another (a memory that beds tend to be thicker than the sampling interval). Interval lengths large enough to dampen this 'within-state' memory resulted in the missing of many relatively thin, but diagnostic lithologies in the section and distorted values for between-state transitions.

In the absence of any meaningful criterion to select thickness of interval between successive observations, each bed in the stratigraphic section can itself be considered as a separate event. In this case, a state can only be involved in a transition to another so that cell values on the main diagonal of the transition matrices will always be zero. One possible solution to the problem this raises is suggested by Carr et al. (1966) in the concept of 'multistorey lithologies' which is also mentioned by Krumbein (1967) and Potter and Blakely (1968). They suggest that if a worker can recognise subdivisions within a lithological state "for example a sandstone following a sandstone" (Potter and Blakely) or "variations such as change in shale colour or a sandstone texture" (Krumbein), then values for within-state transitions are possible. Such a concept is impossible to apply and of no real meaning.

Thus a lithology can be subdivided into a scheme of storeys by virtually any number of criteria so that, in the case of a simple scheme, the number of 'within-state' transitions will be small; for a complex scheme, the number will be large. The important point is that while the main diagonal cell values will vary according to which scheme of multistorey classification is used, the off-diagonal cells will remain immutable, so that the resulting matrix and its significance is largely a function of the worker's subjectivity. The fault lies not in Markov theory but in the illogicality of multistorey division of states. Such a process is the breakdown of an entity into parts which have recognisably different character and so must constitute separate states, as this is done in a precisely similar manner in the division of the state 'rock' into a system of lithological states.

The stratigraphic section is hence most objectively (and meaningfully) considered as a succession of events each representing a different lithology from the preceding, so that successive observations are made in recognisably different beds.

Stationarity

Another condition (important in the theory of Markov chains) is that, for simple analysis, the process involved in the studied sequence should be 'stationary.' A sequence that is satisfactorily described by essentially constant transition probabilities is termed stationary, while, if these are variable, it is 'non-stationary.'

To facilitate interpretation of transition data, a stationary process is desirable, but the geological situation may not be so obliging. In a non-stationary process, the proportion of the different states will change throughout the sequence. Such a situation occurs in the Ayrshire Coal Measure sections, as is demonstrated in their smoothed profiles, (see Figs.27,28,29), where lithological proportions differ markedly along their lengths so that parts are dominated by frequent sandstones, others by frequent shales.

In the following study, coal measure sections are divided into parts according to the predominance of sandstone or shale, and cumulative transition matrices constructed for each type. The partition into two types represents a rigid approach, as these divisions can be presumed to have only an approximate stationarity. However, they represent a closer approach to perfect stationarity and major deviations from this ideal become evident in any detailed study of matrices derived in this manner.

Testing for a first order Markov property

As already indicated, the possession of a first-order Markov property implies a partial dependency between successive events, as opposed to an independent events model where there is no such dependence. Tests for such a property are usually made to check the null hypothesis that a process of independent events is operative.

Krumbein (1967) uses the method of Anderson and Goodman (1957) who apply a chi-square distribution. The sample statistic is:

$$-2 \log_e \lambda = 2 \sum_{ij}^{m} n_{ij} \log_e (p_{ij} / p_j)$$

where n_{ij} = the value of the ij^{th} cell in the transition tally matrix,

p_{ij} = the transition probability of the ij^{th} cell,

p_j = the marginal probability of the j^{th} columns, and the quantity ($-2\log_e\lambda$) for m states is asymptotically distributed as chi-square with $(m - 1)^2$ degrees of freedom.

Conditions of this test are that the transition probability matrix is stationary and that events are separated by equal intervals of time. This test will not accept zero values that appear in any of the matrix cells ($\log_e$ zero equals minus infinity). Krumbein suggests that the test can be modified to compensate for a few zero cells by ignoring these, while subtracting one degree of freedom for each, when statistical limitations are approximately met.

The application of this test to matrices that have zero main diagonal cell elements must strain it beyond these limitations, so that use of the test in these circumstances is statistically invalid. Potter and Blakely (1968) suggest use of a chi-square contingency table modified for use with this type of transition matrix. In this case, the number of degrees of freedom for a matrix of m states is $(m - 1)^2 - m$. Again, the null hypothesis of an independent events model is postulated and the observed tally transition matrix is tested against an expected tally transition matrix assuming an independent events process is operative.

The calculation of an expected independent events tally matrix proceeds as follows. If the cell values in each row of the observed tally matrix are summed, then each row total is the number of occurrences of the state that the row represents. It also follows that the sum of the row totals is the total number of occurrences of all states in the system. On an independent events model for the three-state system (ABC)

$$P\ (X/Y) = P\ (X)$$

where X and Y are all combinations of A, B and C, or, stated more fully, the expected transition probabilities to the state labelled as X equal the probabilities of X occurring as an event anywhere in the sequence. Then

P (X) = state (X) Row Total/Summed row totals and from these two relations, an expected independent events transition probability matrix is computed. These calculations must be modified to allow for the condition that successive observations cannot be made in the same state. (It must be emphasised that this condition usually precludes the idealisation of a perfect independent events matrix, as some sort of memory is assumed that disallows transitions of a state to itself. However, the resulting matrix is a close approach to an ideal independent events matrix if the state proportions are broadly similar). The expected transition probability values are then applied to the row totals of the observed tally matrix to produce a predicted independent events tally matrix representing the same population as that of the observed sample.

The observed tally matrix is then tested against the null hypothesis independent events matrix in the conventional manner of a chi-square contingency table, but omitting main diagonal cells. If the null hypothesis is rejected then a Markov - 1 model is accepted.

Higher Order Markov Models

Remarks have so far been mainly directed to the examination of the first-order Markov model, where only a 'one-step' memory is operative. This model is only a specific case of the generalised

Markov process, in which the state of the system at time $(t - x)$ has influence on the state at time t. This represents an x^{th} order memory.

A superficial consideration of the nature of sedimentary processes leads one to suspect at least the possibility of memories of more than one step. For example, a geological analogy can be conceived of the sequence

ABCBABCBABC

in which the state preceding state B clearly determines the state that follows it and so illustrates the presence of a second order memory (or Markov - 2 property).

Successively higher order memories become progressively less likely in natural situations where the long chains of partial ordering they imply become increasingly susceptible to random peturbations. It follows that the real processes represented in rock sequences that have one-step memories, may have weak two-step memories, but third and higher order memories are unlikely unless the sequence is particularly well-ordered in some complex fashion.

The theory of the presence of a second-order memory in a rock sequence is postulated if a first-order memory has been established. In this case, the null hypothesis is set that only a first-order memory is operative. A first-order Markov model is then used to predict the nature of the $i + 2^{th}$ event, given that of the i^{th}. This introduces the usage of 'tree diagrams' which are diagramatic representations of the range of probable sequences after any given number of events based on one step memories. For the system (ABC), a possible diagram is shown in Fig.30.

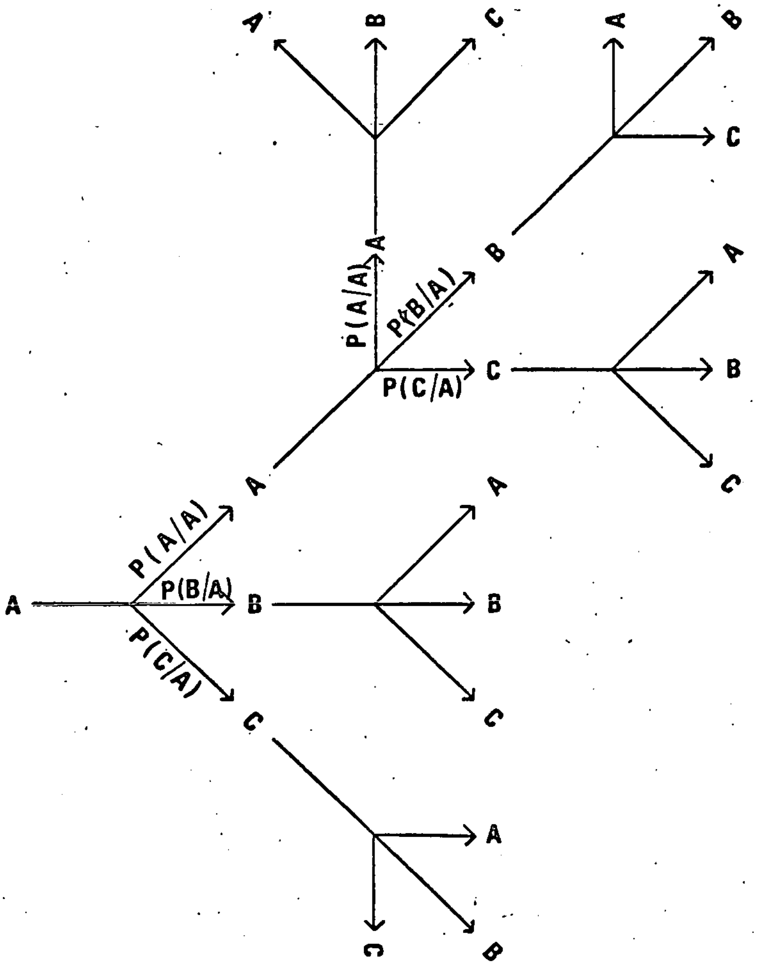


Fig. 30 Tree diagram of system (ABC)

(VARIOUS BRANCHES & TRANSITION PROBABILITIES OMITTED FOR CLARITY)

The probability of the sequence ABAB is then the product of P (B/A) and P (A/B). An extension of this procedure enables the calculation of the probability of the i + 2th step given the state at the ith step, assuming that only a one-step memory is operative.

This calculation can be done directly by squaring the transition probability matrix. The new matrix therefore contains the Markov - 1 predicted probabilities of the i / i + 2 pairs. This is used as the null hypothesis prediction model.

The stratigraphic section is then re-analysed and the number of actual i / i + 2 pairs counted and expressed in the form of a tally matrix. The null hypothesis probability matrix is then converted to a tally matrix representative of the same number of observations as present in the rock sequence and tested against the observed tally matrix as a chi-square contingency test. In this case, the main diagonal cells will be positive and so the number of degrees of freedom therefore $(m - 1)^2$, where m is the number of states. If the null hypothesis is rejected then a second order memory (Markov - 2 property) is proved.

This approach can be extended to establish the presence or absence of higher order memories, but becomes increasingly more cumbersome to apply. However, it seems logical that if only a weak second order memory is proved, the likelihood of significant higher order memories is small.

Chapter 6

MARKOV MODELS APPLIED TO THE AYRSHIRE COAL MEASURE SEQUENCE

Method and Definitions

For the following study, the combined sequences represented in 26 boreholes were used in the analysis of coal measure lithological ordering for properties of Markov models. The stratigraphic ranges of these boreholes is shown in Fig.31, where their coverage can be seen to extend over the Lower, Middle and Upper Coal Measures.

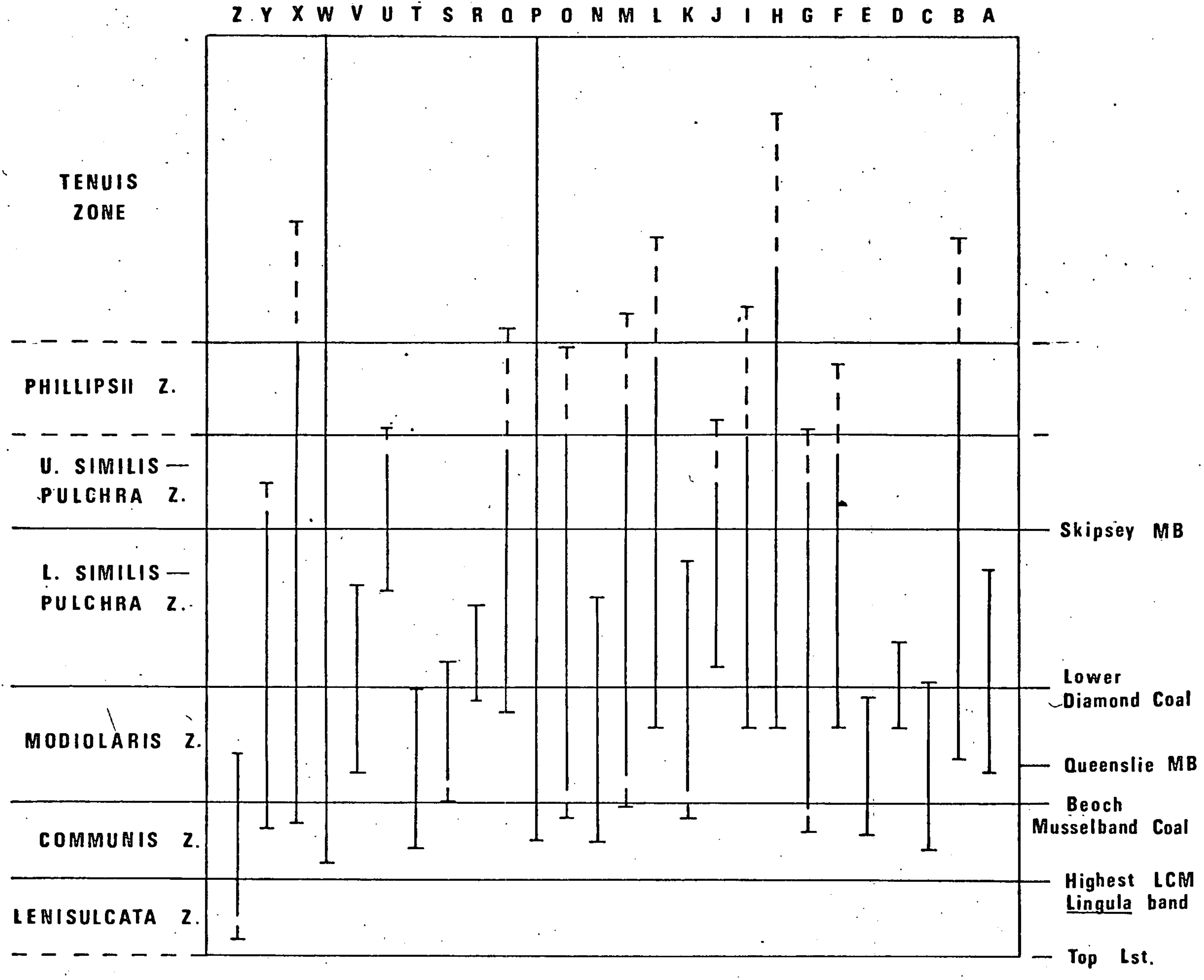
To satisfy approximately the condition of stationarity, the sequences were divided into two groups of fragment termed 'sandy' and 'shaly' according to whether sandstone or shale predominated. The boundary between these fragments was set by reference to their long-term smoothed profiles (Chapter 4), where sections in which the smoothing curve lay below the 'siltstone value' were designated 'shaly,' those above, 'sandy.' (The arbitrariness of such a boundary does not violate the objectivity of Markov model studies). This division was seen to result in a very effective separation between parts of the section largely consisting of thick shale with frequent silt stones and rare, thin sandstones, and parts dominated by thick sandstones and siltstones with a reduced proportion of shale.

Tally matrices constructed for each group were combined in cumulative matrices representing the shaly and sandy section populations. Rather than construct two 'super' tally matrices to describe each type of population group, three cumulative matrices

A	Fairfield No. 1	(10 / 32NW)
B	Adamton Mains No. 1	(12 / 32NE)
C	Newfield No. 1	(5 / 33SE)
D	Fortacres No. 2	(71 / 33SE)
E	Chalmerston	(93 / 40NE)
F	Dalmellington No. 237	(249 / 40NE)
G	Ashentree No. 1	(140 / 41SW)
H	West Tarelgin No. 1	(2 / 41NE)
I	Dalmellington No. 231	(6 / 41NE)
J	Treesmax	(10 / 41NE)
K	Drumbowie No. 2/57	(56 / 41NE)
L	Boghead No. 5	(7 / 42NW)
M	Outmains Farm	(20 / 42NW)
N	Enterkine No. 7	(14 / 42SW)
O	Redcraig	(15 / 42NE)
P	Slatehole	(4 / 42SE)
Q	Carnell No. 2	(60 / 43SE)
R	Hindsward No. 6	(53 / 51NW)
S	Garlaff No. 3	(117 / 51NW)
T	Auchincross No. 14	(5 / 51SW)
U	Upper Red Group No. 3	(105 / 51SE)
V	Main Coal Group No. 10	(123 / 51SE)
W	Kingencleugh	(12 / 52NW)
X	Kenstey Farm	(21 / 52SW)
Y	Rigg No. 1 Diamond	(96 / 52SE)
Z	Mortonmuir No. 16	(136 / 52SE)

BOREHOLES USED IN MARKOV MODEL WORK
Bracketed values refer to borehole number
and Ordnance Survey 6 in. NS sheet number.

FIG. 31 STRATIGRAPHICAL RANGES OF BOREHOLE SECTIONS



representing subgroups were summed for each and independently tested as an additional check on the constancy of the statistical conclusions.

The definition of states was made on the criteria that they should each be readily recognisable and have some potential geological significance. It would obviously be desirable to define as many states as possible, so that the analysed model would be described by a large number of variables. However, a stricture is placed on this ideal in that the number of cells increases as the square of the number of states. The conditions governing statistical procedures are more closely obeyed if there is a reasonable sample number in each cell and, for a large number of cells, this is usually only possible by sampling an impracticably large population of observations.

Six states were chosen for Ayrshire Coal Measure sequences as follows:

"Barren" shales and mudstones - designated A
F/W Lamellibranch-bearing shales and mudstones - " M
Siltstones - " B
Sandstones thinner than 20 feet - " C
Sandstones thicker than 20 feet - " K
Rootlet horizons - " Y

The minimum thickness of a lithology to be recognised as the occurrence of a state, was taken as one foot, with the exception of rootlet horizons, on which no thickness limitation was placed.

These have the property of being easily recognisable and the geological criteria involved in their selection is outlined below.

A and M

While the absence of fresh-water lamellibranchs in certain shales may be a function of non-preservation, it seems possible that some barren shales and mudstones (particularly at seat-earth horizons) represent a different facies from lamellibranch-bearing shales. Such a theory is a sub-hypothesis which does not subjectively alter the presence or absence of Markovian properties. If these two states exhibit statistically insignificant difference in their transition behaviour then the hypothesis that they are different in Markovian terms is rejected.

B

No criterion was obvious for subdividing siltstones into separate types and so these were set as a discrete state.

C and K

Field observations and sub-surface maps of sandstones in the Ayrshire Coal Measures (and in many coalfields elsewhere) reveal the presence of sandstones which, in their thickest development, take the form of sheets, belts and pods of often restricted areal development. These can be contrasted with thin sandstones whose areal and vertical distribution appears more haphazard. The nature of borehole records precludes more sophisticated differentiation of these two types on any grounds but thickness. Bearing in mind the likely overlap of these hypothetical types using this crude criterion, the arbitrary boundary of twenty feet was selected. As in the case of A and M, the hypothesis that they represent different states in Markovian terms is rejected if they show statistically significant similar transition behaviour.

Y

The seatearths that are present in the series were differentiated into their separate lithological types and coded in terms of the states already described. The state Y was thus defined as the vegetation interface at the top of a seatearth. In many cases, this corresponds to a coal, but in others no coal is present and in these Y represents the 'ghost vegetation' which for various reasons is not preserved as a coal. The setting of coal as a state distinct from rootlet horizon was rejected on the grounds that almost all coals (with the exception of many cannels) are underlain by seatearths. The very strong memory that this introduces might endow a biased Markovian property to an effectively amnesic sequence.

The system defined is fairly broad, and so schemes of transitions, resulting from analysis, are of correspondingly simple nature. However, this framework can be expanded to study the systematics of more detailed variation by considering a state as a subsystem and dividing it into substates. This is precisely analagous to dividing the system 'rock' (a state in a larger system of things) into states. An example of this approach is given later, where the state K is subdivided into substates on the basis of grainsize, to analyse the internal variation of this state in terms of Markov characteristics.

To ease the seemingly endless (and essentially repetitive) labour involved in production of Markov model data, the programme BORE ANALYSIS (Appendix F) was used. This accepts borehole data tapes used in conjunction with the earlier programme SMOOTHBORE, and computes transition matrices at one and two step levels, as well as recording bed thicknesses for use in simulation model work that requires lithological thickness distributions.

First Order Markov Model Work

Shaly Group (G)

No sandstones thicker than twenty feet were found in the fragments of section used in the cumulative matrices of this group. Therefore the state K did not occur, and the system was condensed to one of five states. The observed transition tally and transition probability matrices of the three population sub-groups are shown in tables 9 and 10. The transition probability matrices predicted for an independent-events process were calculated for each sub-group (Table 11) and used as the basis for null hypothesis models against which the observed tally matrices were tested.

The chi-square test totals were as follows:

G1	179.5
G2	73.1
G3	145.1

For nine degrees of freedom, the tabulated chi-square value at α0.01 is 21.67, and so the null hypothesis of independent events strongly rejected.

Sandy Group (H)

The system describing this group is in its full six-state form. The procedure used for treating the Shaly Group was repeated. The observed transition tally and transition probability matrices are shown in tables 12 and 13, while the predicted independent-events

KEY TO SYMBOLS IN TABLES 9 TO 24 ; 26, 27, 28.

A = MUDSTONE

M = MUDSTONE + NON-MARINE LAMELLIBRANCHS

B = SILTSTONE

C = SANDSTONE < 20 FEET THICKNESS

K = SANDSTONE ≥ 20 FEET THICKNESS

Y = ROOTLET HORIZON

		A	M	B	C	Y	Totals
	A	-	-	74	27	71	172
	M	-	-	40	11	10	61
G 1	B	102	12	-	60	37	211
	C	29	4	65	-	5	103
	Y	40	46	31	6	-	123
							670
		-	-	114	26	87	227
		-	-	28	9	7	44
G 2		135	9	-	33	30	207
		36	2	34	-	7	79
		55	33	32	11	-	131
							688
		-	-	100	20	82	202
		-	-	32	4	10	46
G 3		113	14	-	57	27	211
		27	1	51	-	11	90
		62	31	28	9	-	130
							679

Table 9 TRANSITION TALLY MATRICES FOR SUB-GROUPS OF SHALY GROUP (G)

		A	M	B	C	Y
	A	-	-	0.43	0.16	0.41
	M	-	-	0.66	0.18	0.16
G 1	B	0.48	0.06	-	0.28	0.18
	C	0.28	0.04	0.63	-	0.05
	Y	0.33	0.37	0.25	0.05	-
		-	-	0.50	0.12	0.38
		-	-	0.64	0.20	0.16
G 2		0.65	0.04	-	0.17	0.14
		0.46	0.02	0.43	-	0.09
		0.42	0.26	0.24	0.08	-
		-	-	0.49	0.10	0.41
		-	-	0.70	0.09	0.22
G 3		0.54	0.06	-	0.27	0.13
		0.30	0.01	0.57	-	0.12
		0.47	0.24	0.22	0.07	-

Table 10 TRANSITION PROBABILITY MATRICES FOR SUB-GROUPS OF SHALY GROUP (G)

		A	M	B	C	Y
	A	-	-	0.48	0.24	0.28
	M	-	-	0.48	0.24	0.28
G 1	B	0.38	0.13	-	0.22	0.27
	C	0.30	0.11	0.37	-	0.22
	Y	0.31	0.11	0.39	0.19	-

	-	-	0.50	0.19	0.31
	-	-	0.50	0.19	0.31
G 2	0.47	0.09	-	0.17	0.27
	0.37	0.07	0.34	-	0.22
	0.41	0.08	0.37	0.14	-

	-	-	0.49	0.21	0.30
	-	-	0.49	0.21	0.30
G 3	0.43	0.10	-	0.19	0.28
	0.34	0.08	0.36	-	0.22
	0.37	0.08	0.39	0.16	-

Table 11 TRANSITION PROBABILITY MATRICES EXPECTED FOR SUB-GROUPS OF SHALY GROUP (G) IF THEY REPRESENT AN INDEPENDENT EVENTS PROCESS

		A	M	B	C	K	Y	Totals
	A	-	-	74	45	7	98	224
	M	-	-	38	17	3	4	62
H1	B	97	13	-	140	4	72	329
	C	57	5	152	-	-	15	229
	K	6	0	15	-	-	0	21
	Y	63	42	51	28	6	-	190
								1055
		-	-	90	45	13	80	228
		-	-	27	20	3	3	53
H2		108	12	-	88	11	54	273
		58	6	96	-	-	17	177
		13	0	22	-	-	0	35
		49	35	38	25	7	-	154
								920
		-	-	120	41	9	116	286
		-	-	26	8	4	5	43
H3		141	11	-	125	15	50	342
		59	2	121	-	-	14	196
		9	0	27	-	-	1	37
		77	30	48	22	9	-	186
								1090

Table 12 TRANSITION TALLY MATRICES FOR SUBGROUPS OF SANDY GROUP (H)

		A	M	B	C	K	Y
H1	A	-	-	0.33	0.20	0.03	0.44
	M	-	-	0.61	0.28	0.05	0.06
	B	0.30	0.04	-	0.43	0.01	0.22
	C	0.25	0.02	0.66	-	-	0.07
	K	0.29	0	0.71	-	-	0
	Y	0.33	0.22	0.27	0.15	0.03	-
H2		-	-	0.39	0.20	0.06	0.35
		-	-	0.51	0.37	0.06	0.06
		0.40	0.04	-	0.32	0.04	0.20
		0.33	0.03	0.54	-	-	0.10
		0.37	0	0.63	-	-	0
		0.32	0.23	0.25	0.16	0.04	-
H3		-	-	0.42	0.14	0.03	0.41
		-	-	0.60	0.19	0.09	0.12
		0.41	0.03	-	0.37	0.04	0.15
		0.30	0.01	0.62	-	-	0.07
		0.24	0	0.73	-	-	0.03
		0.41	0.16	0.26	0.12	0.05	-

Table 13 TRANSITION PROBABILITY MATRICES FOR SUB-GROUPS OF SANDY GROUP (H)

		A	M	B	C	K	Y
H1	A	-	-	0.42	0.30	0.03	0.25
	M	-	-	0.42	0.30	0.03	0.25
	B	0.31	0.09	-	0.32	0.03	0.25
	C	0.27	0.08	0.41	-	-	0.24
	K	0.27	0.08	0.41	-	-	0.24
	Y	0.26	0.07	0.38	0.27	0.02	-
H2		-	-	0.43	0.28	0.05	0.24
		-	-	0.43	0.28	0.05	0.24
		0.42	0.08	-	0.27	0.05	0.24
		0.32	0.07	0.39	-	-	0.22
		0.32	0.07	0.39	-	-	0.22
		0.30	0.07	0.36	0.23	0.04	-
H3		-	-	0.45	0.26	0.05	0.24
		-	-	0.45	0.26	0.05	0.24
		0.38	0.06	-	0.26	0.05	0.25
		0.33	0.05	0.40	-	-	0.22
		0.33	0.05	0.40	-	-	0.22
		0.32	0.05	0.37	0.22	0.04	-

Table 14 TRANSITION PROBABILITY MATRICES EXPECTED FOR SUB-GROUPS OF SANDY GROUP (H) IF THEY REPRESENT AN INDEPENDENT EVENTS PROCESS

models transition probability matrices are shown in Table 14.

For the sub-groups, the chi-square test totals were:

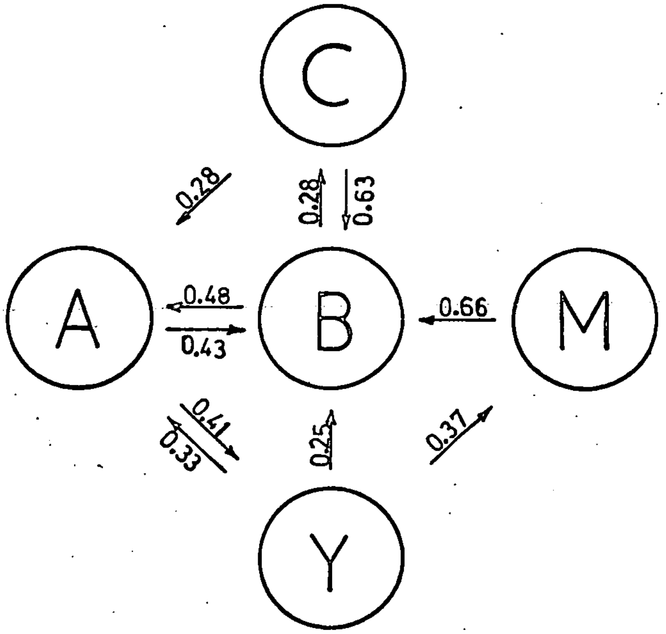
H1	255.9
H2	140.6
H3	230.9

With the inclusion of the state K, the number of degrees of freedom involved is expanded to fifteen where, at α 0.01, the tabulated chi-square value is 30.58. As with the shaly group, the hypothesis of independent-events is therefore overwhelmingly rejected.

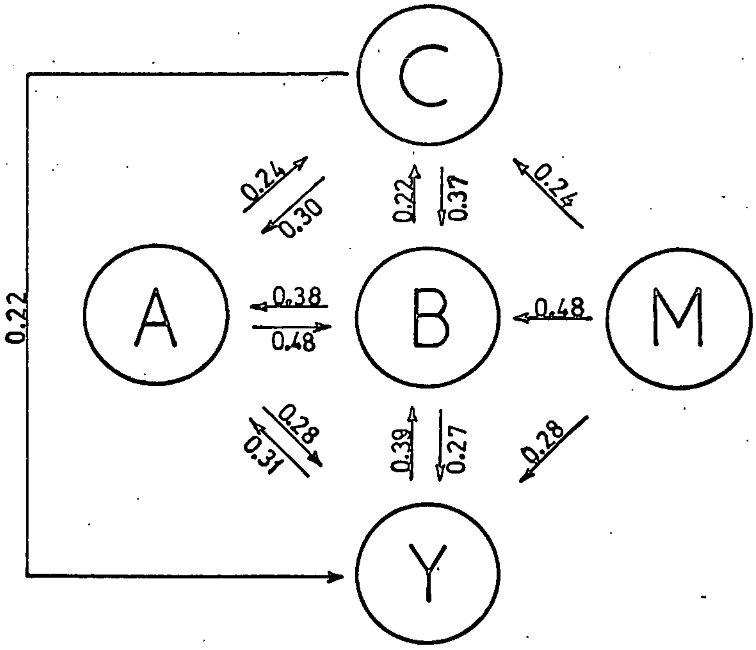
A Markov model of first order is therefore demonstrated as statistically adequate to describe the sequential ordering of lithologies in Ayrshire Coal Measure successions, suggesting a memory of at least one step.

Transition diagrams

The acceptance of a Markov model of first order necessarily implies some scheme of preference of ordering of the various lithologies one to another. The conventional manner of showing such a scheme diagramatically is to represent the states as 'blocks' linked by arrows chosen by the worker for the higher transition probabilities they signify. Examples are shown in Potter and Blakely (1968). The application of this technique to the group G1 gives the diagram of Fig.32i. Such a diagram is unsatisfactory as it reflects the effect of the relative proportions of the states as well as the preferred transitions over and beyond this effect. An illustration of this weakness can be seen by reference to Potter and Blakely (1968) Fig.7, p.165, in which almost all other states in the system



i. G1 OBSERVED TRANSITION PROBABILITIES



ii. G1 INDEPENDENT EVENTS MODEL TRANSITION PROBABILITIES (CHANCE)

Fig. 32 Illustrative transition diagrams of (AMBCY) system for Shaly Group (G) - i. observed, and ii. expected for an Independent Events model.

they consider are shown as having preferred transition to the state 'gray shale.' The authors remark that "the importance of gray shale as the most common lithology is again related to its dominance, since it constitutes over 50 per cent of the section." It follows that a 'transition diagram' can be drawn for an independent-events model, where the high transition probabilities are merely expressions of the higher lithological proportions. The independent-events model for G1 is shown as a transition diagram in Fig. 32 ii. On an independent-events model, the transitions are, by definition, ones of total disorder and so such a transition diagram has no meaning in Markov terms of a one-step memory.

It is therefore clearly desirable to remove the effect of relative state proportions and produce a scheme of transitions that expresses the structure of the proved first-order Markov model. An assessment of which transition types are diagnostic one-step memory links can be made by examination of the individual cell contributions to the total in the chi-square tests. Large cell values are produced by high deviations from the number of transitions predicted by independent-events. These cells represent those transitions that collectively endow the sequence with a first-order Markov property. However, the absence of any statistical criterion to set a level at which cell values are differentiated into Markov-1 and independent-events dictated transitions makes it impossible to extract significant transition types from the matrices as they stand, by any but subjective methods.

An objective procedure to obtain the significant transition types can be made by the proposition of a number of sub-hypothesis. Each state is taken in turn, and its total number and type of transitions to all other states considered. The hypothesis is set that the transitions between two specified states is the number that would be expected on an independent-events model. This is then tested as a chi-square distribution with one degree of freedom and appropriate level of α, applying a continuity correction throughout. There are three possible results of the test:

(1) the null hypothesis is accepted, in which case the number of transitions is that which would be expected in an independent-events process;

(2) the null hypothesis is rejected and the observed value is greater than predicted by independent-events, when there is a significant memory for this transition to occur;

or (3) the null hypothesis is rejected and the observed value is less than predicted, showing a significant memory discouraging the occurrence of this type of transition.

The hypothesis is repeated for all possible permutations of transition types and these grouped into three classes according to the results of the tests. An optimum scheme of transitions can then be constructed from those transition types that have significantly greater totals than independent-events. This expresses the one-step memory structure that represents the Markov-1 model of the sequence.

The method was applied to the G and H groups as follows. In testing each permutation, the α level was chosen as 0.05 for which the tabulated chi-square value is 3.84 for one degree of freedom. Each test result was designated 0, + or -, according to whether independent-events was accepted, or rejected on the grounds that the number of transitions was significantly more, or less, than predicted. The permutation tests were repeated for each sub-group and the results tabulated. The test results do not match perfectly for each permutation from sub-group to sub-group owing to the three effects:

(1) "weak" transition memories will tend to waver between statistical significance and insignificance;

(2) the states that are proportionately minor tend to produce statistically poor sample totals in their permutations with other states;

and (3) the 'pseudo-random' character of the predicted independent-events tally matrices.

However, overall homogeneity of results if fairly strong and consistent with a conclusion as to status of each transition type, based on testing the combined groups of three. The results of these tests for Shaly Group G and Sandy Group H are shown in tables 15 and 16.

An 'optimum transition scheme' for each group was then drawn using only those permutations that have positive test results. These schemes (Fig.33) plot the transitions that involve a positive one-step memory and are a diagramatic representation of the first-order Markovian models proved to satisfy these two groups.

Second-Order Markov Models

The acceptance of a strongly significant one-step memory in the lithological sequence leads logically to the suspicion that two-step or higher memories may be present. The possibility that such higher memories underlie geological situations is readily accepted

	G1	G2	G3	G Total
AB	0	0	0	0
AC	-	-	-	-
AY	+	+	+	+
MB	+	0	+	+
MC	0	0	-	0
MY	-	-	0	-
BA	+	+	+	+
BM	-	-	0	-
BC	+	0	+	+
BY	-	-	-	-
CA	0	0	0	0
CM	-	0	-	-
CB	+	0	+	+
CY	-	-	-	-
YA	0	0	+	0
YM	+	+	+	+
YB	-	-	-	-
YC	-	0	-	-

Table 15 SHALY GROUP (G). RESULTS OF CHI-SQUARE TESTS OF INDIVIDUAL PAIR SEQUENCES AS ONE-STEP MEMORY LINKS (SEE TEXT)

	H1	H2	H3	H Total
AB	-	0	0	0
AC	-	-	-	-
AK	0	0	0	0
AY	+	+	+	+
MB	+	0	+	+
MC	0	0	0	0
MK	0	0	0	0
MY	-	-	0	-
BA	0	0	0	0
BM	-	-	-	-
BC	+	0	+	+
BK	0	0	0	0
BY	0	0	-	0
CA	0	0	0	0
CM	-	0	-	-
CB	+	+	+	+
CY	-	-	-	-
KA	0	0	0	0
KM	0	0	0	0
KB	+	+	+	+
KY	-	-	-	-
YA	+	0	+	+
YM	+	+	+	+
YB	-	-	-	-
YC	-	0	-	-
YK	0	0	0	0

Table 16 SANDY GROUP (H): RESULTS OF CHI-SQUARE TESTS OF INDIVIDUAL PAIR SEQUENCES AS ONE-STEP MEMORY LINKS (SEE TEXT)

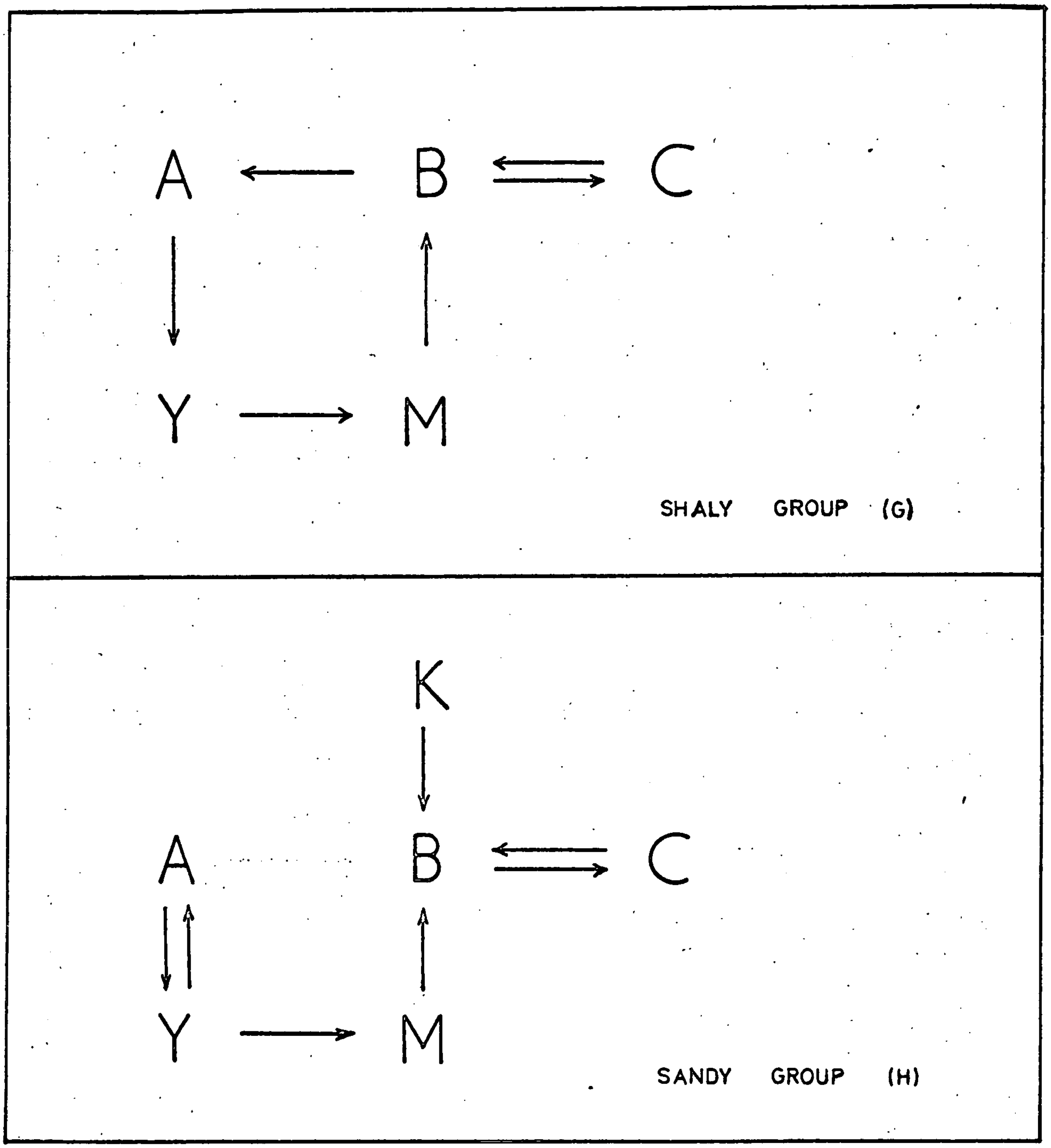


Fig. 33 Markov 1 Transition Schemes

in the literature, although almost all applied work (so far as is known) has been confined to Markov-1 models (an exception is Schwarzacher, 1967). The extension of research to a Markov-2 model is not the addition of complexity for its own sake, but the expansion of a crude transition scheme to a broader picture of lithological ordering. If the real situation has a two-step memory as a significant control, then a one-step memory process, with its blinkered view of life, may be an intolerably crude model.

The presence of a second-order memory in lithological sequences is established in an analogous manner as the first. In this case, the null hypothesis is set that the character of the i + 2th lithology is adequately predicted on a Markov-1 model, given the character of the ith lithology. If the hypothesis is rejected, then a second-order memory is proved that has a control over and beyond the first-order memory involved in the one-step linkages.

The observed population for this test was calculated by counting the various types of (i/i+2) pairs (reading from older to younger) and setting these out as a tally matrix in a precisely similar manner to the one-step transition tally matrix (tables 17 and 19). The Markov-1 prediction model was calculated by squaring the one-step transition probability matrix. The resulting cell values represent the predicted probabilities of the various types of (i/i+2) pairs. These were converted to a predicted tally population by multiplying through by the row totals of the observed population (tables 18 and 20). The observed tally matrix was tested against the null hypothesis matrix as a chi-square contingency table.

The chi-square test values were as follows:

G 1

	A	M	B	C	Y
A	60	27	31	25	20
M	21	14	2	11	9
B	19	15	95	14	58
C	37	1	12	28	26
Y	25	0	60	26	15

G 2

117	25	33	25	24
25	4	8	4	4
31	4	85	15	71
20	8	17	12	23
31	4	63	24	16

G 3

113	23	25	26	14
18	8	3	10	3
23	4	86	16	75
23	8	15	22	21
24	0	75	15	18

Table 17 TWO-STEP TRANSITION TALLY MATRICES FOR SUB-GROUPS OF SHALY GROUP (G)

		A	M	B	C	Y
G 1	A	63	30	33	23	14
	M	24	6	9	11	7
	B	28	16	94	19	44
	C	33	6	17	24	24
	Y	17	2	54	24	31
G 2		121	27	32	26	18
		26	3	6	5	5
		28	8	94	20	55
		25	3	21	11	19
		27	2	57	20	33
G 3		98	26	30	32	15
		21	4	4	9	4
		29	7	100	14	54
		32	6	16	17	18
		18	2	58	17	37

Table 18 TWO-STEP TRANSITION TALLY MATRICES EXPECTED FOR SUB-GROUPS OF SHALY GROUP (G) IF THEY REPRESENT A PURE MARKOV-1 PROCESS

		A	M	B	C	K	Y
H1	A	69	30	50	39	8	17
	M	9	6	15	25	1	6
	B	52	16	148	25	5	82
	C	45	4	18	81	2	78
	K	5	0	2	11	0	3
	Y	32	7	94	48	4	13
H2		78	23	49	38	12	26
		20	6	11	11	1	4
		47	12	119	31	5	58
		44	4	20	45	5	60
		13	0	3	10	1	7
		25	7	70	44	9	16
H3		125	21	51	47	10	34
		10	4	7	13	1	5
		52	8	166	23	8	80
		56	3	25	57	5	48
		9	1	1	12	2	12
		35	3	87	43	11	16

Table 10 TWO-STEP TRANSITION TALLY MATRICES FOR SUB-GROUPS OF SANDY GROUP (H)

		A	M	B	C	K	Y
	A	65	24	58	44	4	18
	M	18	3	15	17	1	9
H1	B	60	19	135	34	6	54
	C	50	10	26	80	4	58
	K	4	1	2	8	0	6
	Y	25	3	72	48	5	45
		81	23	53	41	7	22
		19	2	13	9	1	7
H2		50	15	115	34	9	47
		44	8	30	47	8	40
		9	1	5	9	2	9
		29	3	60	39	7	33
		111	23	62	59	11	21
		15	2	9	9	1	4
H3		61	9	164	27	8	67
		55	6	29	55	7	42
		12	1	4	11	1	8
		30	2	74	36	7	46

Table 20 TWO-STEP TRANSITION TALLY MATRICES EXPECTED FOR SUB-GROUPS OF SANDY GROUP (H) IF THEY REPRESENT A PURE MARKOV-1 PROCESS

Shaly Group (G)

G1.	50.9
G2.	37.1
G3.	46.9

Number of degrees of freedom = 16

For 16 df, the tabulated chi-square value at ∝ 0.01 = 32.0

Sandy Group (H)

H1.	94.0
H2.	59.3
H3.	61.7

Number of degrees of freedom = 25

For 25 df, the tabulated chi-square value at ∝ 0.01 = 44.3.

For two-step transitions, values appear on the main diagonal, so that the number of degrees of freedom expand to 16 in the Shaly group, 25 in the Sandy group. In all tests, the hypothesis of a pure Markov-1 model was rejected and so the presence of a second-order memory accepted as statistically significant.

As in the case of a first-order model, the geologist is interested in what a second-order memory represents in terms of rock ordering. This is not readily appreciated from a study of the two-step matrices, as these are composed solely of (i) and (i+2), without the intervening (i+1) lithology. First-order transition types were extracted by independently testing transition pairs. This method can be extended to second-order memory, by testing the actual occurrence of transition trios against their predicted occurrence on a purely first-order memory model. The observed population was derived by counting the number of the various permutations of transition trios occurring in the sequence. A prediction model was calculated by multiplying the two transition probabilities involved in each permutation, to obtain a two-step probability, which was then multiplied by the appropriate row total on the observed tally matrix to give a prediction value. Each permutation was then tested as a chi-square distribution with one degree of freedom in the same manner as used in testing individual transition pairs. The results of the tests were designated +, - or 0, according to the convention already described, and these were tabulated for the Shaly and Sandy groups (tables 21 and 22).

The conclusions that can be immediately derived from an inspection of these results are:

(1) the possible second-order memory involved in most trios is insignificant;

and (2) those trios that do have some degree of second-order memory control are almost always those that have the rootlet horizon (Y) as first or third member. If Y is the first member then the positive trio is usually one of coarsening-upwards character; if the third member, the trio is usually one of fining-upwards nature.

Combining these conclusions with the observations of first-order transitions, it can be reasoned that the two-step model that attempts to describe these coal measure sequences is one of predominantly one-step memory with two-step memories immediately pre- and post-rootlet horizons.

The use of 'terms'

A transition scheme that illustrates both first and second-order memories (a diagramatic representation of a second-order

ABA	0	MBY	0	CYB	0
ACA	0	MCY	0	CAC	0
AYA	0	BCA	0	CMC	0
ABM	0	BYA	0	CBC	0
ACM	0	BCM	0	CYC	0
AYM	0	BYM	-	CAY	0
ACB	0	BAB	-	CMY	0
AYB	0	BMB	0	CBY	0
ABC	0	BCB	0	YBA	+
AYC	0	BYB	0	YCA	0
ABY	+	BAC	-	YBM	0
ACY	-	BMC	0	YCM	0
MBA	0	BYC	0	YAB	+
MCA	0	BAY	+	YMB	0
MYA	0	BMY	0	YCB	0
MBM	+	BCY	0	YAC	+
MCM	0	CBA	0	YMC	-
MYM	0	CYA	0	YBC	0
MCB	0	CBM	0	YAY	-
MYB	0	CYM	0	YMY	0
MBC	0	CAB	0	YBY	-
MYC	0	CMB	0	YCY	0

Table 21 SHALY GROUP (G). CUMULATIVE RESULTS CHI-SQUARE TESTING OF INDIVIDUAL TRIO SEQUENCES FOR SECOND-ORDER MEMORY PROPERTIES (SEE TEXT)

ABA	0	MBC	0	CYA	0	KMK	0
ACA	0	MYC	0	CBM	-	KBK	0
AKA	0	MBK	0	CYM	0	KYK	0
AYA	0	MYK	0	CAB	-	KAY	0
ABM	0	MBY	0	CMB	0	KMY	0
ACM	0	MCY	0	CYB	0	KBY	0
AKM	0	MKY	0	CAC	0	YBA	0
AYM	0	BCA	0	CMC	0	YCA	0
ACB	-	BKA	0	CBC	0	YKA	0
AKB	0	BYA	0	CYC	0	YBM	+
AYB	0	BCM	0	CAK	0	YCM	0
ABC	-	BKM	0	CMK	0	YKM	0
AYC	0	BYM	-	CBK	0	YAB	+
ABK	0	BAB	-	CYK	0	YMB	0
AYK	+	BMB	0	CAY	+	YCB	0
ABY	0	BCB	0	CMY	0	YKB	0
ACY	0	BKB	0	CBY	+	YAC	+
AKY	0	BYB	0	KBA	0	YMC	0
MBA	-	BAC	-	KYA	0	YBC	0
MCA	0	BMC	0	KBM	0	YAK	+
MKA	0	BYC	0	KYM	0	YMK	0
MYA	0	BAK	0	KAB	0	YBK	0
MBM	0	BMK	0	KMB	0	YAY	-
MCM	0	BYK	0	KYB	0	YMY	0
MKM	0	BAY	+	KAC	0	YBY	-
MYM	0	BMY	0	KMC	0	YCY	-
MCB	0	BCY	0	KBC	0	YKY	0
MKB	0	BKY	0	KYC	0		
MYB	0	CBA	0	KAK	0		

Table 22 SANDY GROUP (H). CUMULATIVE RESULTS OF CHI-SQUARE TESTING OF INDIVIDUAL TRIO SEQUENCES FOR SECOND-ORDER MEMORY PROPERTIES (SEE TEXT)

TERMS OF POSITIVE SIGNIFICANCE

ABA AYA AYM MBA MYM
MBC BCB BAY CBA CBC
CAY YAB YMB YMC YMY

INSIGNIFICANT TERMS

ACB AYB ABC MCA MBM
MCM MCB MBY MCY BCA
BYM BAB BMB BMC CBM
CYM CAB CAC CBY YBA
YCB YAC YBC BCY

TERMS OF NEGATIVE SIGNIFICANCE

ACA ABM ACM AYC ABY
ACY MYA MYB MYC BYA
BCM BYB BAC BYC BMY
CYA CMB CYB CMC CYC
CMY YCA YBM YCM YAY
YBY YCY

<u>Table 23</u> SHALY GROUP (G)♂ STATUS OF TERMS TESTED AGAINST THEIR THEORETICAL OCCURRENCE SET BY AN INDEPENDENT-EVENTS MODEL

TERMS OF POSITIVE SIGNIFICANCE

AYA AYM AKB AYK MBC BYM
BCB BAY CBA CBC CAY CBY
KBA KBC KAY YAB YMB YKB
YMC YAK

INSIGNIFICANT TERMS

ABA AKA AKM ACB AYB ABC
AYC ABK MBA MCA MKA MBM
MCM MKM MYM MCB MKB MBK
MYK MBY MKY BCA BKM BMB
BKB BAK BMK BYK CYM CMC
CMK CBK KBM KYM KAB KMB
KAC KMC KAK KMK KBK KYK
KMY KBY YBA YKA YBM YKM
YCB YAC YBC YMK YBK YMY
YKY

TERMS OF NEGATIVE SIGNIFICANCE

ACA ABM ACM ABY ACY AKY
MYA MYB MYC MCY BKA BYA
BCM BAB BYB BAC BMC BYC
BMY BCY BKY CYA CBM CAB
CMB CYB CAC CYC CAK CYK
CMY KYA KYB KYC YCA YCM
YAY YBY YCY

Table 24 SANDY GROUP (H). STATUS OF TERMS TESTED AGAINST THEIR THEORETICAL OCCURRENCE SET BY AN INDEPENDENT - EVENTS MODEL

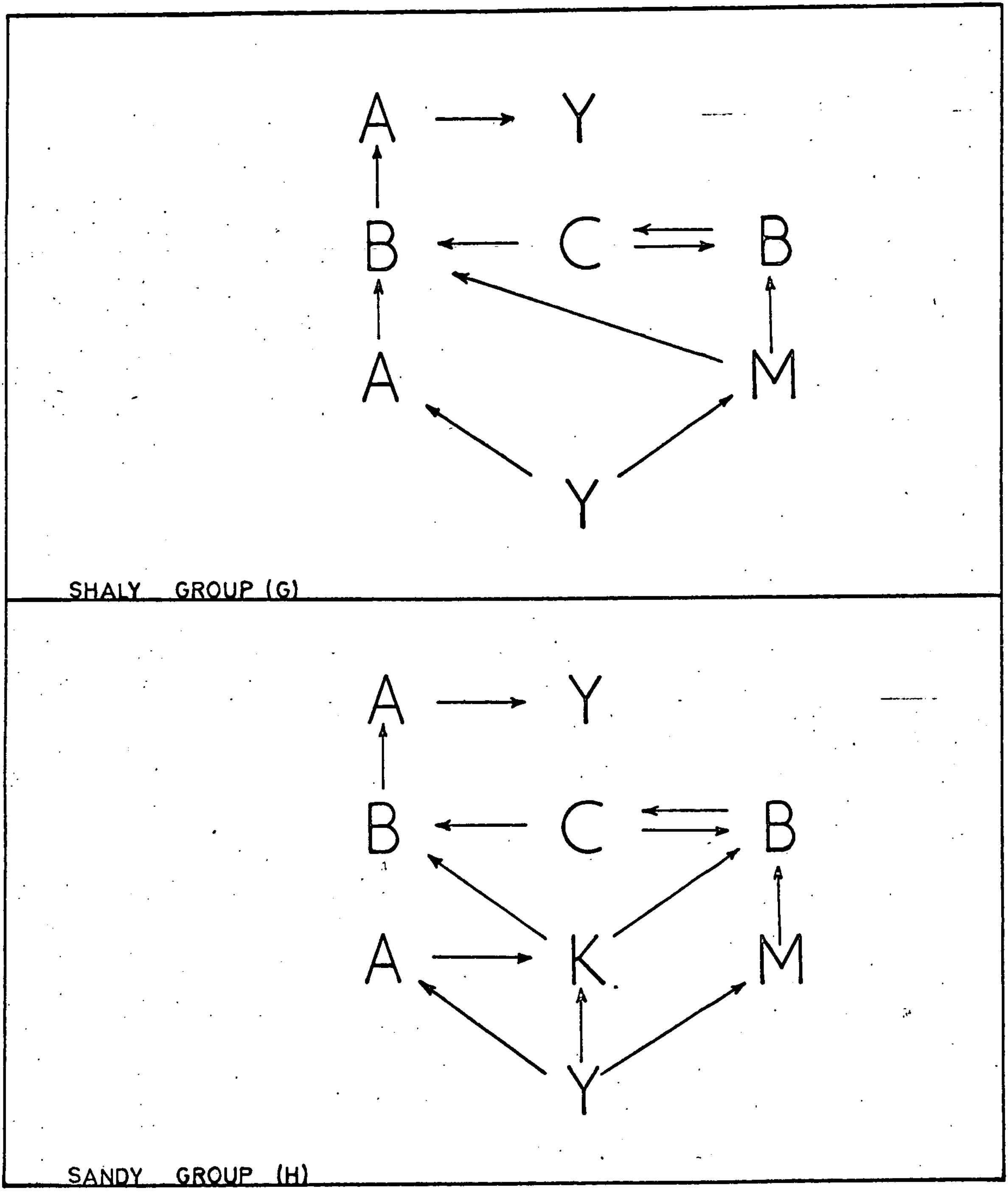


Fig. 34 Term Transition Schemes

model) can now be attempted. This could be done by modifying the one-step transition diagram by the incorporation of positively significant second-order memory elements. A more attractive method is to test the various permutation trios against their occurrence as predicted on an independent-events model, and fit those of positive significance in a transition scheme that simultaneously incorporates both one and two-step memories. The procedure that was used in the extraction model set as independent-events rather than Markov-1.

The trios that have positive significance in these tests can be viewed either as products of first and/or second-order memory elements, or merely as rock groups of three that have a higher occurrence than would be expected randomly. This latter concept roughly coincides with the 'term' of Phillips (1836). The use of terms in the construction of transition diagrams introduces a greater precision, in that the terms can be dove-tailed together in a continuous chain that has less ambiguity than the crude one-step transition diagram. The statistical test result tables for terms of the Shaly and Sandy groups are shown in tables 23 and 24, while the term transition schemes are shown in Fig.34.

Markov Models as Cycle Predictors

The structure of the transition schemes is broadly that of a flow diagram, and it can be reasonably argued that the shortest path from one point to another is likely to be of more frequent occurrence than longer paths. (This is true broadly speaking, providing allowance is made for terms which though statistically significant in their content are infrequent in occurrence). Modal cycles (in the sense of Duff and Walton, 1962) would be predicted from the transition schemes as the following (ordered in frequency):

Shaly Group (G)

M	(Shale)
MBA and ABA	(Shale - Siltstone - Shale)
MBCBA	(Shale - Siltstone - Sandstone - Siltstone - Shale)

Sandy Group (H)

MBCB	(Shale - Siltstone - Sandstone - Siltstone)
KBCB	(Thick Sandstone - Siltstone - Sandstone - Siltstone)
MBCBA	(Shale - Siltstone - Sandstone - Siltstone - Shale)

In Duff and Walton's analysis of the Pennine Coal Measures, modal cycles were:

A	(Shale)
ABA	(Shale - Siltstone - Shale)
AmA	(Shale - Siltstone and Sandstone - Shale)

The broad similarity between the predicted model types and those of actual occurrence (admittedly in another coalfield) carries the implication that a Markov-2 model may be an adequate predictor of cycle types and frequencies. This is not a foregone conclusion, as a model of this type has only a limited amount of information at its disposal (the probabilistic occurrence of terms), while higher order memories peculiar to cycle formation may be present. The possibility of such higher order memories is touched upon by Krumbein (1967) p.9 in his consideration of the problem of the production of distinctively well-spaced marker horizons in simulated stratigraphic sections.

Accordingly, the question whether Markov models would produce realistic cycles was treated in more detail. The borehole sections used in this study were analysed for their content of cycles using the criteria set by Duff and Walton (1962). They selected the coal (or where absent, the top of a seatearth) as the definitive boundary for their cycles and this practice has been adhered to for the following reasons:

(1) the growth of vegetation represents the only consistently recognisable discontinuity in a record of clastic sedimentation seemingly devoid of any diagnostic horizons of more than purely local significance. (The "marine" bands provide the only exception to this remark, but these are usually too infrequent to be practicable as boundaries).

(2) on a second-order model the state Y (rootlet horizon) has a strong character in its placing in lithological sequences unlike the somewhat transient appearance of the other states. Y usually marks the end of one second-order memory link and the beginning of another, which passes upwards into a network of one-step memory linkages before terminating in the second-order memory link immediately preceding the next occurrence of Y.

The minimum thickness of cycles recorded was set at two feet in order to be consistent with cycles predicted by the various mathematical models. The number of states defining each cycle was reduced to four:

A = Shale (combined A and M)
B = Siltstone
C = Sandstone (combined C and K)
Y = Rootlet horizon

The reasons for this were firstly to reduce the enormous variety of permutations of six-state cycles to a distribution of manageable size, and secondly to facilitate comparison with cycles recorded by workers in other coal measure sequences.

The cycles recorded were plotted in the form of a histogram distribution (Fig.35) grouped as permutations in sets of n-member cycles, with the height of column equal to the number counted for each permutation. Inspection of this distribution shows that the modal cycles present in Ayrshire coal measure sections are (in order of frequency):

A
ABA
AB
BA
B
ABCB

These modal types are similar to those observed by Duff and Walton in their studies, indicating local sedimentational controls of broadly similar character.

Mathematical prediction models of cycle occurrence

Mathematical models of various types were computed by use of the programmes ONE-STEP CYCLE and TWO-STEP CYCLE (Appendix G). For Independent-Events and Markov-1 models, the input took the form of a lithological state transition probability matrix as well as the total number of cycles to be generated (made equal to the number of the observed population). In the case of an Independent-Events model, these probabilities were dictated by the proportional occurrence of the states, while for the Markov-1 model, they were the one-step transition probabilities registered on the sequence. The generation of a second order Markov model was achieved by a simple extension of this principle. (See Appendix G for fuller details). The programmes were each independently applied to Shaly and Sandy group data, and the results summed in cumulative distributions.

The performance of these models as predictors of the population of cycle types can only be assessed somewhat qualitatively, as numerical tests would be difficult to apply meaningfully. One reason for this is that the basic data for each model consists of two transition matrices which are only a crude representation of the 'real' transition matrix whose component cells are continuous distributions rather than discrete values. If a model is successful, a good qualitative and loosely quantitative fit is to be expected. There is also the problem of applying a statistically valid test to a very irregular distribution of this kind.

(i) Independent-events model 'cycles'

It will be recalled that the presence of 'modal cycles' does not, in itself, preclude an underlying randomising process. Accordingly, a prediction model based on an independent-events process was generated and is shown in Fig.35. This distribution can be most easily conceived as the 'background noise' in much the same sense as the background of X-ray diffraction traces, which are essentially functions of the machine rather than the mineralogical

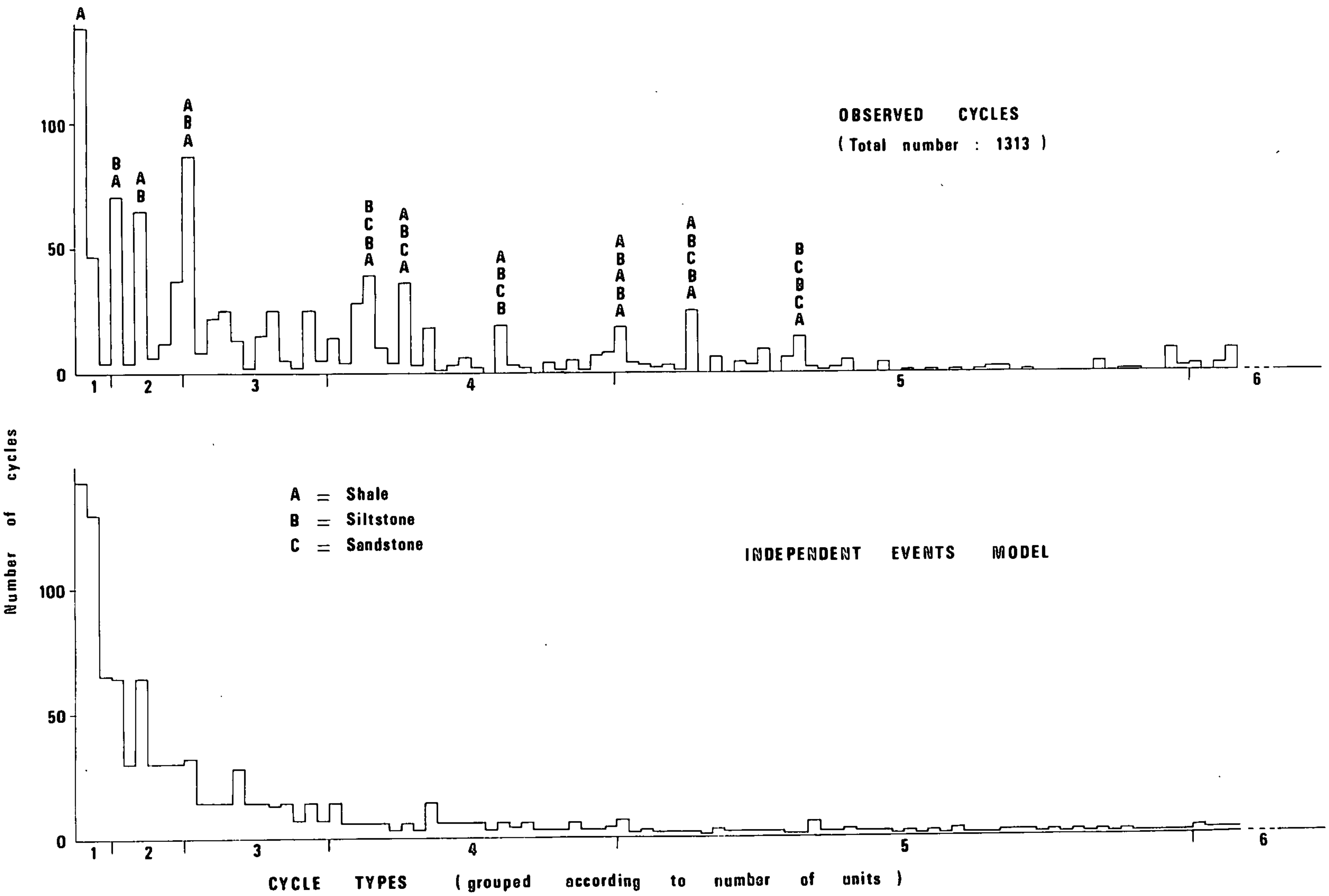


Fig. 35 Cycle Type Frequency Histograms

composition of the analysed sample. The significant deviations of the actual cycle distribution from this background are the expression of processes of a non-random character. Statistical techniques to extract diagnostic non-random cycles by some 'peak to background ratio' method would be of complex and dubious character. Nevertheless, a visual comparison of the actual cycle distribution with its randomised background leads to the following conclusions:

(1) The modal cycles are almost all coincident with major positive deviations of the observed distribution with its background, with the exception of the modes A and BA;

(2) The total of each class of independent-event cycles with the same number of members decreases in an exponential fashion from one member upwards for the independent-events model, whereas for the actual distribution, the number increases to a maximum for three-member cycles, from which it declines. (This relation is shown in Fig.37).

These two observations suggest that one-member cycles are discouraged in nature (at the two-foot level) and that the dominant occurrence of pure shale cycles is more apparent than real. The systematic process that underlies cycles aims for the production of cycles of slightly more complex history of intermediate (3 member) rather than great length. The nature of this history as demonstrated by the character of significant positive deviations, has the overall theme of fine - coarse - fine.

(ii) Markov-1 model cycles

Using one-step transition probability matrices, a cumulative cycle distribution was calculated as that predicted by a Markov-1 model and plotted on the same convention as the other cycle distributions (Fig.36). Inspection of this distribution shows strong qualitative agreement with the observed distribution with regard to the character of the modal cycles. Quantitatively, the fit is fair, with the notable exception of the prediction of an excessive number of pure shale cycles. This disagreement emphasises the short-sighted character of a one-step memory as a sequence predictor, in that the strong memory for first-member shales and shale seatearths results in the prediction of a disparitly large number of pure shale cycles. In the natural situation, a first-member shale will more often tend to initiate a more complex cycle than terminate immediately as a seatearth. This reinforces the suggestion that the underlying systematics tends to aim for cycles of intermediate length.

(iii) Markov-2 model cycles

The cumulative distribution for this model is shown in Fig.36. This distribution is broadly similar to that of the Markov-1 model in its estimates of modal types. Deviations from the Markov-1 model are qualitatively minor, and this is explained by the dominantly one-step memory dictated nature of rock ordering, with the exception of second-order modification in the vicinity of seatearths. The accurate prediction of one-member cycles is a function of its perfect memory for them, as these are rock terms of three members.

Closer comparison of the model histograms indicates that for certain parts of the object population, the Markov-1 model is a

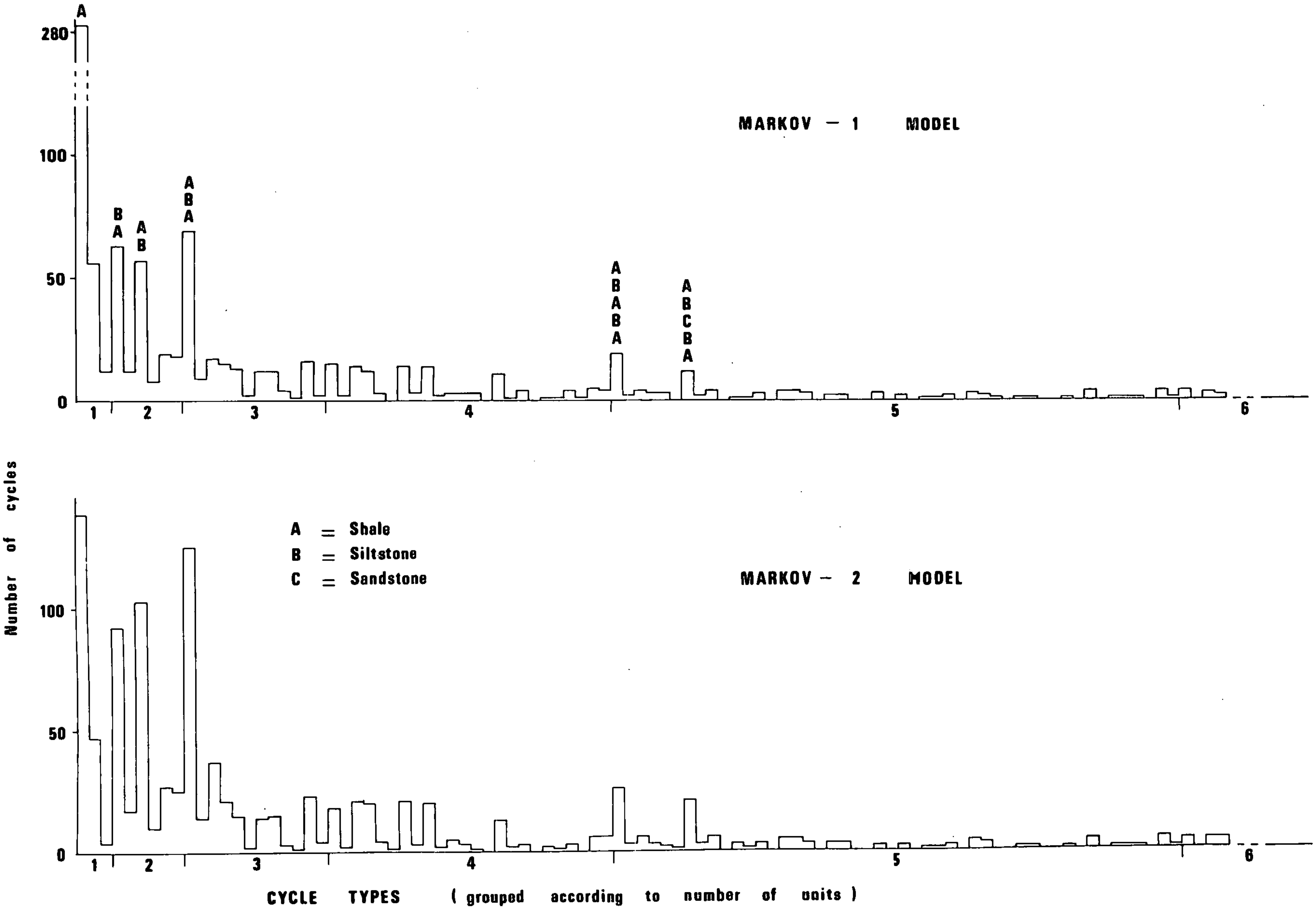
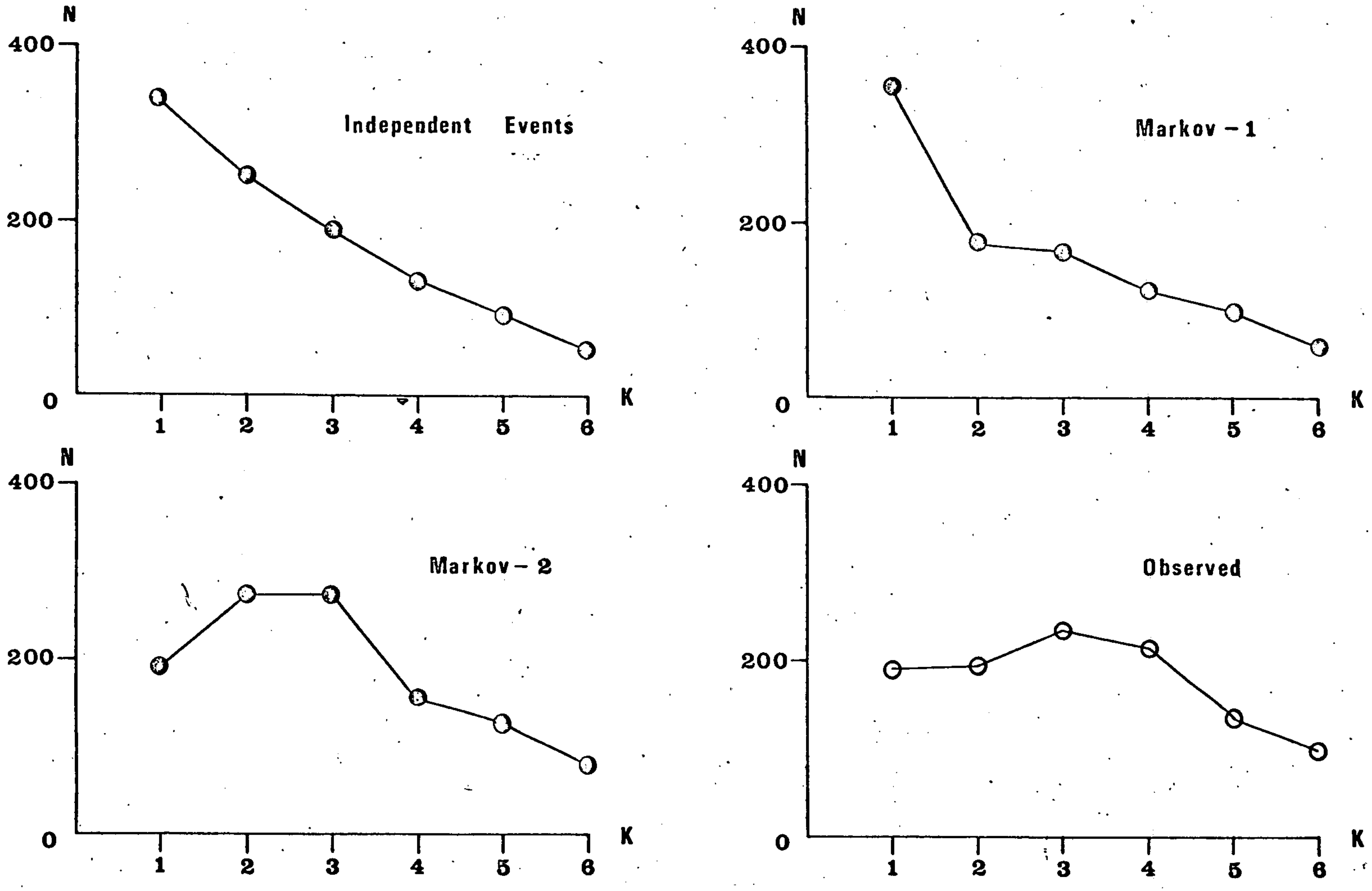


Fig. 36 Cycle Type Frequency Histograms



N = number of cycles ; K = number of units in cycle

FIG. 37 NUMBERS OF UNITS IN OBSERVED AND MODEL CYCLE DISTRIBUTIONS better frequency predictor than that of the Markov-2, and vice-versa in other parts. Accordingly, Markov-1 and Markov-2 models were matched in their power to predict the 'correct' number of each cycle type and the results tabulated. Where the Markov-2 model provided a better estimate, the result was designated +, while an equal or poorer estimate was marked as 0 or -, respectively. The scores were summed in the table below.

NUMBER OF MEMBERS IN CYCLE	+	0	-
2	1	0	5
3	5	2	5
4	12	8	4
5	9	30	9
6	10	74	12

The broad trend of this table indicates that the Markov-1 model is a better predictor of short-length cycle occurrence (other than one member), a worse one for those of intermediate length, and of equal power with a Markov-2 model in estimating long cycle frequencies. (The increasing proportion of zero values with length of cycle is a reflection of the greater likelihood of low sample numbers). This pattern is interpreted as mainly a function of the ideal situation where a cycle is bounded by second-order property terms separated by sequences of essentially first-order character. For two-member cycles, the full development of second-order terms is inhibited and more accurately predicted as a product of first-order elements. For three or four-member cycles, the second-order terms become dominant, while for longer types, the first-order dictated cycle cores are increasingly important so that at this level there is a balance in the predicting power of Markov-1 and Markov-2 models.

The summary of conclusions that can be derived from these models are:

(1) The systematic pattern that underlies cycle formation aims for a cycle of intermediate length (in the region of three members).

(2) The character of this pattern is broadly one of fine to coarse to fine in clastic sedimentation.

(3) The pattern is dominated by a first-order memory, but with significant second-order control immediately preceding and following the occurrence of a vegetation horizon.

Prediction of Longer Sequences

A second-order model would appear to describe adequately lithological ordering for sequences of restricted length, and so such a model is an expression of the sedimentary environmental parameters responsible for the deposition of such sequences. Extension of this model as an accurate predictor of longer successions is impossible as, at this scale, the sequence departs from one dominated by purely local controls to one in which controls of climate, tectonism and long-term sedimentational factors in the basin and source areas become appreciable. The reality of these larger scale controls is evinced by the essential non-stationarity of transition matrices, so that at various points through time there is a change in the dominant rock type, not wholly accounted for by the random fluctuations from the probabilistic core of the small-scale Markov model. Therefore, a model that would satisfy coal measure sections on a zonal or larger scale would have more complex parameters, whose controls would be on two scales, the larger, supposedly climatic/tectonic/long-term sedimentational, and the smaller, local environmental. The preceding Markov models are purely the product of this smaller control.

Auxiliary Analysis

Before attempting to interpret the Markovian transition schemes in terms of their environmental significance, additional analysis was made of the internal variation of the states involved in these schemes. Each state can itself be treated as an independent system and the systematics of its internal changes studied, after sub-states have been defined by a suitable criterion. Ideally, this criterion should be of potential geological meaning. Such an analysis could only be very restricted for sequences derived from Ayrshire boreholes, in that information of a detailed geological character, such as nature of bedding, were of rare and sporadic occurrence. While crude criteria such as colour were common, these were held to be somewhat subjective and of doubtful value. Accordingly, analysis was limited to a study of the internal variation of the thick sandstones in terms of grain-size and the relationships between the thickness of coals and the lithological nature of their roofs and floors.

(1) Internal variation of thick sandstones

The states defined for grain-size variation were as follows:

O = Lithology other than sandstone
K = Conglomeratic sandstone
C = Coarse sandstone
M = Medium-grained sandstone
F = Fine-grained sandstone
A = Silty sandstone

	O	K	C	M	F	A	X
O/	-	22	18	24	15	2	9
K/	2	-	15	17	2	1	11
C/	3	6	-	37	4	4	11
M/	20	12	15	-	42	21	19
F/	17	3	6	21	-	20	13
A/	31	0	5	8	5	-	7
X/	17	5	6	22	12	8	-

i. Transition Tally Matrix

	O	K	C	M	F	A	X
O/	-	0.24	0.20	0.27	0.17	0.02	0.10
K/	0.04	-	0.31	0.36	0.04	0.02	0.23
C/	0.05	0.09	-	0.57	0.06	0.06	0.17
M/	0.15	0.09	0.12	-	0.33	0.16	0.15
F/	0.21	0.04	0.08	0.25	-	0.25	0.16
A/	0.55	0	0.09	0.14	0.09	-	0.13
X/	0.24	0.07	0.09	0.32	0.17	0.11	-

ii. Transition Probability Matrix

Table 25 GRAIN - SIZE VARIATION WITHIN SANDSTONES OF THICKNESS GREATER THAN TWENTY FEET (FOR SYMBOL KEY, SEE TEXT)

X = Uncharacterised sandstone.

The state X was defined to include those sandstone beds for which there were no grain-size designations. Each sandstone thicker than twenty feet was coded in its internal character, transition types counted and the transitions summed in a cumulative matrix (table 25i). The row and column representing X transitions were ignored, and the remaining matrix tested as a chi-square contingency table with 19 degrees of freedom. The test value was 156.6 which strongly exceeded the tabulated chi-square value at α 0.05 of 30.1. A first-order Markov process was hence shown as operating in the grain-size distribution of these sandstones. Examination of the contribution of individual cells to the test value yielded a quick estimate of the character of this process as being one of fining-upwards nature of the form:

K - C - M - F - A

It must be remembered that this is analogous to the 'composite sequence,' so that the placing of states is made in terms of their significant preference of positioning rather than their frequency of occurrence. Thus inspection of the transition probability matrix (table 25ii) shows that these sandstones are most commonly initiated by medium-grained lithologies that fine upwards. The raw internal variation of the coded data used for this model indicates a high variability that suggests that while fining-upwards is the overall theme, this is achieved largely by a storied repetition of this pattern.

(2) Vegetation Horizon (Y) expressed as Coal Thickness

Coals, as distinct from seatearth horizons, were previously ignored in Markovian process work for the reason that the well-known strong association of the two might unfairly bias the potential memory of the sequence as a whole. The separate consideration of coal eliminates any such bias. In this study, coals were subdivided into states on the criterion of thickness, and seatearths without any overlying coal considered as coals of zero thickness. The relation of coal thickness to the nature of its seatearth and the succeeding lithology were examined by a simple approach as follows:

(i) Coal and roof lithology

The nature of the roof was designated as either shale (A), siltstone (B), sandstone thinner than twenty feet (C), and sandstone thicker than twenty feet (K). Roof lithology types were counted for each thickness class of coal from the analysed borehole section data, and the numbers tabulated as table 26(i). These figures were converted into percentages for each coal class in table 26(ii). This shows a strongly systematic pattern in the relation between the character of the roof lithology with the thickness of the coal it overlies. The thicker the coal, the more fine-grained the succeeding lithology, so that, while all coals and even seatearths are preferentially overlain by shales, this tendency becomes increasingly likely, the thicker the coal. (The small sample of thick sandstones obscures any appreciable behaviour with regard to an underlying coal). The clear character of these relations was considered to make statistical tests unnecessary.

The study was extended to consider the character of the shales that overlie the different coal classes. Shales were subdivided

Coal Thickness (inches)	A	B	C	K
0 (seatearth only)	373	197	94	17
1 - 6	238	62	21	5
7 - 18	196	42	19	4
19 - 42	126	21	4	3
42+	44	2	1	1

(i) ROOF LITHOLOGY COUNTS

Coal Thickness (inches)	A	B	C	K
0 (seatearth only)	55	29	14	2
1 - 6	73	19	6	2
7 - 18	75	16	7	2
19 - 42	82	14	3	2
42+	92	4	2	2

(ii) ROOF LITHOLOGY AS o/o

A = shale / B = siltstone / C = sst.<20ft./ K = sst.>20ft.

Table 26 RELATIONSHIP BETWEEN THICKNESS OF COAL AND THE CHARACTER OF THE SUCCEEDING LITHOLOGY (ROOF)

Coal Thickness (inches)	M	A
0 (seatearth only)	139	234
1 - 6	70	168
7 - 18	74	122
19 - 42	71	55
42+	29	15

(i) ROOF SHALE COUNTS

Coal Thickness (inches)	M	A
0 (seatearth only)	37	63
1 - 6	29	71
7 - 18	38	62
19 - 42	56	44
42+	66	34

(ii) ROOF SHALE AS o/o

M = shale + F/W lamellibranchs / A = 'barren' shale

Table 27 RELATIONSHIP BETWEEN THICKNESS OF COAL AND CHARACTER OF SUCCEEDING SHALES

Coal Thickness (inches)	A	B	C
0 (seatearth only)	387	246	48
1 - 6	211	100	15
7 - 18	177	70	14
19 - 42	104	46	4
42+	38	9	1

(i) PAVEMENT LITHOLOGY COUNTS

Coal Thickness (inches)	A	B	C
0 (seatearth only)	57	36	7
1 - 6	65	31	5
7 - 18	68	27	5
19 - 42	68	30	3
42+	79	19	2

(ii) PAVEMENT LITHOLOGY AS o/o

A = shale / B = siltstone / C = sandstone

Table 28 RELATIONSHIP BETWEEN THICKNESS OF COAL AND PRECEDING LITHOLOGY (PAVEMENT) into states M and A according to whether they did or did not (respectively) contain non-marine lamellibranchs. The results are shown in table 27, from which it can be seen that the development of a lamellibranch fauna becomes increasingly likely the thicker the coal.

(ii) Coal and seatearth lithology

No seatearth was found as part of a sandstone thicker than twenty feet, and so the system of seatearth lithologies condensed to ABC. The numerical results (table 28) demonstrate that much the same relation applies as for roof lithologies. Thus while all coals tend to be underlain by a shale seatearth, the probability of this becomes greater with increasing thickness of coal.

Field character of sandstones

The demonstrably different character of thin sandstones (C) and thick (K) in their placing in rock sequences as shown in Markovian process studies, implies that they are representative of different facies. Interpretation of the type of facies they represent cannot be made on the crude criteria of thickness and grain-size variation alone, so that more information on their attributes is required. As such data is minimal in borehole records, field examination was made of a large number of sandstones in South Ayrshire, mainly of Lower and Middle Coal Measure age. Particular attention was paid to those sandstones that show the field relations that coincide with the ordering shown in the Markov transition schemes (Fig.34). Reference to these schemes shows that the optimum placing of thin sandstones is one of initiation and alternation with siltstones, leading to the development of a seatearth. Contrasted with this, thick sandstones significantly tend to be near the base of cycles, underlain either directly by the vegetation horizon or the barren shales immediately following it, and then fine upwards directly to a shale seatearth, or indirectly through an alternation of siltstones and thin sandstones.

'Thick' sandstones

While numerically of less frequent occurrence than thinner sandstones, this group makes up for this in the wealth of its internal characters. Their field-relations are summarised as follows:

Geometry

Usually elongate belts or pods with lensoid cross-sections; sometimes sheet-like developments.

Sequence characteristics

Tend to be floored by dark shales or coal; pass upward into interbedded siltstones and thin sandstones.

Basal contact

Sharp, essentially concordant and sometimes showing washout and flute-cast structures.

Upper contact

Ill-defined.

Grain size

Upper part

Usually fine.

Middle part

Sometimes coarse, usually medium or fine.

Lower part

Coarse or medium; often with basal conglomerate lag of ironstone and siltstone pebbles and log cas

Bedding characters

Upper part

Flaggy beds, internally showing parallel and ripple-drift lamination; rib and furrow.

Middle part

Small scale trough and planar cross-sets as well as irregular flaggy layers.

Lower part

Medium to large-scale trough (and to lesser degree planar) cross-sets; sometimes as massive.

Fauna

Middle and Upper parts

Rare burrows and tracks.

Lower part

Nil.

Flora

Upper part

Common small plant fragments as well as leaves and twigs often orientated in parallelism.

Middle part

Sporadic comminuted fragments.

Lower part

Basal lag branches and trunks; small lenticular coal rafts.

Illustrative Plate

Plate 1.

Sandstone bodies of extremely similar character have been described in coal measure basins all over the world and almost invariably interpreted as the deposits of channels (e.g. Busch (1954), Wanless (1955), Mudge (1956), Potter and Glass (1958), Jablokov, Botvinkina and Feofilova (1961), Clarke (1963), Bluck and Kelling (1963)). However, there is difference in opinion on the origin of the channel fill ranging from marine (tidal channels) through marine alluvial (aggradation of alluvial channels by rise in sea level) to purely alluvial (river channels). In the context of Ayrshire, deposits of the latter types are favoured by the seemingly overwhelmingly freshwater (or possibly brackish) character of the adjacent sediments and the close similarities of internal characters with those of modern river channels.

'Thin' sandstones

This group covers the thickness range between one and twenty feet and is inevitably the product of a spectrum of sedimentary environments, if the coal measures are representative of any reasonable degree of sedimentary facies complexity. However, the transition character of the thin sandstones shown in Markovian work must largely represent the majority of this type. As the thickness distribution of sandstones was found to have a broadly exponential form, declining with thickness, this majority is confined to the 'thinner end' of the distribution. Thus taking thin sandstones alone, those of three feet or less were found to constitute 71% of the whole in the Shaly group, 59% in the Sandy group. Therefore the transition behaviour of the state C mainly represents thin sandstones of this order, while sandstones in the 4 to 20 feet range have transitional properties between this and the state K. Accordingly, generalisations from field observations of thin sandstones were divided into two thickness classes, bearing in mind that those peculiar to the thinner class were more typical of the state C.

Sandstones, thickness 1-3 feet

Geometry

Broadly sheet-like

Sequence characteristics

Usually interbedded with muddy siltstones (or sometimes silty mudstones).

Basal contact

Most commonly sharp, concordant; base planar or rippled.

Upper contact

Often gradational; if sharp, sometimes showing rippled surface with straight crests.

Grain size

Fine to very fine; coarser towards base.

Bedding characters

Often structureless at base, but showing cross, ripple or parallel lamination towards top. Occasional small-scale cross bedding.

Fauna

Nil.

Flora

Finely comminuted plant material common; sometimes leaves and twigs, occasional rootlets.

Sandstones, thickness 4-20 feet

Geometry

Sheets, pods or elongate bodies.

Sequence characteristics

Separated by thin developments of dark sandy shales and siltstones.

Basal contact

Usually sharp, concordant; occasional washout structures.

Upper contact

Usually fairly sharp; planar or rippled surface (straight or, less commonly, lingvoid crests).

Grain size

Fine to medium; either broadly homogeneous or coarsening towards base.

Bedding characters

Often massive, particularly in lower part, or flaggy; otherwise showing cross-bedding decreasing in scale upwards.

Fauna

Rare burrows at base.

Flora

Sparse comminuted plant material (more common in intervening lithologies).

Illustrative plate

Plate 2.

The arbitrary boundary of twenty feet separating these from 'thick' sandstones means that there must be a gradation in properties between the two states. The resulting overlap means that many C sandstones (particularly the thicker ones) must represent channel deposits, and field observations of channel-cut structures support this view. The rest are probably the products of environments peripheral to the channel network, so that some are possibly levee and crevasse-splay sediments, while others representative of outer parts of levee areas, floodbasins and more remote parts of the alluvial plain.

A Model for Ayrshire Coal Measure Deposition

Attention has long been directed at the deltaic model as a suitable process to produce the lithological and palaeontological attributes of carboniferous coal-measure sequences in the northern hemisphere. The characteristic interdigitation of sediments of marine and non-marine character in these formations points to an environment at the continental/marine boundary. Much of the sediment would appear to be of non-marine character, derived directly from an inland source area, resulting in a broadly fresh-water environment punctuated at various times by marine conditions. The degree of this balance between marine and non-marine varies both according to the area and the age of the rocks studied within the coal measures, so that remarks directed to Ayrshire sequences have generalised, but not specific, application elsewhere. In Ayrshire, the influence of open marine conditions would appear to be relatively minor for the following reasons:

(1) the fauna found in the 'marine bands' is generally of a very restricted kind. Goniatites and other orthodox marine forms are rarely found, and the characteristic assemblage is one of dwarfed Lingula (often taken as an indicator of brackish water, particularly in the absence of diagnostic marine forms, e.g. Bennison (1961));

(2) almost all these marine bands are limited to the

lower part of the Lower Coal Measures and the upper part of the Middle (with the notable exception of the Queenslie [Katharina] Marine Band);

and (3) the areal distribution of the marine bands is often of local tongue-like developments rather than blanket occurrence, indicating a somewhat desultory marine transgression (see Mykura (1967), Fig.11).

These arguments against a pronounced direct marine influence are all based on palaeoecology, in the absence of any widely accepted geochemical criterion or recognition of exclusive sedimentary rock attributes of undisputed marine origin. However, it is possible that 'non-marine' lamellibranchs (and in particular, Naiadites) had some degree of salinity tolerance and that somewhat brackish conditions prevailed at various times (e.g. see Maclennan, 1943). This sweetness of water could be the result of large-scale dilution of sea-water by heavy discharge from the delta distributaries and/or a physical barrier from the open sea such as an offshore bar as suggested by Robertson (1948). Alternatively, it could be a simple function of distance from shore-face, so that for most of Coal Measure time, Ayrshire would be the site of a delta plain with the shoreline set outside the area.

The Ayrshire succession is therefore envisaged as deposition in primarily fresh-water or brackish conditions punctuated by infrequent phases of marine conditions of a limited character. In the context of a delta, this would favour interpretation to be directed at top-set delta plain deposits and to a lesser extent those of a delta front in which marine conditions played a restricted role.

Studies of the complex of environments to be found in deltas of the present day have been made on examples all over the world. The Mississippi is the most extensively investigated, though potentially not perhaps the best model. While the characteristics of each delta is to a large extent dictated by a combination of specifically local controls such as climate, shape of the depositional basin, offshore marine current configuration, and so on, they have many features in common, enabling meaningful generalisations to be made. For this study consideration is made of the delta plain and front environments, for reasons already explained.

Delta plain

In a typical delta, the topset plain consists of a mosaic of subenvironments which is complex in pattern and constantly changing in distribution character. It can basically be divided into a network of distributaries and minor channels separated by areas of 'wet lands,' 'dry lands,' and open bodies of water. These channels vary from straight to highly sinuous in plan configuration and carry the coarser fraction of the sediment from the source area towards the delta front. The network is dynamic rather than static, so that its distribution pattern changes in response to varying conditions in source supply and internal mechanisms of lateral erosion and accretion, crevassing, channel cut-off and so on. The channel complex thus migrates into the intervening areas, while its abandoned parts become incorporated into the environment of the interdistributory plain. The distributaries are normally lined by natural leeves built up from sediment deposited in overbank flooding and these often form the only significant topography of the delta plain.

The distributary banks may be breached at various points at times of flood, leading to the deposition of lobes of sediment from the channel (known as crevasse splays) into the peripheral floodbasins.

The areas that divide these drainage arteries usually consist of areas of open water or, where filled in, by marshes or swamps. The size of these bodies of water range from small ponds and pools to large lakes, of which some have drainage outlets while others have not. All have a tendency to fill with sediment and eventually become swamp or marsh areas (Fosberg, 1964). On the other hand, the formation of these lakes is usually "a stage in the deterioration or partial burial of the marsh" (Kolb and Van Lopik, 1966). It seems that there is an intricate interplay between the vegetational and open water environments, controlled by subsidence, drainage and other factors. Deposition in these areas is normally of very fine-grained and organic sediment except at those times when flooding in the distributary network manifests itself and coarser material is either directly flooded in or is carried by the rudimentary drainage patterns operative in the swamps and lakes.

Delta front

In this part of the delta, marine influence becomes apparent in an interchange of freshwater, brackish and marine environments in a regime of transitional character. The bodies of water contained in the areas separating distributaries are usually larger and more frequent and take the forms of bays and lagoons as well as lakes of varied salinity. Fauna and flora change to forms with appropriate salinity tolerances. At points where the distributaries discharge at the front, current velocity is reduced, and coarser material is deposited as distributary mouth bars, while the finer fraction is carried seawards. Coastal marine currents redistribute the coarser load along the margins of the delta front as offshore bars, beaches and allied morphological forms.

Results of the Markovian studies of Ayrshire Coal Measure sequences are constructed in terms of these two broad classes of environment.

Environmental Interpretation of Markovian Models

The transition schemes for the Shaly and Sandy groups (Fig.34) show a strong similarity, the only difference being the presence of thick sandstones in the Sandy group and the significant occurrence of shale-siltstone-shale (ABA and MBA) terms in the Shaly group. The two schemes can thus be combined in the generalised plan of Fig.38. Examination of the structure of this diagram is made by analysis of the terms from which the two schemes are constructed. These terms can be envisaged as 'memory elements' that possess indigenous first and second order Markovian properties. The terms are considered in grouped form as to their environmental significance.

(1) Cycle boundary terms.

The elucidation of the events that lead to the termination of one cycle of clastic sedimentation, colonisation by vegetation and the renewal of normal deposition in the following cycle are fundamental to the explanation of coal measure cyclic phenomena. Lithological variation within the cycle is a less controversial field for which mechanisms of conventional sedimentary control are usuall

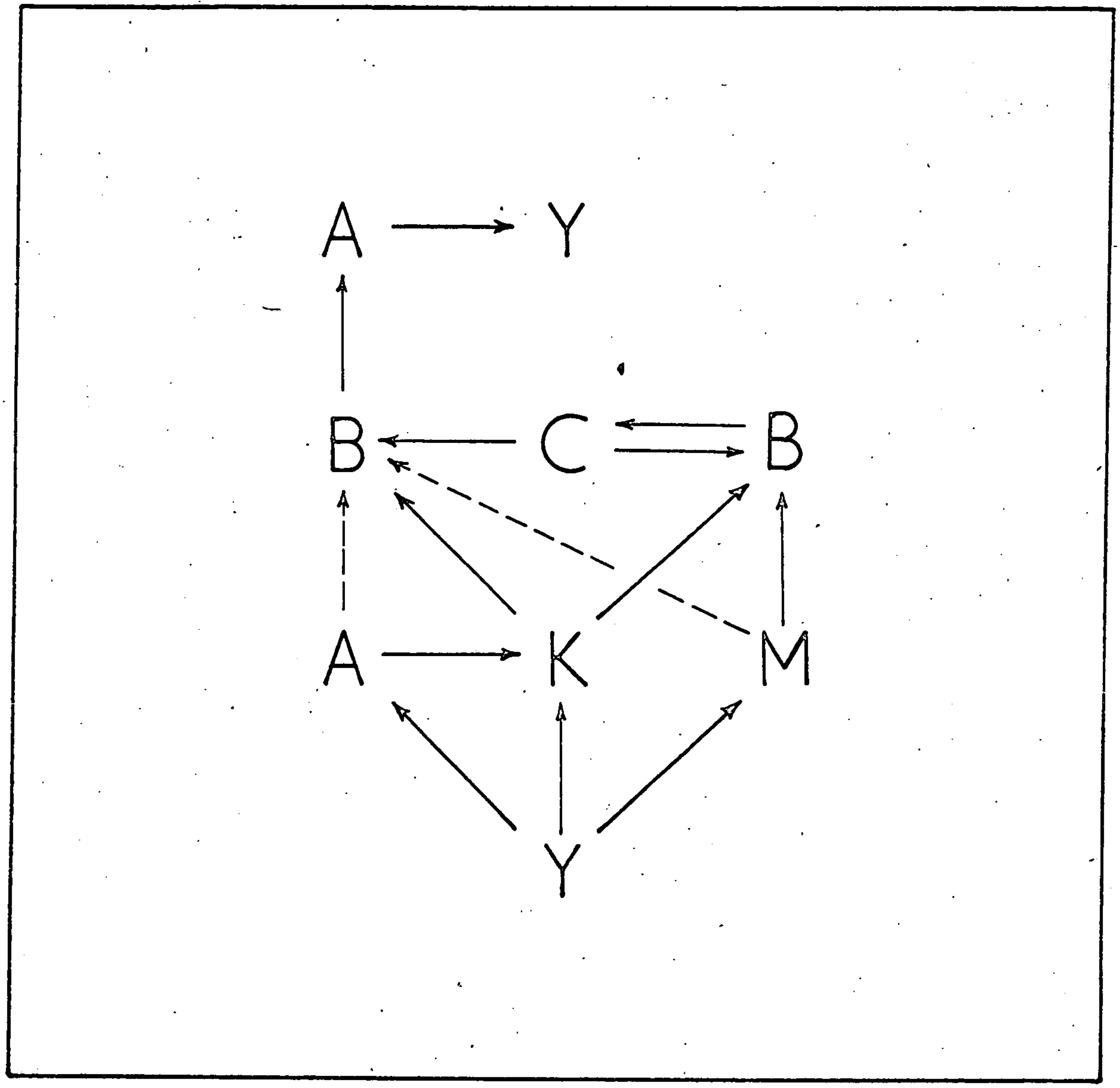


Fig. 38 Combined Term Transition Scheme for Shaly and Sandy Groups (Solid arrows - applicable to both groups ; broken arrows - for Shaly Group alone.)

postulated. However, particularly in the case of the initiation of a new cycle, theories have ranged from sudden subsidence, induced by tectonics (Bott, 1964) or compaction (Van der Heide, 1950), to sudden rise in sea level, perhaps glacially controlled (Wanless and Shepard, 1936), breakdown in beach bar (Robertson, 1952), and other mechanisms of a relatively catastrophic nature.

The terms representative of this phase of cyclic development are those that contain the vegetation horizon (Y) as a component state. With regard to Markovian properties, this group has distinct differences with those of other lithological terms. It has previously been mentioned that second-order memories exhibited in the rock sequence are almost all confined to those terms in which the state Y is the first or third member. Thus, of fourteen rock terms of positive second order memory character drawn from the analysis of the Shaly and Sandy groups, twelve are of this type. The inference that can be drawn from this is that the deposition that immediately precedes and follows colonisation by vegetation (that may be represented as a coal or merely a seatearth) is of 'programmed' character as opposed to the more short-term nature of the first-order memory that dominates the lithological ordering of the more central parts of cycles.

(i) Terms (1.2.Y)

Examination of the terms with Y as third member (those of the seatearth regime) shows that the significant composition of this type is mainly one of a fining-upwards sequence, those drawn from the Sandy group being of a coarser character than those of the Shaly group. The development of lithologies immediately preceding the colonisation by vegetation and formation of seatearths has been a matter for speculation for many years, involving as it does the possibility of vegetationally-controlled sedimentation and geochemical and mechanical reworking of the substrate. Research (partly for economic reasons) has been mainly directed at the clay mineralogical variation of these interesting rocks. This has been centred to a large degree on the problem of whether such clay minerals are produced by post-depositional leaching and plant-root activity or by deposition of materials altered outside the depositional basin. Thus while Stout (1923), Huddle and Patterson (1961) and others advocate the former theory, supporters of the latter include Grim and Allen (1938), Schultz (1958) and Wilson (1965). However, while these authors have their differences regarding the development of the clay mineralogy of seatearths, their opinions regarding the overall sequence of events during their deposition have broad similarities. The observation of Stout that there is no consistent relationship between the thickness of a coal and the thickness of its seatearth is endorsed by most authors. From this, Stout, Wilson and Huddle and Patterson all argue that the vegetation that established roots in the seatearth and to a debatable degree altered its characteristics, took place in aerated conditions. This preceded a phase when conditions became progressively more stagnant, decay slowed, and an accumulation of peat allowed whose root systems were for the main part confined to the peat mass. The authors part company on the question of the extent of the geochemical effect of the primary vegetation so that Huddle and Patterson consider that this marks a phase of extensive leaching in acid swamp waters whereas Wilson holds that leaching is minor and that the growth of vegetation is largely incidental to the character of its "allocthonous" soil. Wilson notes that there is a decrease in quartz content moving upwards through the seatearth and, together with Schultz, postulates that this fining-upwards character is due to a progressive reduction in transporting capacity of the depositing medium. He ascribes this to the establishment of the primary vegetation which reduces the velocity of water currents (and hence grain size of the deposited sediment) until the circulation of water is restricted to the point of semi-stagnancy, when anaerobic conditions favour the accumulation of peat. Such a hypothesis is supported by Markovian model studies, firstly because the second-order memory elements point to a systematic fining-upwards in gradation of sediment and secondly, the virtual restriction of this type of memory to terms initiated or terminated by the state Y indicates a vegetational control of sedimentation.

The observation that there is a fairly close relationship between the thickness of a coal and the likelihood that it will be floored by a shale seatearth (Table 28) can be interpreted largely as a function of primary vegetation cover. If initial conditions favour a strongly successful development of this vegetation, then reduction of transported sediment to shale grade is more effective, and stagnancy encouraged with the prospect of correspondingly greater peat accumulation.

(ii) Terms (1.Y.3)

These terms express the relation (if any) between the character of the seatearth and that of the first member of the succeeding cycle. It has already been shown (Tables 26 and 28) that thicker coals have a greater tendency to be preceded and followed by finer-grained sediments (particularly shale) than thin coals, and so it would seem reasonable that there might be a second-order memory relationship between the states preceding the following Y of the Fine-Y-Fine, Coarse-Y-Coarse type. However, such a relationship appears to be virtually non-existent, as only two such terms have a significant second-order memory, so that the character of the group as a whole is described by the two one-step memory links they represent.

The two exceptions are the terms BYM (negatively significant in both Shaly and Sandy groups) and AYK (positively significant). The first implies that there is a preference against coals with siltstone seatearths being succeeded by lamellibranch-bearing shales. This is presumably an amplification of the already established relationship that thick coals have a greater tendency to be floored by shale rather than siltstone seatearths and are more often succeeded by fossiliferous shale.

The explanation of the positive AYK term dwells more in the realm of speculation. While inspection of other terms shows that thick sandstones tend to significantly either directly overlie coals or their immediately succeeding shales, the connection of the thick sandstone, with the nature of the seatearth is puzzling. The sample of thick sandstones was too small to make deductions regarding the relationship between the preferred placing of a thick sandstone and the thickness of the coal it overlies, but the positive character of the AYK term suggests that they may have a preference to succeed thick coals. If these sandstones were at all erosional, this hypothesis would be very difficult to verify. Jablokov, Botvinkina and Feofilova (1961) report associations of this type in Russian coal measure basins and suggest that such occurrences mark the site of ancient "river valleys" where there was a greater development of both coal-forming vegetation and alluvium, though this tendency is not always shown in the resulting rock sequence as the repeated development of channel activity would lead to the greater role of washouts and hence destruction of coal seams. (For an example of a coal overlain by a thick sandstone, see Plate 1).

To summarise, the overall character of this type of term seems to be one of first-order memory links rather than of second-order memory in which the character of a seatearth might be used to predict statistically the nature of the first member of the succeeding cycle.

(iii) Terms (Y.2.3)

Like the terms preceding the vegetation horizons, this group contains significant second-order memory properties, suggesting a similar programmed development of sedimentation, though with the difference of showing an overall coarsening-upwards character. Such a pattern seems to belie the somewhat catastrophic flooding advocated by many authors to terminate the growth of coal-forming peats, implying that the return to normal sedimentation is fairly abrupt. The paucity of marine bands precludes direct flooding by the sea in Ayrshire cycles in the majority of cases, though analagous theories of widespread flooding of peat swamps by brackish or fresh water could be put forward. However, the resumption of clastic sedimentation would appear to be gradual because:

(1) the presence of significant second-order memory elements at this level suggests an orderly

sequential rather than abrupt development of lithologies;

and (2) the broad pattern that relates thickness of coal with the character of the overlying lithology indicates that the development of peat to some degree dictates the nature of the initial sediments that bury it.

It therefore seems likely that at some stage, sediment-bearing waters enter the swamp area and vegetation control again restricts sedimentation, so that deposits are initially of fine grade but coarsen as this control wanes with the introduction of aerated waters, cessation of peat formation and increasing transporting power of the incoming waters.

However, there still remains the problem of the nature of the mechanism that caused the cessation of swamp conditions and the initiation of a new cycle of clastic sedimentation. The types of possible mechanism can be classified as external or internal relative to the flood-plain environment. External factors such as climate change, eustatic rise in sea-level, regional episodic subsidence can be largely disregarded on the criterion of scale, in that their effects would be expected to be regional, whereas most cycles are of relatively local significance. Internal factors are therefore favoured. Tectonic subsidence within individual basins can be invoked as a broad background control, as the number and thickness of cycles increases towards the interior of depositional basins (Wills, 1956; Read and Dean, 1967), but there is no evidence that such movement was abruptly episodic. The role of compaction of sediment and, in particular, water-logged peat is probably an important controlling factor once sedimentation has been renewed over the swamp, but seems unlikely as the control that begins such a phase, in that compaction of sediment under its own weight will be gradual and self-compensating.

Reference to the deterioration and burial of swamps on modern delta-plains suggests that this is caused by change of sedimentation patterns combined with vegetational controls in the context of overall subsidence. Kolb and Van Lopik (1966) p.47, state that in the Mississippi delta plain, "factors involved in the growth of inland lakes that initiate as depressions in the marsh surface are complex. Impounding of water through distributary growth, faulting, and subsidence under the influx of clayey sedimentation from nearly alluvial streams may, singly or in combination, bring about the formation of a large inland lake." Duff (1967), drawing on Anderson's description of conditions operative in the deltate peat swamps of Sarawak (Anderson 1963, 1964), suggests that coal swamps may have been limited in their accumulation of peat by edaphic factors, when a failure to keep pace with subsidence could lead to change in drainage pattern and renewed sedimentation.

A combination of sedimentational and vegetational controls would thus appear as the most likely mechanism to terminate old cycles of clastic deposition and initiate new ones, explaining the localised extent of many cycles, the development of programmed second-order Markovian characteristics at this level, and having the appeal of uniformitarianism, in that some sort of complex mechanism of this nature appears to be operative in modern deltaic plains.

(2) Internal cycle terms

(i) Terms involving thick sandstones

Reference to the transition scheme (Fig.30) shows that the significant occurrence of thick sandstones within cycles take the form:

Y(A)KB(CB)AY

This, expressed more fully, means that thick sandstones tend to occur preferentially at the base of cycles lying directly on the coal or seatearth or separated from this by an intervening thickness of shale devoid of fresh-water lamellibranchs. The sandstone then fines upwards to a seatearth in either a simple fashion or, more raggedly, through interbedded siltstones and thin sandstones. Such a sequence bears strong similarity to the cycle proposed by Woodland and Evans (1964) as representative of the Pennant Coal Measures of South Wales.

The origin of many of these sandstone bodies as river channels has already been touched upon (p.104), so that theories are phrased in this context. The observation that sandstones of this facies often tend to overlie coal has been made in many other coalfields (e.g. Jablokov, Botvinkina and Feofilova, 1961; Clarke, 1963; Woodland and Evans, 1964) and the second-order memory involved in their placing suggests a rather systematic mechanism. These channels are likely to be erosional to some extent, and if this is great, then their basal contacts should lie on a variety of lithologies and so their sequential placing would be somewhat random. This suggests that the erosional depth of the sandstones is not very great and probably limited to the cycles in which they were deposited. In other coal basins there are very varied reports of the depths to which channel sandstones cut so that, for instance, they may reach scales of a hundred feet in the Pennsylvanian (Wanless *et al.*, 1963), while Kosanke *et al.* (1960) consider that the evidence for unconformity at the base (and hence downward cutting) is less than 20% of the areal distribution of any one channel in Illinois cyclotherms, while there are no unconformities for some. Beerbower (1961) and Swann (1964) emphasise the contemporanity of channel formation and the deposition of adjacent lithologies in many sequences and consider erosion at the base of channels to be minor. Jablokov, Botvinkina and Feofilova (1961) suggest that many of the Russian coal measure sandstones are penecontemporaneous with coal formation and that this demonstrates the simultaneous development of active channels with adjacent swamps. It would seem that unconformities produced by Ayrshire channel sandstones are of relatively mild character from the significant placing of these bodies on or just above the coal, which further suggests some specific control. As the coal and shales would be relatively easy to erode, it is possible that the level of the coal may be the deciding factor. Clarke (1963) put forward a theory to explain these observations in which he envisaged a building-up of the upper surface of the channel slightly above the surrounding plain by repeated floodings of channel sediment. The lower surface would be set by the river's grade profile between lakes or, in the case of a major channel, between land and sea. By this or a similar mechanism, many of the river channels could flow through swamp areas while the limitation of their downward erosion to their "aggrading level" would position their floors in the vicinity of the subsequently formed coal horizon.

The sandstones internally become successively finer in grain-size moving upwards (p.99) while there is an accompanying downward movement through flow regime of the depositing medium as expressed by diagnostic bedding forms (p.103). The change in these characters is usually not orderly but somewhat pulsatory in character, suggesting variation through time of conditions within the channel of alternating periods of spate and quieter conditions. The overall fining-upward profile however, agrees well with channel models of both modern and ancient environments (e.g. Jahns, 1947; Schanter, 1951; Glenn and Dahl, 1959; Bernard and Major, 1963; Kolb, 1962; Allen, 1965), where coarse channel lag deposits are succeeded by a point bar complex whose grain-size decreases upwards. Channel-fill deposits resulting from cut-off (a frequent occurrence in many deltaic plains) also show fining-upward characters as currents become progressively weaker and finally cease. Such cut-off channels may become lakes of the ox-bow type which gradually silt up and are encroached by vegetation (a simple grading up to seatearth and coal), or they may persist for some time as sites of limited drainage with episodic deposition by currents of silts and sands before final colonisation by vegetation.

(ii) Terms involving thin sandstones

While alternations of siltstones and thin sandstones often directly follow thick sandstone developments marking the decline in current activity in channel reaches, similar series are found in predominantly shaly sequences, where significant cycles involving thin sandstones can be represented as:

YMBCB(CB)AY

The cycle is preferentially started with a lamellibranch-bearing shale which is succeeded by an alternation of siltstones and thin sandstones before fining to a shale seatearth. The first-order memory character of the contributing terms suggests simple sedimentational mechanisms of short-term nature.

The field attributes of the sandstones points to their deposition in fairly shallow water by traction currents probably of the lower part of the low flow regime. The source of the sand would ultimately be the distributory channel network, though the context of many of these sandstones would be one of deposition in intervening lakes and ponds at varying distances from the adjacent channels, so that some may be representative of levee deposits. Channel-derived sediment would migrate into these basins to fill these to a level where the development of marsh and swamp would take an active hand. Towards the delta front, lakes would often have a brackish character or even take the form of lagoons or bays though, in the seeming absence of evidence of strong marine currents, the environmental differences between these and more inland lakes would be mainly a function of salinity.

The siltstone/thin sandstone alternation would therefore appear to indicate episodic influx of coarser sediment from channels, possibly at times of flood by overbank spill and the enroachment of levees on adjacent lakes or crevassing into these areas. Alternatively, in the complex pattern of drainage through the delta plain, these 'lakes' could at times serve as sluggish drainage systems with consequent silting-up and colonisation by vegetation.

<u>(iii) Shale/Siltstone terms</u>

The terms of MBA and ABA found to be significant (in simple first-order properties) only in the shale-dominated parts of the coal measure succession would seem to form an extension of the environment represented by sandstone/siltstone alternations. In this case, the depositional area was probably at a greater distance from any distributory so that disturbing influences of channel-flood sands would be minor and derivation from this source limited to silt brought by feeble currents into the more remote parts of lakes and ponds. Here deposition of mud would predominate and lamellibranch faunas flourish. These areas were probably fairly shallow and of transient nature where subsidence and other factors competed with infilling by sediment and the spread of vegetation.

Combining these various types of postulated environment into one all-embracing scheme, the depositional situation can be broadly conceived as a deltaic topset plain with the appearance of delta front or near delta front conditions at various times and places. The setting would be of a network of distributaries and minor channels migrating laterally and modifying its pattern by crevassing and cut-offs. These channels were probably banded by levee developments acting as temporary barriers from the intervening areas which consisted largely of marshes and swamps, together with lakes and ponds, in a mosaic arrangement of constantly changing pattern as a result of the interplay of factors of sedimentation, subsidence and active control by vegetation in colonisation and possibly later edaphic decay. Nearer the delta front, these stretches of water would be larger and more brackish with possible occurrence of lagoons and bays or even arms of the sea, though the latter seems to have been of quasi-marine character. At various times, and more particularly in parts nearer the active channels, sands and silts would flood into the lakes over the levees or through breaches in the channel banks as crevasse splays contributing to their infilling and so encouraging the spread of swamps.

Chapter 7

COAL MEASURE SEQUENCE SIMULATION MODELS

Introduction

In the last few years, mathematical simulation models have made a sudden appearance in the geological literature. Encouraged by the success of these models in such fields as business, social sciences, medicine and military strategy, an extension to geological problems is a logical step. The natural systems encountered in geology exhibit the same complex intertwining of variables that defy full analysis by simple deterministic and statistical methods. While conventional studies reveal broad relationships between variables, generally taken in small groups at a time, simulation models can be used to study the interplay of almost any number of variables in a dynamic manner, and so approximate to a far better appreciation of the natural situation. The process of simulation is essentially the translation of the model of the system studied through time so that the theoretical performance of the system is reproduced. Simulations can be made with various objectives in mind. One is to describe a conceptual model in dynamic terms when rather arbitrary estimates of variables that are thought to be control parameters are used to produce estimates of the behaviour of real or hypothetical situations. Another is to use the simulation in more rigorous fashion as an analytical tool to test in some quantitative manner hypotheses concerning processes that are considered to operate in the system studied.

Geological simulation studies published include marine sedimentation (Harbaugh, 1966; Schwarzacher, 1966), salt dome development (Howard, 1967), evaporite sedimentation (Briggs and Pollack, 1967), brachipod time-trend curves (Fox, 1967), delta sedimentation (Bonham-Carter and Sutherland, 1968) and stratigraphic sequences (Carr *et al*., 1966; Potter and Blakely, 1967; Schwarzacher, 1967; Krumbein, 1967, 1968) and others. Most of these models have been of broad conceptual character and comparison of their performance with the system simulated has generally been made visually. Oertel and Walton (1967) point out that while such intuitive evaluation is inevitable to some degree, objective and, if possible, mathematical criteria are preferable. The complexity of natural situations is such that visual comparisons cannot usually be trusted. If Zeller (1964) can produce from the Lawrence Kansas Telephone Directory, lithological sequences that are acceptable to the human eye as reasonable simulations, then the use of this member as an objective arbiter is rather limited.

Therefore, if the simulation model is to be used as something more than either a dynamic qualitative conceptual model or a teaching toy, it must be constructed so that its performance characteristics can be quantitatively compared with data from the natural system. Then the simulation can be used as an analytical method to test hypotheses of specific character.

With regard to stratigraphic sequence simulation, Schwarzacher (1968) p.19, considers that "Little has been learned, however, about the mechanics of sedimentation from such experiments. The reason for this is largely the complexity of natural processes. It is possible that some progress can be made by severely restrictin the scope of such investigations." This suggests that, at the outset, limited problems should be studied in which relatively simple simulations are computed to answer specific questions. Experimentation of this kind should be ordered in development from simple to complex in the conventional scientific manner.

Because of the somewhat random character of natural processes, most models (though not all) have been of a probabilistic nature and the technique of translating them through time achieved by variants of the 'Monte Carlo' method. This intriguing title was originally a code name used by Von Neumann and Ulam at Los Alamos in 1944 for secret work on the atom bomb in connection with the probabilistic problems involved with random neutron diffusion in fissile material. In Monte Carlo methods, the basic mechanism is the operation of a random number series on the probability distributions of the model variables, by means of which the process simulation is moved forward a step at a time.

Simple simulations can be produced very easily by using pencil and paper and referring to random number tables, but in the event of any complexity, the exercise is extremely time-consuming and so is done preferably by a computer. The generation of random numbers within a digital computer is most conveniently achieved by the use of a function. As it is in the nature of the beast that the systematic structure of a function precludes the production of a perfectly random series of numbers, the result is really of pseudo-random character. However, these functions are devised so that departure from randomness as assessed by statistical tests, is insignificant. The computer used for the following simulations was the ERCC KDF9, whose 'pseudo-random number generator' is a routine termed 'real function random k' (see Appendix H). A series of six hundred numbers produced by this function were tested and found to have a serial correlation coefficient of - 0.04, which demonstrates the essentially random character of sequences of numbers generated by functions of this type.

Monte Carlo models of Ayrshire successions

The probabilistic variables used in the simulation studies were derived from the Markovian and Indedendent Events models used in the previous sections. It was shown earlier that the Markov models were adequate qualitative (and loosely quantitative) predictors of lithological ordering in Ayrshire Coal Measure sequences in terms of short lengths expressed as cycles. (The essential non-stationarity of long sequences indicated controls of a higher level over and beyond these models. These controls would have to be incorporated to enable acceptably accurate simulation of extended sections). Such models are merely assessments of the sequential character of lithologies idealised as discrete events, with no estimate of the significance of such factors as thickness of succeeding lithologies or thickness of complete cycles. Consideration of the role of these attributes can be made within a simulation model. The hypothesis is set that the thickness of cycles can be adequately predicted on a Markov model of ordering in which the thickness of each component lithology can be selected randomly from the appropriate thickness population.

A series of simulated cyclic successions were generated for Independent Events, Markov-1 and Markov-2 models using the variables of transition probability matrices and thickness frequency distributions as input. The pseudo-random number generator was operated on this data to produce simulated Coal Measure stratigraphical sections. A more detailed explanation of procedure is given in Appendix H, together with the programmes used. The simulations produced as computer output took the form of symbolised graphic sections. Diagramatic examples of these are shown in Figs.39 and 40 together with appropriate borehole sections with which interesting comparisons can be made.

A thickness frequency distribution of cycles was computed for each simulation. The object population of this distribution representing the natural system was prepared from actual cycles culled from borehole sections used in Markov work.

The first feature of interest in the object population is that the average thickness of cycles compiled from the Sandy Group section parts (23.2 feet) is greater than that representative of the Shaly Group (18.6 feet). This accords well with observations in the literature that sandier cycles tend to be thicker than those dominated by shale e.g. Duff and Walton (1962) p.247. These figures also provide a useful check on the efficiency of the computed simulation models, in that average thickness of simulation cycle populations should be approximately the same as for the object population. (This conclusion may be surprising, but can best be understood if one imagines scrambling a natural section into random order. The independent events result contains the same number of vegetation horizons and therefore the same number of cycles; the total thickness remains constant, and therefore the average thickness of the 'random cycle' is the same as for the original section). The various simulation estimates of average

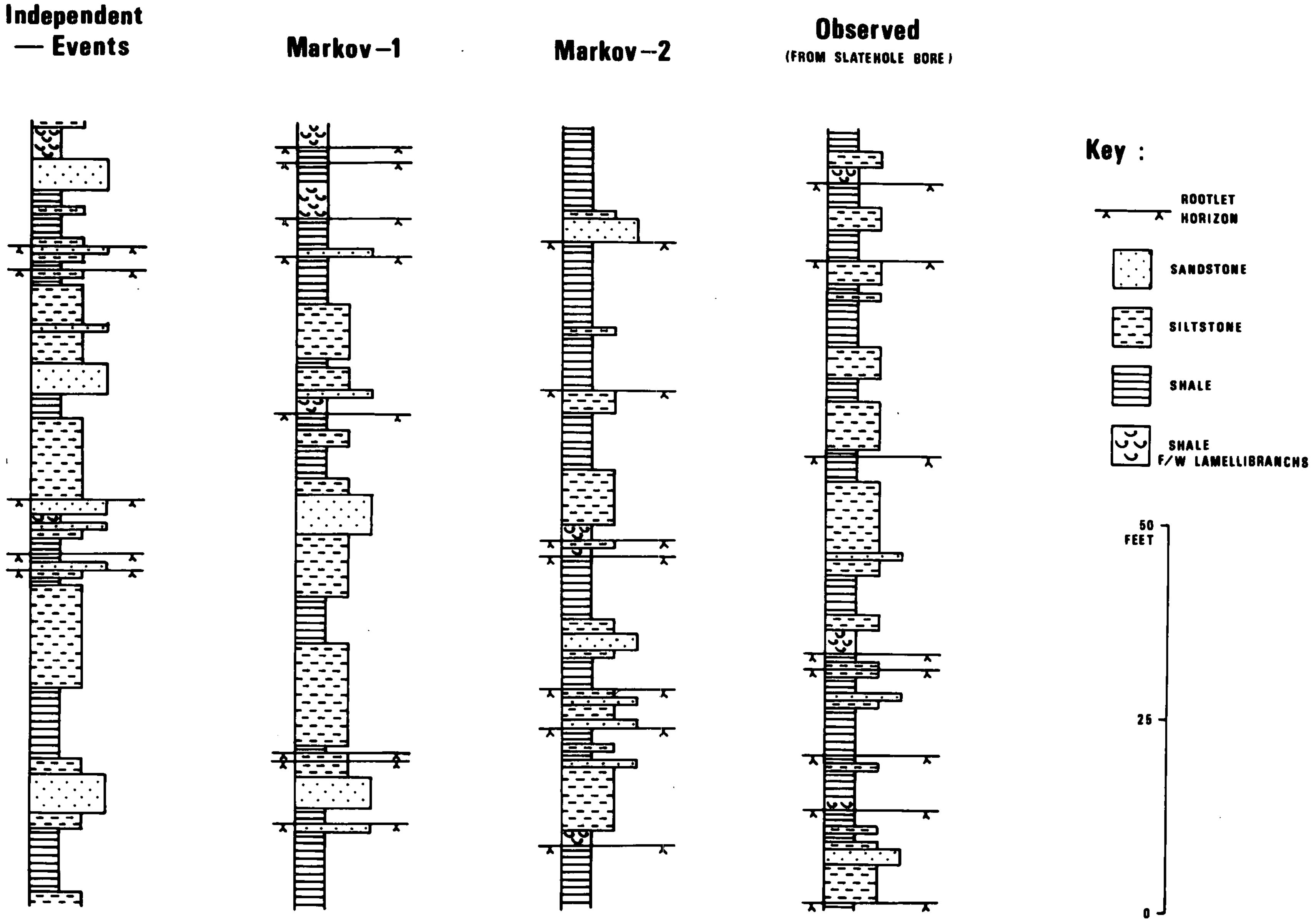


Fig. 39 Shaly Group (G) simulation model successions

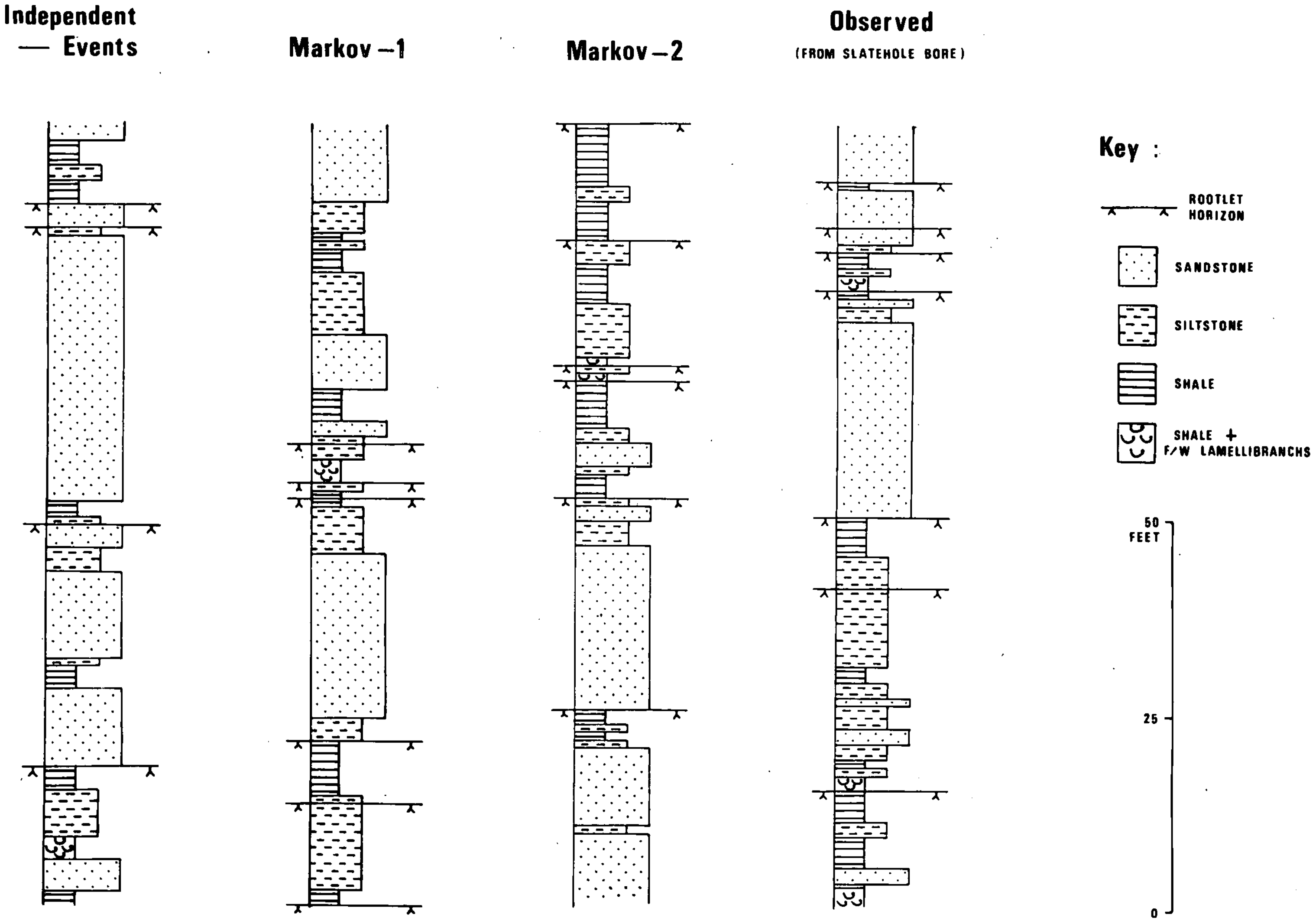


Fig. 40 Sandy Group (H) simulation model successions

cycle thickness are shown below and their sensible agreement shows them as adequate working models.

AVERAGE THICKNESS OF CYCLE (FEET)	I.E.	MARKOV-1	MARKOV-2	ACTUAL
Shaly Group	17.3	19.3	18.8	18.6
Sandy Group	22.9	25.0	23.6	23.2
All	20.4	22.4	21.4	21.2

The cycle thickness distributions were tabulated as grouped data with class interval of five feet together with the distribution of the object population (Table 29). Visual comparison of the various model data shows a generalised trend in closer prediction with the power of the Markov model. Each model population was independently tested as a chi-square distribution on the hypothesis that it was drawn from the same population as that of the object distribution. The method used was that set by Krumbein and Graybill (1965) p.172. The test values were as follows:

Independent Events Model	152.1
First-Order Markov "	150.9
Second-Order " "	40.5

The number of degrees of freedom is 15 when, at α 0.05, the tabulated chi-square value is 25.0, from which it follows that the hypothesis that any of these models are statistically adequate predictors of cycle thicknesses is rejected. This failure can be attributed to the following factors acting singly or in combination:

(1) the model does not satisfactorily predict the internal ordering of lithologies (considered as events) within cycles;

(2) there is a significant relationship between the thickness of a lithology and the character and thickness of the succeeding lithology;

and (3) there is a broader 'external' control that regulates thickness of cycles.

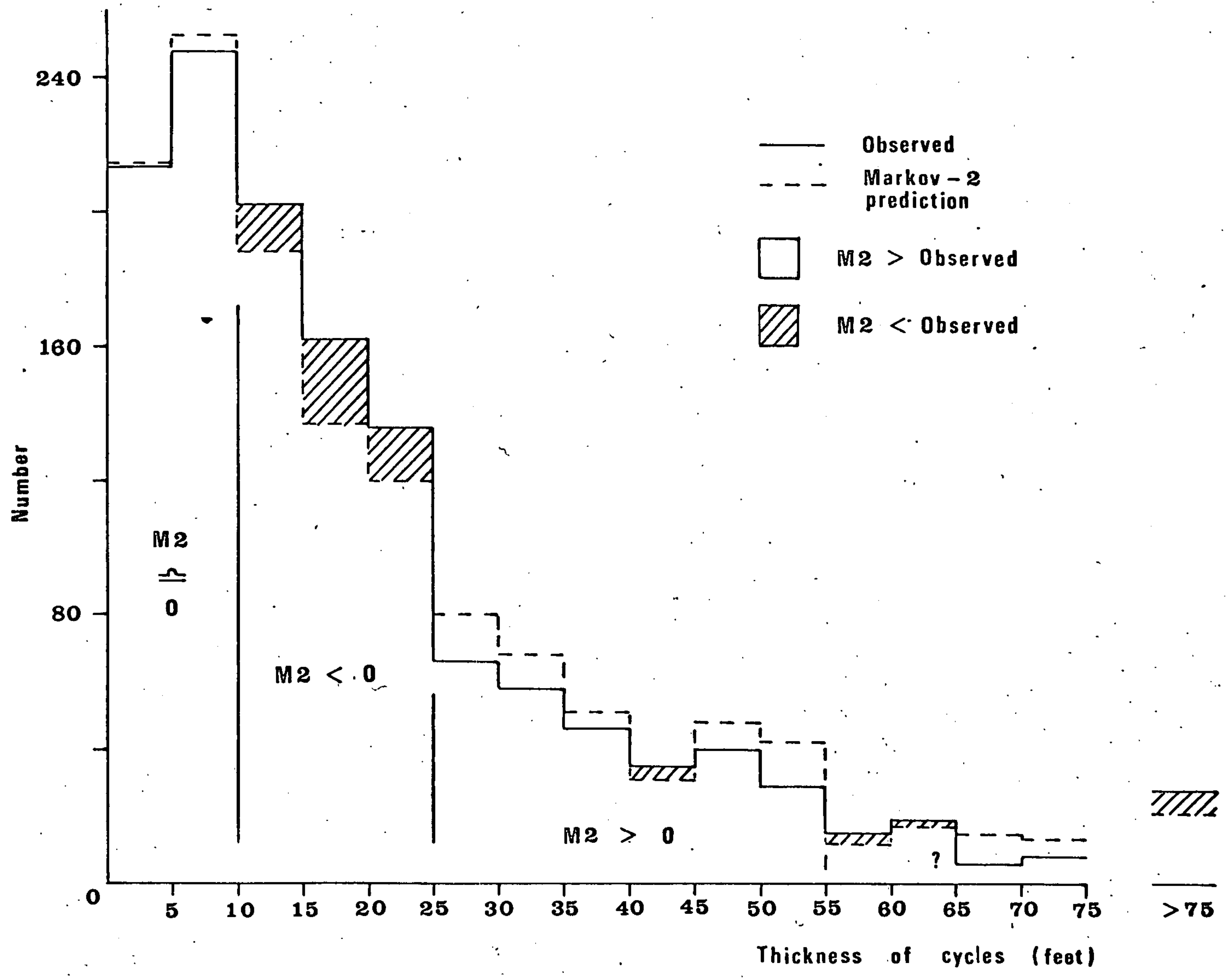
Examination of the model class counts used in this test (Table 29) shows that in the case of the Independent Events and Markov-1 models, the significant deviation from the object population is largely the result of excessive estimates of very thin and very thick cycles, with underestimation of the frequency of intermediate types. The Markov-2 model shows a much closer approach to the ideal, and interesting comparisons can be made with the object population by superimposing the two distributions as in Fig.41. This shows a close parallelism in pattern and the existence of a broad trend underlying the difference between the two populations. For cycles less than 10 feet in thickness, the frequencies are very similar; in the range 10 to 25 feet, the number of Markov-2 cycles are consistently less; in the range 25 to 55 feet, greater. (For cycles thicker than 55 feet, the sample numbers are too low and the relations too ragged to allow interpretation).

This relationship can be usefully compared with the Markov-2 prediction model of numbers and types of cycles of different internal ordering (Fig.37). In this case, the model predicted a higher number of cycles of two and three members, and consistently lower numbers for those of higher than three, relative to the object population. As there is a broad positive relationship between the number of members in a cycle and the cycle's thickness, it follows

CLASS INTERVAL (FEET)	I.E.	M-1	M-2	OBSERVED
2 - 5	300	272	214	213
6 - 10	242	224	253	248
11 - 15	181	182	188	202
16 - 20	112	155	137	162
21 - 25	85	74	120	136
26 - 30	72	62	80	66
31 - 35	58	62	68	58
36 - 40	39	46	51	46
41 - 45	35	31	31	35
46 - 50	29	33	48	40
51 - 55	27	24	42	29
56 - 60	24	28	12	15
61 - 65	17	19	17	19
66 - 70	19	19	15	6
71 - 75	11	12	14	8
>75	60	68	21	28

Table 29 GROUPED CYCLE THICKNESS DISTRIBUTIONS FOR INDEPENDENT EVENT (I.E.), MARKOV - 1 (M-1), MARKOV - 2 (M-2) SIMULATION MODEL AND OBJECT POPULATIONS

FIG. 41 CYCLE THICKNESS HISTOGRAMS : M2 v. OBSERVED



that the deviations between the Markov-2 and object cycle thickness populations is the reverse of what would be expected if these deviations were merely the function of the inability of the Markov-2 model to accurately predict cycle types.

It therefore seems likely that some sort of 'thickness control' is present and that the thicknesses of cycles are not purely a function of lithological state ordering in conjunction with arbitrary thicknesses of the component members. The nature of this control can be inferred from the character of the Markov-2 cycle thickness deviations. These suggest that this factor discourages the formation of relatively thick cycles (thicker than 25 feet) with corresponding encouragement of thinner cycles (with the exception of those of 10 feet or less whose occurrence is much as predicted).

Investigations of the periodicities of certain horizons in sedimentary sequences has been made in recent years by power spectral analysis and other techniques which seek to isolate significant harmonies that are present. Both Schwarzacher (1967) and Carss (1967) analysed Carboniferous sections and found fundamental periodicities in the range 100-150 feet, which showed broad agreement with the "average" thickness of measured cyclothems (here defined on a marine horizon-to-marine horizon basis) reported in the orthodox geological literature. Both Schwarzacher and Carss favour the view that such harmonics are response elements in a process model of crustal readjustment to sediment loading. (Possible alternatives of biological or climatic control are also mentioned by Schwarzacher)

It will be appreciated that the seatearth-to-seatearth cycles considered in this study are of a lower order of magnitude than the marine bed bounded cyclothems, both in terms of absolute thickness and in the sense that many cycles are contained between marine band horizons in Ayrshire. The low value range of preferred cycle thickness (10-25 feet) makes it unlikely that the controlling factor is one of readjustment responding to isostatic effects or current movements in the mantle.

In the context of a modern environment, Coleman and Gagliano (1964) have demonstrated a cyclic development of sediments in the Mississippi which is caused by an interplay of sedimentary and subsidence controls. In the Mississippi delta, there is intermittent lateral movement of the local sources of sediment, so that areas subject to active distributary sedimentation become abandoned deltaic lobes and change to marsh, lacustrine, lagoonal or open marine environments, while the reverse happens in adjacent parts of the delta. This variation is the response to the interplay between the controls of active distributary sedimentation and overall subsidence, resulting in a lateral and vertical alternation of sedimentary facies of cyclic type.

It is suggested that a mechanism of this kind is the cause of the systematic factor that appears to underlie the thickness distribution of the Ayrshire Coal Measure cycles. It has the appeal of uniformitarianism, would produce cycles of the right order of magnitude, and is consistent with the interpretation of the ordering of rock types within the cycles made in the Markov analysis earlier. In such a scheme, there would be a sense of equilibrium between the amount of subsidence within an area and its tendency to become a locus of active coarse clastic deposition. For cycles thinner than ten feet, subsidence would be insufficient to encourage migration of sediment courses from elsewhere, so that cycles at this level are satisfactorily described by a Markov-2 model of internal ordering and choice of fairly arbitrary thicknesses for the lithologies. Cycles thicker than 55 feet would mark a delayed response of facies migration to prolonged subsidence. However, cycles in the intermediate range (25-55 feet) would represent the products of the optimum balance between the two controls of distributary source migration and subsidence in an environment of the deltaic type.

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PLATE 1

THICK SANDSTONES

Lower Coal Measures sandstone body resting directly on the Pennyvenie Two foot - Seven inch Coal (left of centre). Internal characters, lithological association, and lensoid geometry suggest origin as a fresh - water channel deposit.
Cummock Burn, Dalmellington, South Ayrshire.

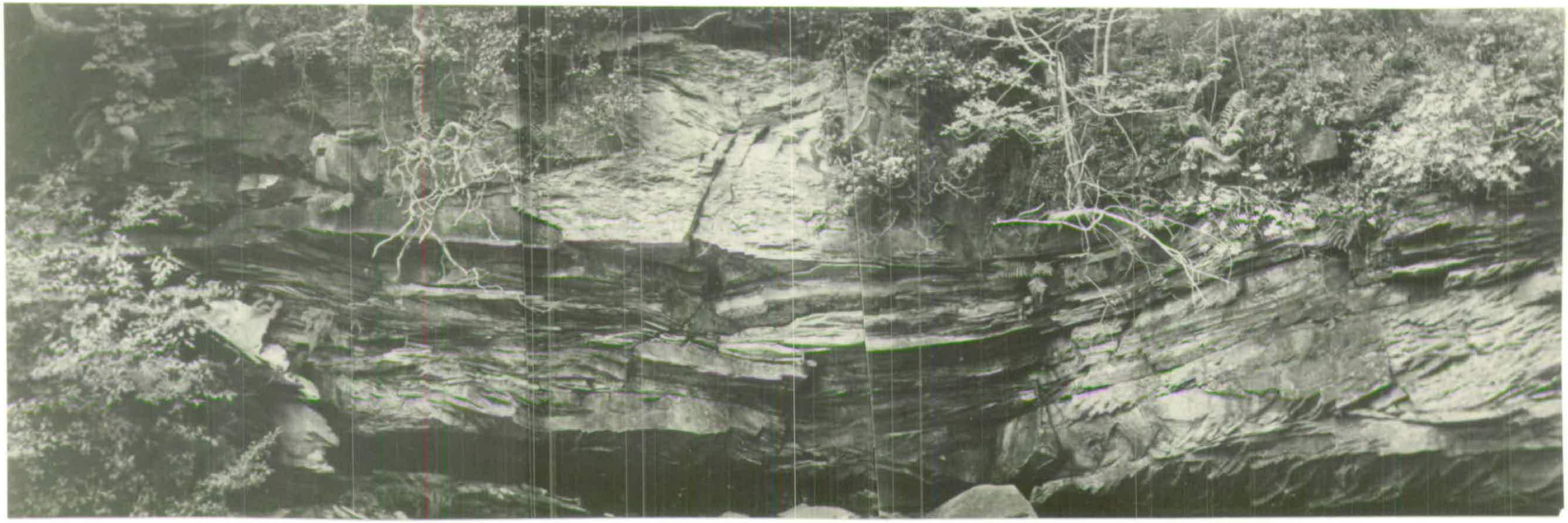
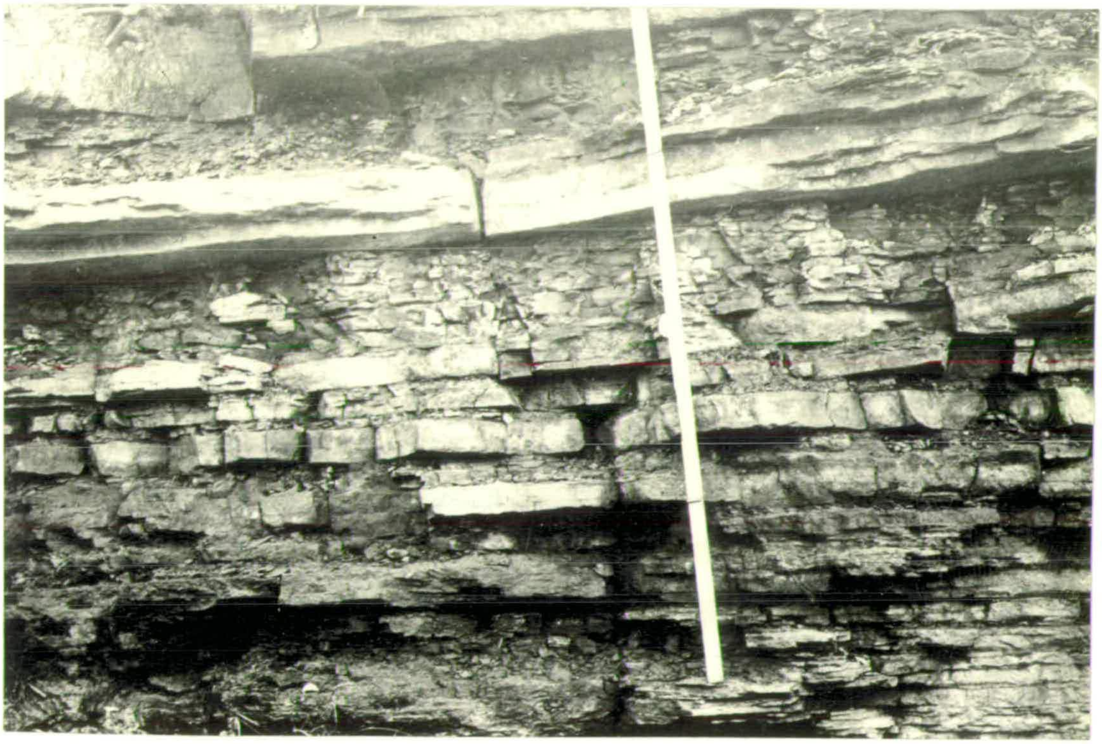


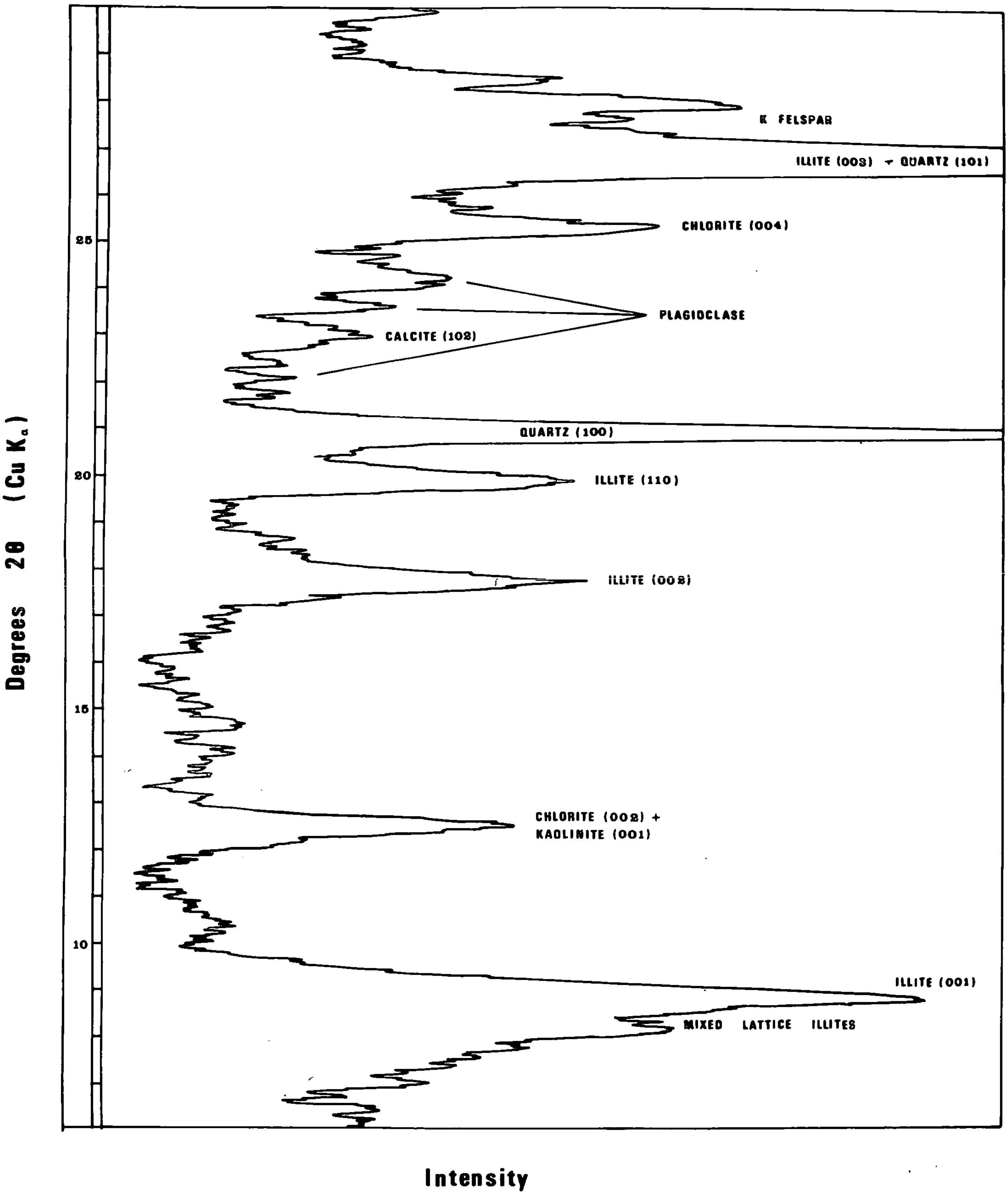
PLATE 2

THIN SANDSTONES

Typical Lower Coal Measures thin sandstone sequences. Thin sandstones interbedded with siltstones, silty mudstones, and sandy mudstones.
Cummock Burn, Dalmellington, South Ayrshire.



APPENDICES A - I


K FELSPAR
ILLITE (003) + QUARTZ (101)
CHLORITE (004)
PLAGIOCLASE
CALCITE (102)
QUARTZ (100)
ILLITE (110)
ILLITE (002)
CHLORITE (002) +
KAOLINITE (001)
ILLITE (001)
MIXED LATTICE ILLITES
25
20
15
10
Degrees 2θ (Cu Kα)
Intensity

SHALE

APPENDIX B

Analysis of trace elements in a Middle Coal Measure mudstone

The mudstone was collected from a core of the Craigmark No.30 Bore (sited two miles north-west of Dalmellington) at an horizon twelve feet above the Queenslie (Katharina) Marine Band, here represented by a fauna of dwarfed *Lingula* and fish scales. The sample is a dark grey, carbonaceous, slightly silty mudstone, containing traces of *Anthraconaia* sp., which is taken to indicate that the depositing medium was one of fresh or slightly brackish water. It was analysed by D.H. Doff on a Phillips 1212 Automatic X-ray Fluorescence Spectrometer for the elements shown in the table below, where the analysis is compared with values representing the 'average shale' of Turekian and Wedepohl (1961).

	Craigmark No.30 Mudstone Sample	Average Shale (Turekian and Wedepohl, 1961)
Ba	867	580
As	9	13
Zn	2046	95
Cu	48	45
Ni	81	68
Co	62	19
Mn	321	850
Ti	1.03%	0.46%
V	144	130
Cr	159	90
Pb	49	20
S	0.07%	0.24%
P	513	700

(Parts in ppm except where indicated as percent).

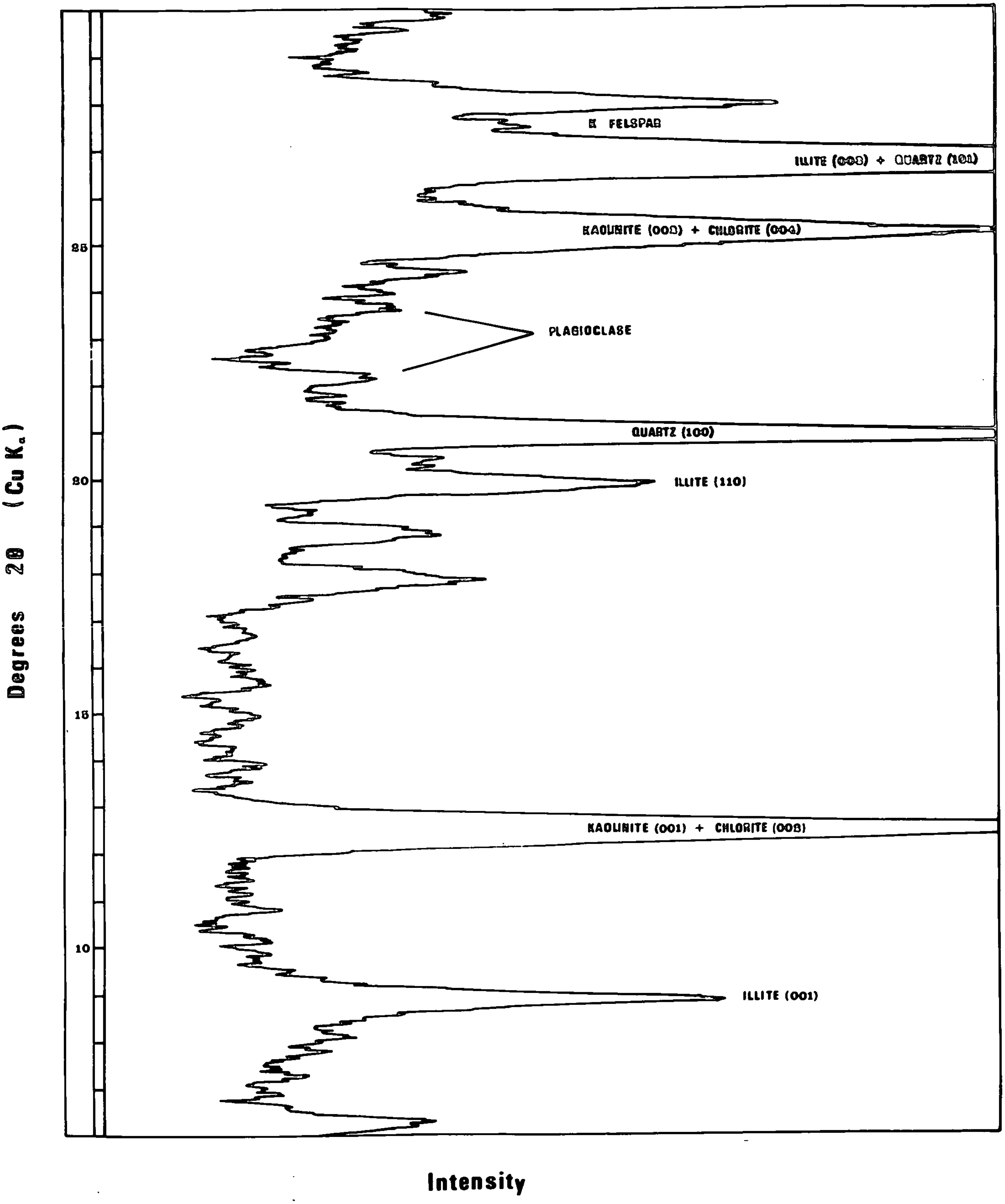
Studies by Nicholls and Loring (1962) are of particular interest, as they undertook the investigation of trace element analyses of a rock interval that both encompasses the time horizon represented by this mudstone and has a very similar lithological association to the cored section of the Craigmark No.30 Bore. However, their study was conducted in a North Wales coalfield, so that geochemical characters peculiar to that area preclude direct quantitative comparisons. Nicholls and Loring concluded that the development of the trace element content was due to a mixture of the factors of detrital introduction, precipitation from solution, and sorption by organic matter and clay minerals.

The most striking feature of the present analysis is the anomalously high zinc content. The relatively low proportion of sulphur is argument against significant sulphide precipitation as the main cause of this. The moderately high titanium content suggest the possibility of detrital material introduction as a strong influence on the trace element proportions. However, there are no obvious zinc-mineralised zones in nearby potential source areas. Cannon _et al_. (1968) have noted that a modern descendent of the Carboniferous flora, _Equisetum_, is a zinc accumulator and this factor could have a minor bearing in this problem. More likely, however, is sorption by decaying carbonaceous matter during sedimentation and burial.

Appendix C

X-ray Diffraction of a Coal Measures Seatearth

In hand-specimen, the sample is a pale creamy-grey, slightly silty mudstone, which is transected by numerous vertical rootlet traces, but appears otherwise structureless. The sample was collected from an horizon approximately thirty feet above the Queenslie Marine Band (i.e. Middle Coal Measures) in Cummock Burn, Dalmellington.



MUDSTONE SEATEARTH

APPENDIX D

Definition of a clastic coding scale used in smoothing operations

The rock types recorded in an object succession must be translated as a numerical system for Spencer's smoothing formula to be applied, while the coding must be designed to be geologically meaningful. Now, there is a broad positive correlation between grain-size and sedimentary environment defined in terms of transporting current strength, so that, for the lithologies represented in the Ayrshire Coal Measures, a natural scale will range from low for shales to high for conglomerates.

The problem now centres on the actual numerical values to ascribe within this range. If the Wentworth scale is applied directly, then the raw values represent drastically disproportionate extremes. A logarithmic index, such as the 'phi-scale,' gives a more acceptable coding system in terms of a sensible smoothing result. Vistelius (1961) p.707 sets the values of his number scale, "in compliance with the granulometric composition of the rocks or the general type of sedimentation activity." His criteria are vague, but, in fact, it is impossible to arrive at an absolutely geologically meaningful scale, because of the lack of specific information (such as the nature of the depositional environment) from which to build it.

The feature with which this study is concerned is essentially the geometry of the long-term trend, which is interpreted as broad changes in the grade of material supplied to the area through time. The use of several reasonable scales for the fine to coarse spectrum will only distort the geometry of the 'real trend' to varying degrees, registered in terms of accentuating or reducing profile peaks, but not converting peaks to troughs. The geometric shape is therefore preserved and the use of a sensible scale will enable valid interpretation of long-term changes to be made. The scale chosen for the lithologies of the Ayrshire Coal Measures is shown in table 8.

APPENDIX E

Atlas Autocode (AA) Programme SMOOTHBORE

Input data consists of the name of the object succession terminated by a full-stop, the length (or an overestimate of this) of the section in feet, followed by a string of numbers representing the coding of the section at foot interval observations terminated by the value -1. The coding system is that shown in Table 8 with modifications as follows:

Shale + non-marine lamellibranchs = 55
Siltstone + " " = 66
Shale seatearth = 77
Siltstone " = 88
Sandstone " = 99

These additional states allow the recording of non-marine lamellibranc and seatearth horizons.

Spencer's 21-term smoothing formula is applied to the raw data (one foot level) and trends calculated to third degree level. The third degree trend is sampled at ten foot intervals and the smoothing formula reapplied for three further degrees of smoothing. The result is two trends: a 'medium term' trend (one foot interval) and a 'long term' trend (ten foot interval). The parameters of these are fed off-line to a Calcomp 564 digital graph plotter, which draws the trends as scale profiles against which positions of non-marine lamellibranch and seatearth horizons are marked.

```
%BEGIN
%INTEGER I,NME,N',NO,C
%INTEGERARRAY NOME(1:30)
NME=0
%CYCLE I=1,1,30
READ SYMBOL(NOME(I))
%IF NOME(I)='.' %THEN ->1
NME=NME+1
%REPEAT
1: READ(N')
%COMMENT N' IS LENGTH (OR OVERESTIMATE) OF SECTION  %C
          IN FEET

%BEGIN
%INTEGER Y,YR,NA,NB
%REALARRAY LT(0:N'),LV(0:N'/5),MS(1:N'),RTS(1:N')

%BEGIN
%INTEGER YR',F,X,D,E,B,J,K
%REAL S,T,Z,A
%REALARRAY L(0:1,1:N')
%ROUTINESPEC MUSSELS(%REAL W)
%ROUTINESPEC ROOTS(%REAL WR)

Y=0 ; YR=0 ; YR'=0
%CYCLE I=1,1,N'
READ(L(0,I+10))
%IF L(0,I+10)=-1 %THEN NO=I+19
%IF L(0,I+10)=-1 %THEN ->2
%COMMENT ROUTINES 'MUSSELS' & 'ROOTS' RECORD HORIZONS %C
          OF MUSSELBANDS AND SEATEARTHS
MUSSELS(55) ; MUSSELS(66)
ROOTS(77) ; ROOTS(88) ; ROOTS(99)
%IF L(0,I+10)=55 %OR L(0,I+10)=77 %THEN L(0,I+10)=2
%IF L(0,I+10)=66 %OR L( ,I+10)=88 %THEN L(0,I+10)=9
%IF L(0,I+10)=99 %THEN L(0,I+10)=20
%REPEAT

2: D=0
NA=NO-19
3: J=0
%CYCLE C=0,1,3 ; B=J+(-1)C
%COMMENT C IS NUMBER OF DEGREES OF SMOOTHING = 3
S=0 ; %CYCLE I=1,1,10
S=S+L(J,I+10) ; %REPEAT
T=S/10 ; %CYCLE I=1,1,10
L(J,I)=T ; %REPEAT
S=0 ; %CYCLE I=1,1,10
S=S+L(J,NO-20+I) ; %REPEAT
T=S/10 ; %CYCLE I=NO-9,1,NO
L(J,I)=T ; %REPEAT
```

```
%COMMENT SPENCER'S 21 TERM SMOOTHING FORMULA  %C
         APPLIED TO SECTION
%CYCLE K=11,1,NO-10
A =60*L(J,K)+57*(L(J,K-1)+L(J,K+1))
A =A+47*(L(J,K-2)+L(J,K+2))+33*(L(J,K-3)+L(J,K+3))
A =A+18*(L(J,K-4)+L(J,K+4))+6*(L(J,K-5)+L(J,K-5))
A =A-2*(L(J,K-6)+L(J,K+6))-5*(L(J,K-7)+L(J,K+7))
A =A-5*(L(J,K-8)+L(J,K+8))-3*(L(J,K-9)+L(J,K+9))
A =A-L(J,K-10)-L(J,K+10)
L(B,K)=A/350
%REPEAT

J=B
%REPEAT

%CYCLE I=0,1,NO-19
%IF D=3 %THEN ->4
LT(I)=L(1,I+10)
->5
4: LV(I)=L(1,I+10)
5: %REPEAT
%IF D=3 %THEN ->6
D=3
NO=INT PT((NO-20)/10)+20
NB=NO-19
%CYCLE E=11,1,NO-10
L(0,E)=L(1,E+((E-10)*9))
%REPEAT
->3

%ROUTINE MUSSELS(%REAL W)
%UNLESS L(0,I+10)=W %THEN ->7
Y=Y+1 ; MS(Y)=I
7: %END

%ROUTINE ROOTS(%REAL WR)
%UNLESS L(0,I+10)=WR %THEN ->8
YR'=YR'+1 ; %IF YR'=I %THEN ->8
YR'=I ; YR=YR+1 ; RTS(YR)=I
8: %END

6: %END

%BEGIN
%REALARRAY LT'(0:N'),LV'(0:N'/5)

%CYCLE I=0,1,NA
LT'(I)=I ; %REPEAT
%CYCLE I=0,1,NB
LV'(I)=I*10 ; %REPEAT
```

```
%COMMENT GRAPH PLOTTER OUTPUT ROUTINES OF THIRD  %C
         ORDER SMOOTHINGS AT ONE-FOOT AND TEN-FOOT  %C
         INTERVAL BASED OBSERVATIONS PLUS SEATEARTH %C
         AND MUSSELBAND HORIZONS
INITIALISE PLOTTER(564)
SETPLOT(0,0,100,70,0)
SCALE(5,5,0.04,0.4,0)

LINEGRAPH(LT',LT,NA,1,0,0,0)

CURVE(LV',LV,NB,LV'(0),LV'(NB),5,0.5,1,0,0,0)

AXIS(0,0,1,100,INT(NA/100)+2)
%CYCLE I=INT(NA/100)+1,-1,0
ANNOTATE(I*100,-2,0.5,90) ; PRINT(I*100,3,0)
%REPEAT
AXIS(0,0,2,5,7)
%CYCLE I=5,-1,0
ANNOTATE(-5,5*I-1,5,90) ; PRINT(5*I,2,0)
%REPEAT

ANNOTATE(-5,30,5,90) ; %CAPTION MSS
ANNOTATE(-5,33,5,90) ; %CAPTION RTS
%CYCLE I=1,1,Y
ANNOTATE(MS(I)+14,30,20,90) ; %CAPTION -
%REPEAT
%CYCLE I=1,1,YR
ANNOTATE(RTS(I)+14,33,20,90) ; %CAPTION -
%REPEAT

ANNOTATE(INT(NA/100)*100+200,0,10,90)
%CYCLE I=1,1,NME
PRINT SYMBOL(NOME(I)) ; %REPEAT

CLOSE PLOTTER

%END
%END
%ENDOFPROGRAM
```

APPENDIX F

Atlas Autocode (AA) Programme BORE ANALYSIS

Input data used for this programme is the same as for SMOOTHBORE (Appendix E). Positions of non-marine lamellibranch and seatearth horizons are calculated and printed. A 'medium term' and 'long term' trend are computed using Spencer's smoothing formula and these shown in histogram form on line-printer output.

The succession is then divided into 'sandy' and 'shaly' fractions the division between the two types being marked where the long term trend intersects the siltstone coding value (9). The result is two sets of sequence type, dominated in one by coarse sediments, in the other by fine, within which the condition of stationarity is more closely approached than for the total undivided succession. Fractional parts of less than fifty feet length are rejected as constituting unacceptably small samples for the analysis of lithological transitions that follows.

Each fractional sequence is considered in turn and the following data estimated and printed:

(i) the character of the sequence (SANDY or SHALY);

(ii) the position of the sequence within the total succession;

(iii) the thickness of the lithologies shale (1); shale with non-marine lamellibranchs (2); siltstone (3); siltstone with non-marine lamellibranchs (4); sandstone (5); shale (7), siltstone (8) and sandstone (9) seatearths within the sequence;

(iv) the absolute proportions of these lithologies (feet);

(v) the percentage of the sequence accounted for by shale (A), siltstone (B), and sandstone (C):

(vi) the one-step, one-foot transition tally matrix of the six lithology system of (iii);

(vii) the one-step state (zero diagonal) transition tally matrix of the condensed four-state system shale (A), siltstone (B), sandstone (C), rootlet horizon (Y);

(viii) the one-step state transition probability matrix derived from (vii);

(ix) the sequence represented in the fragment coded as A. Ao. B. BO. C. AY. BY. CY (equivalent to lithologies 1 to 8, respectively) together with lithological thicknesses;

(x) the two-step state transition tally matrix for the four-state (A. B. C. Y) system;

(xi) the two-step state transition probability matrix derived from (x).

```
%BEGIN
%COMMENT  LITHOLOGY 1 = A = SHALE      %C
          LITHOLOGY 2 = 55 = AO = SHALE + MUSSELS
%COMMENT  LITHOLOGY 3 = B= SILTSTONE    %C
          LITHOLOGY 4 = 66 = BO = SILTST. + MUSSELS
%COMMENT  LITHOLOGY 5 = C = SANDSTONE
%COMMENT  LITHOLOGY 6 = 77 = AY = SHALE SEATEARTH   %C
          LITHOLOGY 7 = 88 = BY = SILTST. SEATEARTH  %C
          LITHOLOGY 8 = 99 = CY = SANDST. SEATEARTH
%COMMENT  IN CONDENSED FORM :      %C
          A = A + AO         %C
          B = B + BO         %C
          C = C
%COMMENT  Y = INTERFACE AT TOP OF AY, BY, CY
%INTEGER N,I,B,C,J,K,N',TITLE
NEWLINES(6)
%COMMENT TITLE IS NAME OF SECTION
%COMMENT N' IS LENGTH (OR OVERESTIMATE) OF SECTION (FEET)
%CYCLE I=1,1,30
READ SYMBOL(TITLE)  ;  PRINT SYMBOL(TITLE)
%IF TITLE='.' %THEN ->62
%REPEAT
62: READ(N')

%BEGIN
%INTEGERARRAY LP(1:N')
%REALARRAY LT(1:(N'/10)+10)

%BEGIN
%INTEGER P,F,X,D,E,Y
%INTEGERARRAY R(1:800)
%REAL S,T,Z,A
%REALARRAY RA(1:800),L(0:1,1:N'+1)
%ROUTINESPEC FEATURE(%REAL W)

Y=0
%CYCLE I=1,1,N'+1
READ(L(0,I+10))
%IF L(0,I+10)=-1 %THEN N=I+19
%IF L(0,I+10)=-1 %THEN ->78
LP(I)=INT(L(0,I+10))
%COMMENT  DEPTHS IN FEET OF SEATEARTH AND MUSSELBAND   %C
          HORIZONS RECORDED BY ROUTINE 'FEATURE'
FEATURE(55) ; FEATURE(66)
FEATURE(77) ; FEATURE(88) ; FEATURE(99)
%IF L(0,I+10)=55 %OR L(0,I+10)=77 %THEN L(0,I+10)=2
%IF L(0,I+10)=66 %OR L(0,I+10)=88 %THEN L(0,I+10)=9
%IF L(0,I+10)=99 %THEN L(0,I+10)=20
%REPEAT
78: D=0
```

```
22: J=0
%COMMENT C IS NUMBER OF DEGREES OF SMOOTHING = 3
%CYCLE C=0,1,3
B=J+(-1)C
S=0
%CYCLE I=1,1,10
S=S+L(J,I+10)
%REPEAT
T=S/10
%CYCLE I=1,1,10
L(J,I)=T
%REPEAT
S=0
%CYCLE I=1,1,10
S=S+L(J,N-20+I)
%REPEAT
T=S/10
%CYCLE I=N-9,1,N
L(J,I)=T
%REPEAT

%COMMENT SPENSER'S 21 TERM SMOOTHING FORMULA      %C
         APPLIED TO SECTION
%CYCLE K=11,1,N-10
A= 60*L(J,K) +57*(L(J,K-1)+L(J,K+1))
A= A+ 47*(L(J,K-2)+L(J,K+2)) +33*(L(J,K-3)+L(J,K+3))
A= A+ 18*(L(J,K-4)+L(J,K+4)) +6*(L(J,K-5)+L(J,K+5))
A= A -2*(L(J,K-6)+L(J,K+6)) -5*(L(J,K-7)+L(J,K+7))
A= A -5*(L(J,K-8)+L(J,K+8)) -3*(L(J,K-9)+L(J,K+9))
A= A -L(J,K-10) -L(J,K+10)
L(B,K)=A/350
%IF C=3 %AND D=3 %THEN LT(K-10)=L(B,K)
%REPEAT
J=B

%REPEAT

%IF D=3 %THEN ->14

NEWLINES(3)
%CAPTION LENGTH_OF_SECTION_=_
PRINT(N-20,5,0) ; %CAPTION _FEET
NEWLINES(3)
%CAPTION MUSSELS_AND_SEATEARTHS_AT
NEWLINES(2)
%COMMENT PRINTOUT OF DEPTHS OF SEATEARTH AND     %C
         MUSSELBAND HORIZONS
%CYCLE C=1,1,Y
PRINT(R(C),4,0) ; SPACES(2)
PRINT(RA(C),3,0) ; NEWLINE
%REPEAT
```

```
14: NEWLINES(3)
%CAPTION SMOOTHING_SET_3_=
%IF D=3 %THEN %CAPTION__(2ND_SMOOTHING_SEQUENCE)
NEWLINES(2)

%COMMENT LINE PRINTER HISTOGRAMS OF THIRD ORDER SMOOTHINGS%C
         AT ONE FOOT AND THEN TEN FOOT INTERVAL OBSERVATIONS
%CYCLE I=1,1,N
PRINT (I-10,5,0)
SPACES(2)
Z=(L(1,I))
%IF Z>=0.5 %THEN ->66
%IF Z<0 %THEN Z=MOD(Z)
X=INT(Z)
%CYCLE F=0,1,X
PRINT SYMBOL ('O')
%REPEAT
->99
66: X=INT(Z)
%CYCLE P=1,1,X
PRINT  SYMBOL ('A')
%REPEAT
99: NEWLINE
%REPEAT

%IF D=3 %THEN ->44
D=3
N=INT PT((N-20)/10) +20
%CYCLE E=11,1,N-10
L(0,E)=L(1,E+((E-10)*9))
%REPEAT
->22

%ROUTINE FEATURE(%REAL W)
%UNLESS L(0,I+10)=W %THEN ->86
Y=Y+1 ; R(Y)=I ; RA(Y)=W
86: %END

44: %END

%BEGIN
%INTEGER CN,STEP,Z1,Z2,SHALE,SILT,SAND,ALL,THICK,COUNT,DA
%INTEGERARRAY TRA(1:50),TRB(1:50),MF(1:8),M(1:8,1:8), %C
S(1:4,1:4),TK(1:8),TH(1:8,1:100),RL(6:8),T(1:4), %C
BUZ(1:500),BUX(1:500)
%REALARRAY PR(1:4,1:4)
%ROUTINESPEC CODING(%INTEGER F1,F2,F3)
%ROUTINESPEC SEQUENCE(%INTEGER ZX)
```

```
CN=1
TRA(1)=10
%IF LT(1)<=9 %THEN TRB(1)=2
%IF LT(1)>9 %THEN TRB(1)=1
%COMMENT THE PARTITION OF THE SECTION INTO   %C
          'SHALY' AND 'SANDY' FRAGMENTS
%CYCLE I=2,1,N-20
%IF LT(I-1)<=9 %AND LT(I)>9 %THEN ->12
%IF LT(I-1)>9 %AND LT(I)<=9 %THEN ->13
->47
12: CN=CN+1 ; TRA(CN)=(I-1)*10 ; TRB(CN)=1 ; ->47
13: CN=CN+1 ; TRA(CN)=(I-1)*10 ; TRB(CN)=2
47: %REPEAT
CN=CN+1 ; TRA(CN)=(N-20)*10
%IF LT(N-20)<=9 %THEN TRB(CN)=2
%IF LT(N-20)>9 %THEN TRB(CN)=1

NEWLINES(6)
%CAPTION FRAGMENT_ANALYSIS ; NEWLINES(3)
%CYCLE I=1,1,CN-1
%UNLESS TRA(I+1)-TRA(I)<50 %THEN ->15
%CAPTION FRAGMENT<50 ; NEWLINE
PRINT(TRA(I),4,0) ; SPACES(2) ; PRINT(TRA(I+1),4,0)
NEWLINE
15: %IF TRB(I)=1 %THEN %CAPTION SANDY
%IF TRB(I)=2 %THEN %CAPTION SHALY
SPACES(2) ; %CAPTION FRAGMENT ; SPACES(4)
%IF TRA(I+1)-TRA(I)<50 %THEN ->16
PRINT(TRA(I),4,0) ; %CAPTION --- ; PRINT(TRA(I+1),4,0)
NEWLINES(2)
STEP=1

%CYCLE B=TRA(I+1)-2,-1,TRA(I)
%UNLESS LP(B)=0 %THEN ->17
LP(B)=LP(B+1)  ;  ->184
%COMMENT  TRANSLATION OF SECTION INTO LITHOLOGIES   %C
          A, AO, B, BO, C, AY, BY, CY
17: CODING(1,5,1) ; CODING(6,15,3) ; CODING(16,40,5)
CODING(55,55,2) ; CODING(66,66,4) ; CODING(77,77,6)
CODING(88,88,7) ; CODING(99,99,8)
184: %REPEAT

%CYCLE B=1,1,8 ; MF(B)=0
%CYCLE C=1,1,8
M(B,C)=0
%REPEAT ; %REPEAT
34: %CYCLE B=1,1,4 ; %CYCLE C=1,1,4
S(B,C)=0 ; PR(B,C)=0
%REPEAT ; %REPEAT
%IF STEP=2 %THEN ->35
```

```
%CYCLE B=1,1,8 ; TK(B)=1
%CYCLE C=1,1,100
TH(B,C)=1
%REPEAT ; %REPEAT
%CYCLE B=6,1,8 ; RL(B)=0 ; %REPEAT

%CAPTION LITHOLOGICAL_THICKNESSES ; NEWLINES(2)
%COMMENT PRINTOUT OF THICKNESS OF LITHOLOGIES   %C
         AND THEIR PROPORTIONS (FT. & PERCENT)
%CYCLE B=TRA(I+1)-2,-1,TRA(I)
J=LP(B+1) ; K=LP(B)
%UNLESS J>5 %AND K<6 %THEN ->18
RL(J)=RL(J)+1
18: M(J,K)=M(J,K)+1
%IF J=K %THEN TH(J,TK(J))=TH(J,TK(J))+1
%UNLESS J=K %THEN TK(J)=TK(J)+1
%REPEAT
%CYCLE B=1,1,8
%CAPTION LITHOLOGY_ ; PRINT(B,1,0) ; NEWLINE
%IF TK(B)=1 %THEN ->19
%CYCLE C=1,1,TK(B)-1
PRINT(TH(B,C),3,0) ; NEWLINE
%REPEAT
19: %REPEAT
%CYCLE B=1,1,8 ; %CYCLE C=1,1,8
MF(B)=MF(B)+M(C,B)
%REPEAT ; %REPEAT
NEWLINES(2)
%CAPTION LITHOLOGICAL_PROPORTIONS ; NEWLINE
%CYCLE B=1,1,8
%CAPTION LITHOLOGY_ ; PRINT(B,2,0) ; SPACES(2)
PRINT(MF(B),3,0) ; NEWLINE
%REPEAT
NEWLINES(3)
SHALE=MF(1)+MF(2)+MF(6)
SILT=MF(3)+MF(4)+MF(7)
SAND=MF(5)+MF(8)
ALL=SHALE+SILT+SAND
%CAPTION SHALE ; PRINT(SHALE/ALL,0,3)
%CAPTION __SILT ; PRINT(SILT/ALL,0,3)
%CAPTION __SAND ; PRINT(SAND/ALL,0,3)
NEWLINES(3)

%COMMENT CALCULATION AND PRINTOUT OF TRANSITION   %C
         TALLY MATRIX OF 6- LITHOLOGY SYSTEM
%CAPTION THE_AAOBBOCAYBYCY_TALLY_MATRIX_(ONE_STEP_-_ONE_FOOT)
NEWLINES(2)
%CYCLE B=1,1,8 ; %CYCLE C=1,1,8
PRINT(M(B,C),4,0) ; SPACES(2)
%REPEAT ; NEWLINE ; %REPEAT ; NEWLINES(3)
```

```
S(1,1)=0
S(1,2)=M(1,3)+M(1,4)+M(2,3)+M(2,4)+M(1,7)+M(2,7)+M(6,7)
S(1,3)=M(1,5)+M(2,5)+M(6,8)+M(1,8)+M(2,8)
S(1,4)=RL(6)
S(2,1)=M(3,1)+M(3,2)+M(4,1)+M(4,2)+M(3,6)+M(4,6)+M(7,6)
S(2,2)=0
S(2,3)=M(3,5)+M(3,8)+M(4,5)+M(4,8)+M(7,8)
S(2,4)=RL(7)
S(3,1)=M(5,1)+M(5,2)+M(5,6)+M(8,6)
S(3,2)=M(5,3)+M(5,4)+M(5,7)+M(8,7)
S(3,3)=0
S(3,4)=RL(8)
S(4,1)=M(6,1)+M(6,2)+M(7,1)+M(7,2)+M(8,1)+M(8,2)
S(4,2)=M(6,3)+M(6,4)+M(7,3)+M(7,4)+M(8,3)+M(8,4)
S(4,3)=M(6,5)+M(7,5)+M(8,5)
S(4,4)=0

%COMMENT PRINTOUT OF TRANSITION TALLY AND PROBABILITY %C
         MATRICES OF CONDENSED ( SHALE . SILTSTONE    %C
         SANDSTONE . ROOTS ) SYSTEM
37: %CYCLE B=1,1,4 ; T(B)=0 ; %REPEAT
%CAPTION THE_ABCY_TALLY_MATRIX_(STEP_
PRINT(STEP,1,0) ; %CAPTION ) ; NEWLINES(2)
%CYCLE B=1,1,4 ; %CYCLE C=1,1,4
PRINT(S(B,C),4,0) ; SPACES(2)
T(B)=T(B)+S(B,C)
%REPEAT ; NEWLINE ; %REPEAT ; NEWLINES(3)

%CAPTION THE_ABCY_TRANSITION_PROBABILITY_MATRIX_(STEP_
PRINT(STEP,1,0) ; %CAPTION ) ; NEWLINES(2)
%CYCLE B=1,1,4 ; %CYCLE C=1,1,4
%IF T(B)=0 %THEN PR(B,C)=0
%IF T(B)=0 %THEN ->101
PR(B,C)=S(B,C)/T(B)
101: PRINT(PR(B,C),0,3) ; SPACES(2)
%REPEAT ; NEWLINE ; %REPEAT ; NEWLINES(3)
%IF STEP=2 %THEN ->16

%COMMENT PRINTOUT OF SEQUENCE CONTAINED IN FRAGMENT
%CAPTION ACTUAL_SEQUENCE ; NEWLINES(2)
STEP=2  ;  THICK=1
->34
35: COUNT=1
Z1=TRA(I+1)-1 ; BUZ(1)=Z1
SEQUENCE(Z1)
%CYCLE B=TRA(I+1)-2,-1,TRA(I)
Z2=LP(B)
%IF Z2=Z1 %THEN THICK=THICK+1
%IF Z2=Z1 %THEN ->36
PRINT(THICK,1,0) ; THICK=1 ; SEQUENCE(Z2)
COUNT=COUNT+1 ; BUZ(COUNT)=Z2
```

```
Z1=Z2
36: %REPEAT
DA=1
%CYCLE B=1,1,COUNT
%IF BUZ(B)=1 %OR BUZ(B)=2 %THEN BUX(DA)=1
%IF BUZ(B)=3 %OR BUZ(B)=4 %THEN BUX(DA)=2
%IF BUZ(B)=5 %THEN BUX(DA)=3
%IF BUZ(B)>5 %THEN BUX(DA)=BUZ(B)-5
%IF B=COUNT %THEN ->68
%UNLESS BUZ(B)>5 %AND BUZ(B+1)<6 %THEN ->68
BUX(DA+1)=4 ; DA=DA+1
68: DA=DA+1
%REPEAT
Z1=BUX(1) ; Z2=BUX(2)
%CYCLE B=3,1,DA-1
J=BUX(B)
%IF J=Z2 %THEN ->59
S(Z1,J)=S(Z1,J)+1
Z1=Z2 ; Z2=J
59: %REPEAT

%COMMENT CALCULATION OF SECOND ORDER TRANSITION TALLY %C
         AND PROBABILITY MATRICES FOR CONDENSED       %C
         ( A.B.C.Y ) SYSTEM
NEWLINES(3) ; %CAPTION TWO_STEP ; NEWLINES(2)
->37

16: NEWLINES(5)
%REPEAT

%ROUTINE CODING(%INTEGER F1,F2,F3)
%INTEGER F4
%CYCLE F4=F1,1,F2
%IF LP(B)=F4 %THEN LP(B)=F3
%IF LP(B)=F4 %THEN ->41
%REPEAT
41: %END

%ROUTINE SEQUENCE(%INTEGER ZX)
%IF ZX=1 %THEN %CAPTION A ; %IF ZX=2 %THEN %CAPTION AO
%IF ZX=3 %THEN %CAPTION B ; %IF ZX=4 %THEN %CAPTION BO
%IF ZX=5 %THEN %CAPTION C ; %IF ZX=6 %THEN %CAPTION AY
%IF ZX=7 %THEN %CAPTION BY ; %IF ZX=8 %THEN %CAPTION CY
%END

%END
%END
%ENDOFPROGRAM
```

APPENDIX G

Atlas Autocode (AA) Programmes ONE-STEP CYCLE (M1) and TWO-STEP CYCLE (M2)

The total number of cycles observed within the rock succession studied is set as the initial value of the input data for both programmes. This stipulates the total number of predicted cycles to be generated for each model so that the simulated cycle distributions can be directly compared with the observed distribution in a quantitative manner.

In the case of ONE-STEP CYCLE, this is followed by a state transition probability matrix of the shale (A) - siltstone (B) - sandstone (C) - rootlet horizon (Y) system. Multiplication of appropriate pair transition probabilities gives gross probabilities of the occurrence of any cycle within an infinite variety of cycle types. Further multiplication by the population total yields a model estimate of its frequency which is directly comparable with its observed occurrence. The programme is used for the construction of model distributions for a Markov-1 process, where one-step transition probabilities are used, and for an Independent Events model, where the probabilities are set by the proportional occurrence of the states within the succession studied.

The prediction of a cycle distribution for a Markov-2 model is performed by a modification of this programme in TWO-STEP CYCLE, where the input matrix takes the form of *a priori* probabilities of occurrence of the first two members of a cycle, together with transsition probabilities of trios representing all other possible state combinations. The computational procedure is then analogous with ONE-STEP CYCLE, and the output for both programmes consists of a print-out of all cycle types (coded in the A.B.C.Y system), together with their predicted numbers of occurrence up to, and including, six member cycles.

```
%BEGIN
%COMMENT MARKOV-1 AND I.E. MODELS PREDICTION    %C
         OF NUMBERS OF CYCLE TYPES
%INTEGER MR,MT
READ(MT)
%COMMENT MT IS NUMBER OF DATA SET MATRICES
%CYCLE MR=1,1,MT

%BEGIN
%INTEGER Q,R,S,T,U,V,N,Z,Z',X
%REALARRAY P(1:4,1:4)
%ROUTINESPEC ROCKPRINT(%INTEGER G)

READ(N)
%COMMENT N IS TOTAL NUMBER OF CYCLES IN    %C
         OBSERVED POPULATION
%CYCLE Q=1,1,4 ; %CYCLE R=1,1,4
READ(P(Q,R))
%REPEAT ; %REPEAT
%COMMENT P(4:4) IS TRANSITION PROBABILITY MATRIX
NEWLINES(6)
%CAPTION FOR_FIRST_ORDER_MARKOVIAN_MODEL
NEWLINE
%CAPTION TOTAL_NUMBER  ;   PRINT(N,3,0)
NEWLINES(4)

%COMMENT PRINTOUT OF CYCLE TYPES AND PREDICTED NUMBER
Z=0
%CAPTION ONE_MEMBER_CYCLES ; NEWLINES(2)
%CYCLE Q=1,1,3
PRINT SYMBOL('Y') ; ROCKPRINT(Q) ; PRINT SYMBOL('Y')
SPACES(4) ; X= INT(P(4,Q)*P(Q,4)*N) ; Z=Z+X
PRINT(X,3,0)  ; NEWLINE
%REPEAT ; NEWLINES(2)
%CAPTION TOTAL_ONE_MEMBER=_ ; PRINT(Z,3,0)
NEWLINES(4)

Z'=Z
%CAPTION TWO_MEMBER_CYCLES ; NEWLINES(2)
%CYCLE Q=1,1,3 ; %CYCLE R=1,1,3
%IF Q=R %THEN ->11
PRINT SYMBOL('Y') ; ROCKPRINT(Q) ; ROCKPRINT(R)
PRINT SYMBOL('Y')
X=INT(P(4,Q)*P(Q,R)*P(R,4)*N)
Z=Z+X ; SPACES(4)
PRINT(X,3,0) ; NEWLINE
11: %REPEAT ; %REPEAT ; NEWLINES(2)
%CAPTION TOTAL_TWO_MEMBER=_ ; PRINT(Z-Z',3,0)
NEWLINES(4)
```

```
Z'=Z
%CAPTION THREE_MEMBER_CYCLES ; NEWLINES(2)
%CYCLE Q=1,1,3 ; %CYCLE R=1,1,3 ; %CYCLE S=1,1,3
%IF Q=R %OR R=S %THEN ->22
PRINT SYMBOL('Y') ; ROCKPRINT(Q) ; ROCKPRINT(R)
ROCKPRINT(S) ; PRINT SYMBOL('Y')
X=INT(P(4,Q)*P(Q,R)*P(R,S)*P(S,4)*N)
Z=Z+X ; SPACES(4)
PRINT(X,3,0) ; NEWLINE
22: %REPEAT ; %REPEAT ; %REPEAT ; NEWLINES(2)
%CAPTION TOTAL_THREE_MEMBER=_ ; PRINT(Z-Z',3,0)
NEWLINES(4)

Z'=Z
%CAPTION FOUR_MEMBER_CYCLES ; NEWLINES(2)
%CYCLE Q=1,1,3 ; %CYCLE R=1,1,3 ; %CYCLE S=1,1,3
%CYCLE T=1,1,3
%IF Q=R %OR R=S %THEN ->33
%IF S=T %THEN ->33
PRINT SYMBOL('Y') ; ROCKPRINT(Q) ; ROCKPRINT(R)
ROCKPRINT(S) ; ROCKPRINT(T) ; PRINT SYMBOL('Y')
X=INT(P(4,Q)*P(Q,R)*P(R,S)*P(S,T)*P(T,4)*N)
Z=Z+X ; SPACES(4)
PRINT(X,3,0) ; NEWLINE
33: %REPEAT ; %REPEAT ; %REPEAT ; %REPEAT ; NEWLINES(2)
%CAPTION TOTAL_FOUR_MEMBER=_ ; PRINT(Z-Z',3,0)
NEWLINES(4)

Z'=Z
%CAPTION FIVE_MEMBER_CYCLES ; NEWLINES(2)
%CYCLE Q=1,1,3 ; %CYCLE R=1,1,3 ; %CYCLE S=1,1,3
%CYCLE T=1,1,3  ; %CYCLE U=1,1,3
%IF Q=R %OR R=S %THEN ->44
%IF S=T %OR T=U %THEN ->44
PRINT SYMBOL('Y') ; ROCKPRINT(Q) ; ROCKPRINT(R) ; ROCKPRINT(S)
ROCKPRINT(T) ; ROCKPRINT(U) ; PRINT SYMBOL('Y')
X=INT(P(4,Q)*P(Q,R)*P(R,S)*P(S,T)*P(T,U)*P(U,4)*N)
Z=Z+X ; SPACES(4)
PRINT(X,3,0) ; NEWLINE
44: %REPEAT ; %REPEAT ; %REPEAT ; %REPEAT ; %REPEAT
NEWLINES(2)
%CAPTION TOTAL_FIVE_MEMBER=_ ; PRINT(Z-Z',3,0)
NEWLINES(4)

Z'=Z
%CAPTION SIX_MEMBER_CYCLES ; NEWLINES(2)
%CYCLE Q=1,1,3 ; %CYCLE R=1,1,3 ; %CYCLE S=1,1,3
%CYCLE T=1,1,3 ; %CYCLE U=1,1,3 ; %CYCLE V=1,1,3
%IF Q=R %OR R=S %THEN ->55
%IF S=T %OR T=U %THEN ->55
```

M1

```
%IF U=V %THEN ->55
PRINT SYMBOL('Y') ; ROCKPRINT(Q) ; ROCKPRINT(R)
ROCKPRINT(S) ; ROCKPRINT(T) ; ROCKPRINT(U)
ROCKPRINT(V) ; PRINT SYMBOL('Y')
X=INT(P(4,Q)*P(Q,R)*P(R,S)*P(S,T)*P(T,U)*P(U,V)*P(V,4)*N)
Z=Z+X ; SPACES(4)
PRINT(X,3,0) ; NEWLINE
55: %REPEAT ; %REPEAT ; %REPEAT ; %REPEAT ; %REPEAT ; %REPEAT
NEWLINES(2)
%CAPTION TOTAL_SIX_MEMBER=_ ; PRINT(Z-Z',3,0)
NEWLINES(4)

%CAPTION TOTAL_ACCOUNTED_FOR_=_
PRINT(Z,3,0) ; NEWLINES(20)

%ROUTINE ROCKPRINT(%INTEGER G)
%IF G=1 %THEN PRINT SYMBOL('A')
%IF G=2  %THEN PRINT SYMBOL('B')
%IF G=3 %THEN PRINT SYMBOL('C')
%END

%END
%REPEAT
%ENDOFPROGRAM
```

M2

```
%BEGIN
%COMMENT MARKOV-2 MODEL PREDICTION OF NUMBERS    %C
         OF CYCLE TYPES
%INTEGER MR,MT
READ(MT)
%COMMENT MT IS NUMBER OF DATA SET MATRICES
%CYCLE MR=1,1,MT

%BEGIN
%INTEGER Q,R,S,T,U,V,N,Z,Z',X
%REAL SN,H1,H2,H3,H4
%REALARRAY A(1:4,1:4),B(1:4,1:4),C(1:4,1:4),D(1:4,1:4)
%ROUTINESPEC ROCKPRINT(%INTEGER G)
%ROUTINESPEC TERMINATOR(%INTEGER L,M)
%ROUTINESPEC INTERM(%REALNAME H',%INTEGER I,J,K)

READ(N)
%COMMENT N IS NUMBER OF CYCLES IN OBSERVED POPULATION
%COMMENT A-C(4:4) ARE MARKOV-2 TRANSITION PROBABILITIES %C
         D(4:4) ARE A PRIORI PROBABILITIES OF    %C
         INITIAL TWO MEMBERS IN CYCLE
```

```
%CYCLE Q=1,1,4  ;  %CYCLE R=1,1,4
READ(A(Q,R))  ;  %REPEAT  ;  %REPEAT
%CYCLE Q=1,1,4  ;  %CYCLE R=1,1,4
READ(B(Q,R))  ;  %REPEAT  ;  %REPEAT
%CYCLE Q=1,1,4  ;  %CYCLE R=1,1,4
READ(C(Q,R))  ;  %REPEAT  ;  %REPEAT
%CYCLE Q=1,1,4  ;  %CYCLE R=1,1,4
READ(D(Q,R))  ;  %REPEAT  ;  %REPEAT
NEWLINES(6)
%CAPTION FOR_SECOND_ORDER_MARKOV_MODEL
NEWLINE
%CAPTION TOTAL_NUMBER  ;  PRINT(N,3,0)
NEWLINES(4)

%CAPTION ONE_MEMBER_CYCLES  ;  NEWLINES(2)
%CAPTION OCCURRENCE_AND_NUMBER_=_OBSERVED_OCCURENCE
NEWLINES(4)

%COMMENT PRINTOUT OF CYCLE TYPES AND PREDICTED NUMBER %C
         FOR MARKOV-2 MODEL
Z=0
%CAPTION TWO_MEMBER_CYCLES  ;  NEWLINES(2)
%CYCLE Q=1,1,3  ;  %CYCLE R=1,1,3
%IF Q=R %THEN ->11
PRINT SYMBOL('Y')  ;  ROCKPRINT(Q)  ;  ROCKPRINT(R)
PRINT SYMBOL('Y')
TERMINATOR(Q,R)
X=INT(D(Q,R)*SN*N)
Z=Z+X  ;  SPACES(4)
PRINT(X,3,0)  ;  NEWLINE
11: %REPEAT  ;  %REPEAT  ;  NEWLINES(2)
%CAPTION TOTAL_TWO_MEMBER=_  ;  PRINT(Z,3,0)
NEWLINES(4)

Z'=Z
%CAPTION THREE_MEMBER_CYCLES  ;  NEWLINES(2)
%CYCLE Q=1,1,3  ;  %CYCLE R=1,1,3  ;  %CYCLE S=1,1,3
%IF Q=R %OR R=S %THEN ->22
PRINT SYMBOL('Y')  ;  ROCKPRINT(Q)  ;  ROCKPRINT(R)
ROCKPRINT(S)  ;  PRINT SYMBOL('Y')
INTERM(H1,Q,R,S)  ;  TERMINATOR(R,S)
X=INT(D(Q,R)*H1*SN*N)
Z=Z+X  ;  SPACES(4)
PRINT(X,3,0)  ;  NEWLINE
22: %REPEAT  ;  %REPEAT  ;  %REPEAT  ;  NEWLINES(2)
%CAPTION TOTAL_THREE_MEMBER=_  ;  PRINT(Z-Z',3,0)
NEWLINES(4)

Z'=Z
%CAPTION FOUR_MEMBER_CYCLES  ;  NEWLINES(2)
```

```
%CYCLE Q=1,1,3  ;  %CYCLE R=1,1,3  ;  %CYCLE S=1,1,3
%CYCLE T=1,1,3
%IF Q=R %OR R=S %THEN ->33
%IF S=T %THEN ->33
PRINT SYMBOL(´Y´)  ;  ROCKPRINT(Q)  ;  ROCKPRINT(R)
ROCKPRINT(S)  ;  ROCKPRINT(T)  ;  PRINT SYMBOL(´Y´)
INTERM(H1,Q,R,S)  ;  INTERM(H2,R,S,T)
TERMINATOR(S,T)
X=INT(D(Q,R)*H1*H2*SN*N)
Z=Z+X  ;  SPACES(4)
PRINT(X,3,0)  ;  NEWLINE
33: %REPEAT  ;  %REPEAT  ;  %REPEAT  ;  %REPEAT
NEWLINES(2)
%CAPTION TOTAL_FOUR_MEMBER=_  ;  PRINT(Z-Z´,3,0)
NEWLINES(4)

Z´=Z
%CAPTION FIVE_MEMBER_CYCLES  ;  NEWLINES(2)
%CYCLE Q=1,1,3  ;  %CYCLE R=1,1,3  ;  %CYCLE S=1,1,3
%CYCLE T=1,1,3  ;  %CYCLE U=1,1,3
%IF Q=R %OR R=S %THEN ->44
%IF S=T %OR T=U %THEN ->44
PRINT SYMBOL(´Y´)  ;  ROCKPRINT(Q)  ;  ROCKPRINT(R)
ROCKPRINT(S)  ;  ROCKPRINT(T)  ;  ROCKPRINT(U)
PRINT SYMBOL(´Y´)
INTERM(H1,Q,R,S)  ;  INTERM(H2,R,S,T)
INTERM(H3,S,T,U)  ;  TERMINATOR(T,U)
X=INT(D(Q,R)*H1*H2*H3*SN*N)
Z=Z+X  ;  SPACES(4)
PRINT(X,3,0)  ;  NEWLINE
44: %REPEAT  ;  %REPEAT  ;  %REPEAT  ;  %REPEAT
%REPEAT  ;  NEWLINES(2)
%CAPTION TOTAL_FIVE_MEMBER=_  ;  PRINT(Z-Z´,3,0)
NEWLINES(4)

Z´=Z
%CAPTION SIX_MEMBER_CYCLES  ;  NEWLINES(2)
%CYCLE Q=1,1,3  ;  %CYCLE R=1,1,3  ;  %CYCLE S=1,1,3
%CYCLE T=1,1,3  ;  %CYCLE U=1,1,3  ;  %CYCLE V=1,1,3
%IF Q=R %OR R=S %THEN ->55
%IF S=T %OR T=U %THEN ->55
%IF U=V %THEN ->55
PRINT SYMBOL(´Y´)  ;  ROCKPRINT(Q)  ;  ROCKPRINT(R)
ROCKPRINT(S)  ;  ROCKPRINT(T)  ;  ROCKPRINT(U)
ROCKPRINT(V)  ;  PRINT SYMBOL(´Y´)
INTERM(H1,Q,R,S)  ;  INTERM(H2,R,S,T)  ;  INTERM(H3,S,T,U)
INTERM(H4,T,U,V)  ;  TERMINATOR(U,V)
X=INT(D(Q,R)*H1*H2*H3*H4*SN*N)
Z=Z+X  ;  SPACES(4)
PRINT(X,3,0)  ;  NEWLINE
```

```
55: %REPEAT ;  %REPEAT  ; %REPEAT  ;  %REPEAT
%REPEAT  ;  %REPEAT  ;  NEWLINES(2)
%CAPTION TOTAL_SIX_MEMBER=_  ;  PRINT(Z-Z',3,0)
NEWLINES(4)

%CAPTION TOTALACCOUNTED_FOR_IN_RANGE_2-6_=_
PRINT(Z,3,0)  ;  NEWLINES(20)

%ROUTINE ROCKPRINT(%INTEGER G)
%IF G=1 %THEN PRINT SYMBOL('A')
%IF G=2 %THEN PRINT SYMBOL('B')
%IF G=3 %THEN PRINT SYMBOL('C')
%END

%ROUTINE TERMINATOR(%INTEGER L,M)
%IF L=1 %THEN SN=A(M,4)
%IF L=2 %THEN SN=B(M,4)
%IF L=3 %THEN SN=C(M,4)
%END

%ROUTINE INTERM(%REALNAME H',%INTEGER I,J,K)
%IF I=1 %THEN H'=A(J,K)
%IF I=2 %THEN H'=B(J,K)
%IF I=3 %THEN H'=C(J,K)
%END

%END
%REPEAT
%ENDOFPROGRAM
```

APPENDIX H

Atlas Autocode (AA) Programmes MONTE CARLO MARKOV 1 (M1) and MONTE CARLO MARKOV 2 (M2)

Input data for both programmes consists of a value representing the number of simulated beds required, and a state transition probability matrix of the system shale (A), shale containing non-marine lamellibranchs (M), siltstone (B), sandstone less than twenty feet in thickness (C), sandstone more than twenty feet in thickness (K), rootlet horizon (Y). These data are followed by a thickness distribution of each state (with the exception of Y) recorded as percent. The values of the transition probability matrix are dictated by the type of model set, so that for a Markov-1 model, it is one of one-step transitions, for a Markov-2 model, one of two-step transitions for all trio permutations, while in the case of an Independent Events model, the values are determined by the relative proportions of the lithological state occurrences.

The transition probability matrix and lithological thickness distributions are stored as integer arrays. The initial state of the simulation system is arbitrarily defined a shale (A). A random number in the range one to a hundred is called from the pseudo-random number generator 'real function random k' and used to select a cell in the shale (A) row of the transition probability matrix array. This cell contains the identity of the succeeding lithology which is now the new state of the simulation system and is printed. Another random number is called and selection made of a cell in the state's thickness distribution to ascribe a bed thickness to this step. The procedure is reiterated the number of times set in the data by operation of the random number generator on the appropriate array populations so that the system moves through a sequence of states and, in doing so, describes a simulated rock succession. The printout result takes the form of a graphic log, in which the lithologies are shown in symbol form indexed with values for the thickness of the beds represented by each step.

```
%BEGIN
%COMMENT MONTE CARLO MODEL BASED ON MARKOV-1 MATRIX
%REAL XA,ZA
%REALARRAY P(1:6,1:6)
%INTEGER B,C,R,L,M,TQ,NT,FR,TH,D,E,TITLE,Z
%INTEGERARRAY T(1:5,1:100),S(1:6,1:100)
%REALFNSPEC RANDOM K(%REALNAME X,%INTEGER N)

NEWLINES(6)
%CYCLE B=1,1,30
READ SYMBOL(TITLE)
PRINT SYMBOL(TITLE)
%IF TITLE='.' %THEN ->11
%REPEAT

11: READ(E)  ;  D=1
%COMMENT E IS NUMBER OF SIMULATED BEDS REQUIRED
%COMMENT P(6,6) IS TRANSITION PROBABILITY MATRIX
%CYCLE B=1,1,6
R=0
%CYCLE C=1,1,6
READ(P(B,C))
%IF P(B,C)=0 %THEN ->1
L=INT(P(B,C)*100)
%CYCLE M=R+1,1,R+L
S(B,M)=C
%REPEAT
R=R+L
1: %REPEAT
%REPEAT

%COMMENT T(5,100) IS MATRIX OF LITHOLOGICAL THICKNESS %C
         DISTRIBUTIONS
%CYCLE B=1,1,5
R=0
%CYCLE C=1,1,50
READ(TQ)
READ(NT)
%CYCLE M=R+1,1,R+NT
T(B,M)=TQ
%REPEAT
R=R+NT  ;  %IF R=100 %THEN ->2
%REPEAT
2: %REPEAT

NEWLINES(2)
%CAPTION MONTE_CARLO_SIMULATION  ;  NEWLINE
%CAPTION (BEGINNING_WITH_OLDEST_LITHOLOGY)
NEWLINE
%CAPTION CODING:  ;  NEWLINE
```

```
%CAPTION A_=_SHALE  ;  NEWLINE
%CAPTION M_=_SHALE_WITH_F/W_LAMELLIBRANCHS
NEWLINE
%CAPTION B_=_SILTSTONE  ;  NEWLINE
%CAPTION C_=_SANDSTONE_<20_FEET_THICK  ;  NEWLINE
%CAPTION K_=_SANDSTONE_>20_FEET_THICK  ;  NEWLINE
%CAPTION Y_=_SEATEARTH  ;  NEWLINE
%CAPTION (THICKNESSES_IN_FEET)
NEWLINES(3)

XA=3  ;  ZA=RANDOM K(XA,0)
%CYCLE B=1,1,E
FR=0
3:  ZA=RANDOM K(XA,1)  ;  Z=INT(100*ZA)
%IF Z=0 %THEN Z=1  ;  %IF FR=1 %THEN ->4
D=S(D,Z)  ;  %IF D=6 %THEN ->5
FR=1  ;  ->3
4: TH=T(D,Z)
%IF D=1 %THEN %CAPTION AAAA
%IF D=2 %THEN %CAPTION MMMM
%IF D=3 %THEN %CAPTION BBBB
%IF D=4 %THEN %CAPTION CCCC
%IF D=5 %THEN %CAPTION KKKK
SPACES(2)  ;  PRINT(TH,3,0)
5: %IF D=6 %THEN %CAPTION YYYY
NEWLINE
%REPEAT

%REALFN  RANDOM K(%REAL %NAME  X, %INTEGER  N)
%REAL  X',Y; %INTEGER  I
X'=X
%M  %CODE
->1 %UNLESS  N=1;! PRODUCE NEXT NUMBER
**X'
*FIX
*=C13
*SHL C 13
*SHL -8
*SETB 154643
*=M 13
*SETB 44646
*=I 13
*SETB 77
*=C 13
*Q 13
*XD
*ERASE
*SHL+9
*SHL-9
```

```
*ZERO
*NOT
*NEG
*SHL+46
*OR
*STAND
**=X'
3: X=X'
%RESULT  = X'

1: ->2 %UNLESS  N=0;!INITIALISE
**X'
*FIX
*=RC13
*ZERO
*SHADC 13
*I 13
*SHL+46
*OR
*STAND
**=X'
*ERASE
->3
2:->4 %UNLESS  N>=2 ; !NORMAL DISTRIBUTION
Y=0
%CYCLE  I=1,1,N
Y=Y+RANDOM K(X,1)
%REPEAT
%RESULT  = Y
%END %OF %M  %CODE
4: %CAPTION ~N<0_IN_RANDOM_~; %STOP
%END

%ENDOFPROGRAM
```

```
%BEGIN
%COMMENT MONTE CARLO MODEL BASED ON MARKOV-2 MATRIX
%REAL XA,ZA,PROB
%INTEGER BA,TITLE,E,R,CA,TQ,NT,DA,S,D,Z,FR,DS,L,TH
%INTEGERARRAY T(1:5,1:100),A(1:6,1:100),M(1:6,1:100),  %C
B(1:6,1:100),C(1:6,1:100),K(1:6,1:100),Y(1:6,1:100)
%ROUTINESPEC MOG(%INTEGERARRAYNAME Q)
%REALFNSPEC RANDOM K(%REALNAME X,%INTEGER N)

NEWLINES(6)
%CYCLE BA=1,1,30
READ SYMBOL(TITLE)
%IF TITLE ='.' %THEN ->1
%REPEAT
1:READ(E)
%COMMENT E IS NUMBER OF SIMULATED BEDS REQUIRED
MOG(A)  ;  MOG(M)  ;  MOG(B)  ;  MOG(C)  ;  MOG(K)  ;  MOG(Y)

%COMMENT T(5,100) IS MATRIX OF LITHOLOGICAL THICKNESS
         DISTRIBUTIONS
%CYCLE BA=1,1,5
R=0
%CYCLE CA=1,1,50
READ(TQ) ;  READ(NT)
%CYCLE DA=R+1,1,R+NT
T(BA,DA)=TQ
%REPEAT
R=R+NT  ;  %IF R=100  %THEN ->2
%REPEAT
2: %REPEAT

NEWLINES(2)
%CAPTION MONTE_CARLO_ SIMULATION  ;  NEWLINE
%CAPTION FOR_COMBINED_MARKOV_ONE_AND_TWO   ;  NEWLINE
%CAPTION (BEGINNING_WITH_OLDEST_LITHOLOGY)
NEWLINE
%CAPTION CODING:  ;  NEWLINE
%CAPTION A_=_SHALE  ;  NEWLINE
%CAPTION M_=_SHALE_WITH_F/W_LAMELLIBRANCHS
NEWLINE
%CAPTION B_=_SILTSTONE  ;  NEWLINE
%CAPTION C_=_SANDSTONE_LESS_THAN_20_FEET_THICK
NEWLINE
%CAPTION K_=_SANDSTONE_GREATER_THAN_20_FEET_THICK
NEWLINE
%CAPTION Y_=_SEATEARTH  ;  NEWLINE
%CAPTION (THICKNESSES_IN_FEET)
NEWLINES(3)

S=1  ;  D=6
XA=3  ;  ZA= RANDOM K(XA,0)
```

```
%CYCLE BA=1,1,E
FR=0
3: ZA=RANDOM K(XA,1)  ;  Z=INT(100*ZA)
%IF Z=0 %THEN Z=1
%IF FR=1 %THEN ->11
DS=D
%IF S=2 %THEN ->4  ;  %IF S=3  %THEN ->5
%IF S=4 %THEN ->6  ;  %IF S=5 %THEN ->7
%IF S=6 %THEN ->8
D=A(D,Z)  ;  ->9
4:  D=M(D,Z)  ;  ->9
5:  D=B(D,Z)  ;  ->9
6:  D=C(D,Z)  ;  ->9
7:  D=K(D,Z)  ;  ->9
8:  D=Y(D,Z)
9:  %IF D=6 %THEN ->10
FR=1  ;  ->3
11:  TH=T(D,Z)
%IF D=1 %THEN %CAPTION AAAA
%IF D=2 %THEN %CAPTION MMMM
%IF D=3 %THEN %CAPTION BBBB
%IF D=4 %THEN %CAPTION CCCC
%IF D=5 %THEN %CAPTION KKKK
SPACES(2)  ;  PRINT(TH,3,0)
10:  %IF D=6 %THEN %CAPTION YYYY
NEWLINE  ;  S=DS
%REPEAT

%ROUTINE MOG(%INTEGERARRAYNAME Q)
%CYCLE BA=1,1,6
R=0
%CYCLE CA=1,1,6
READ(PROB)
%IF PROB=0 %THEN ->22
L=INT(PROB*100)
%CYCLE DA=R+1,1,R+L
Q(BA,DA)=CA
%REPEAT
R=R+L
22:  %REPEAT
%REPEAT
%END

%REALFN  RANDOM K(%REAL %NAME  X, %INTEGER  N)
%COMMENT AS FOR MONTE CARLO M1 PROGRAMME
....................
....................
%END

%ENDOFPROGRAM
```

APPENDIX I

Base Map of Trend Surfaces